



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 02:01 PM EST

PDB ID : 5XAG  
Title : Crystal structure of tubulin-stathmin-TTL-Compound Z2 complex  
Authors : Zhang, H.; Luo, C.; Wang, Y.  
Deposited on : 2017-03-12  
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

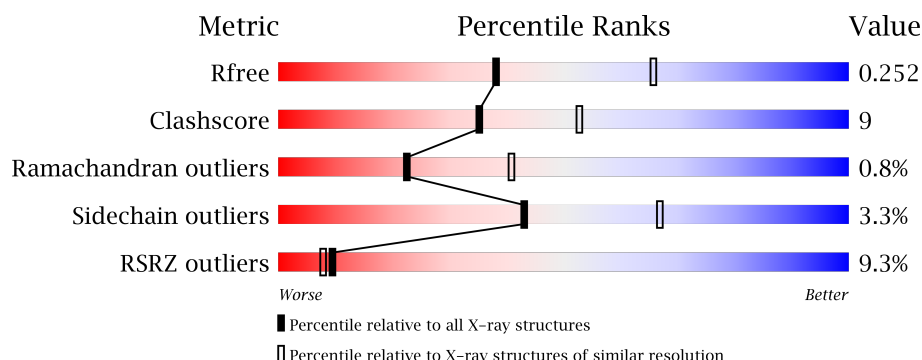
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

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>3%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
2	D	445	<div> <div>9%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div> </div>
3	E	189	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>15%</div> <div>• 37%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	378	

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
12	IMD	C	508	-	-	-	X
12	IMD	C	509	-	-	-	X
12	IMD	E	201	-	-	-	X
6	MG	C	503	-	-	-	X
7	GOL	A	504	-	-	-	X
7	GOL	B	503	-	-	-	X
7	GOL	B	504	-	-	-	X
7	GOL	B	505	-	-	X	X
7	GOL	C	501	-	-	-	X
7	GOL	C	505	-	-	-	X
7	GOL	C	506	-	-	-	X
7	GOL	D	504	-	-	-	X

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 17705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	10	0
			3476	2206	585	660	25			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2204	588	667	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	9	0
			3376	2125	569	655	27			
2	D	421	Total	C	N	O	S	0	3	0
			3321	2089	562	642	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	1	0
			997	616	181	195	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	3	0
			2609	1689	434	472	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

- 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		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

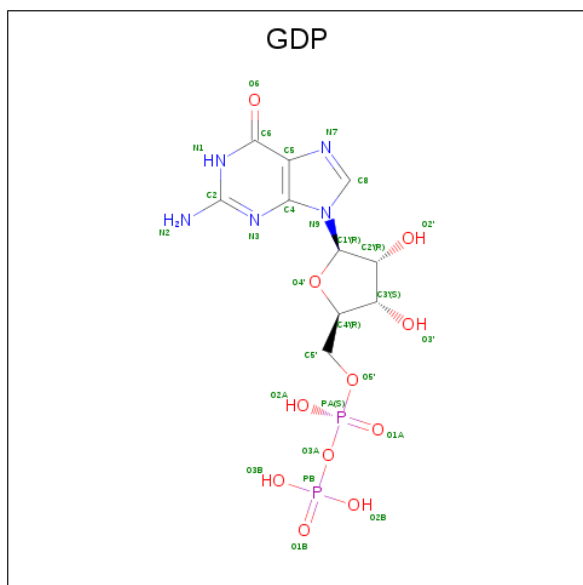


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

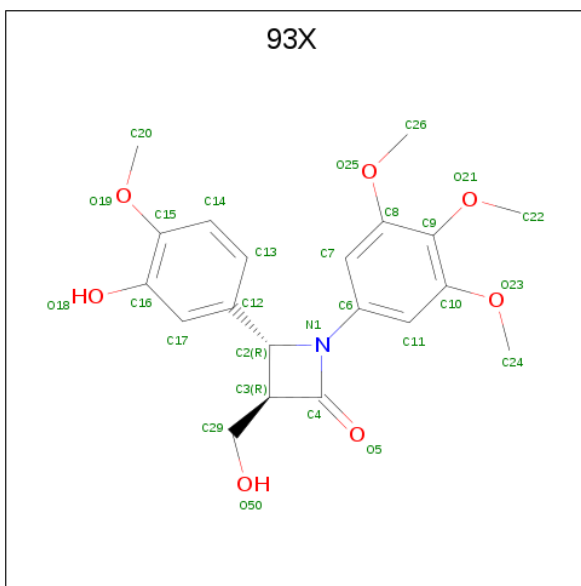
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





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

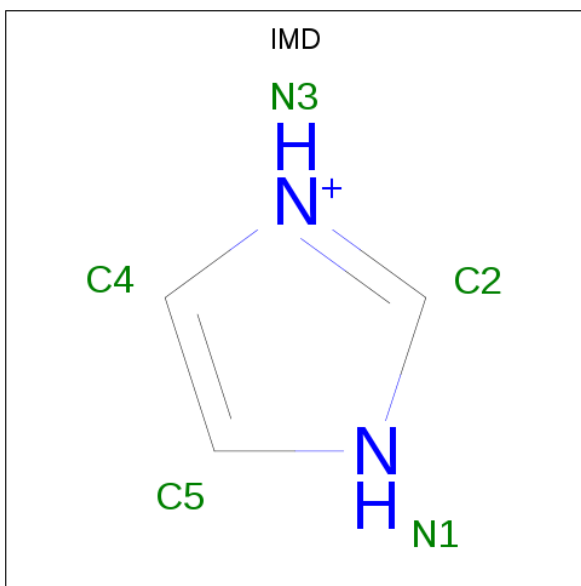
- Molecule 11 is (3 {R},4 {R})-3-(hydroxymethyl)-4-(4-methoxy-3-oxidanyl-phenyl)-1-(3,4,5-trimethoxyphenyl)azetidin-2-one (three-letter code: 93X) (formula: C<sub>20</sub>H<sub>23</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			28	20	1	7		
11	D	1	Total	C	N	O	0	0
			28	20	1	7		

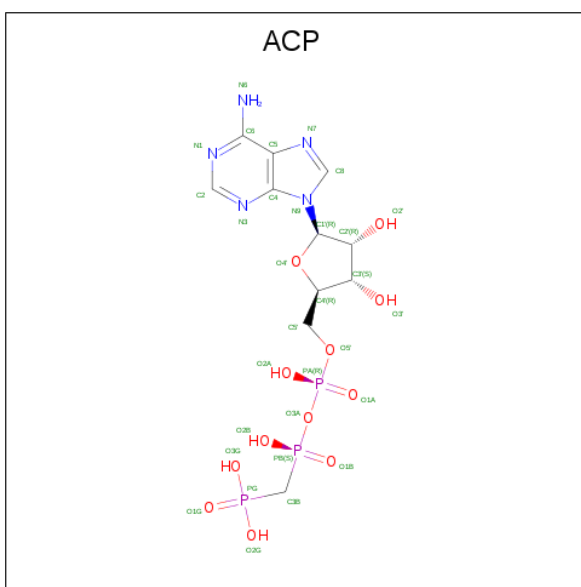


- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	N	0	0
			5	3	2		
12	C	1	Total	C	N	0	0
			5	3	2		
12	E	1	Total	C	N	0	0
			5	3	2		

- Molecule 13 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
13	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

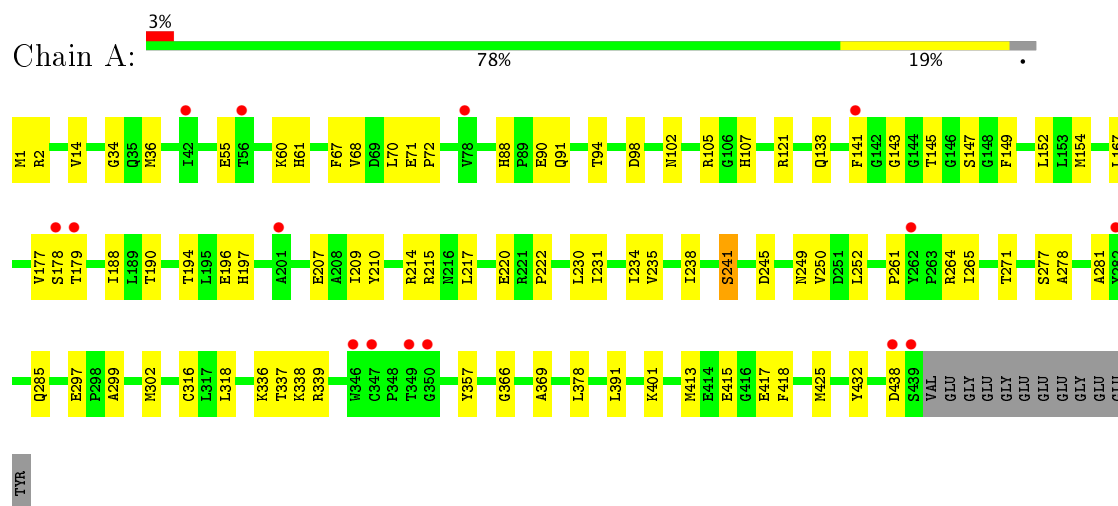
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	20	Total	O	0	0
			20	20		
14	B	20	Total	O	0	0
			20	20		
14	C	48	Total	O	0	0
			48	48		
14	D	9	Total	O	0	0
			9	9		
14	E	15	Total	O	0	0
			15	15		
14	F	18	Total	O	0	0
			18	18		

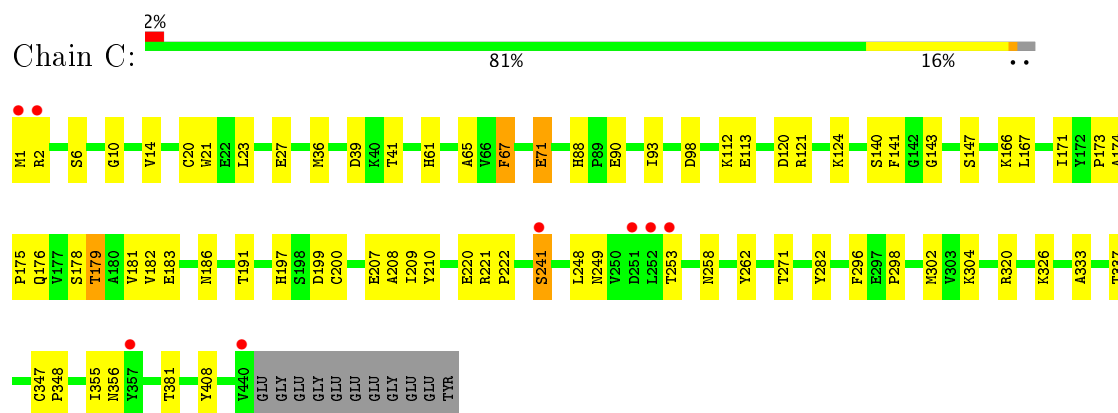
### 3 Residue-property plots [i](#)

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.

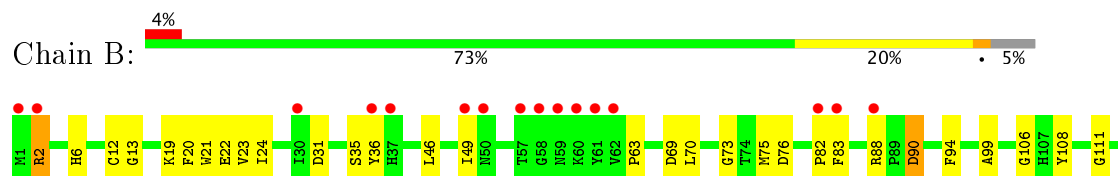
#### • Molecule 1: Tubulin alpha-1B chain

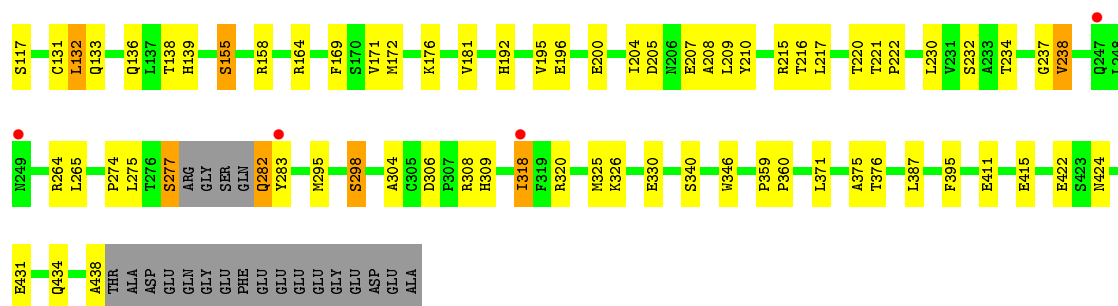


#### • Molecule 1: Tubulin alpha-1B chain

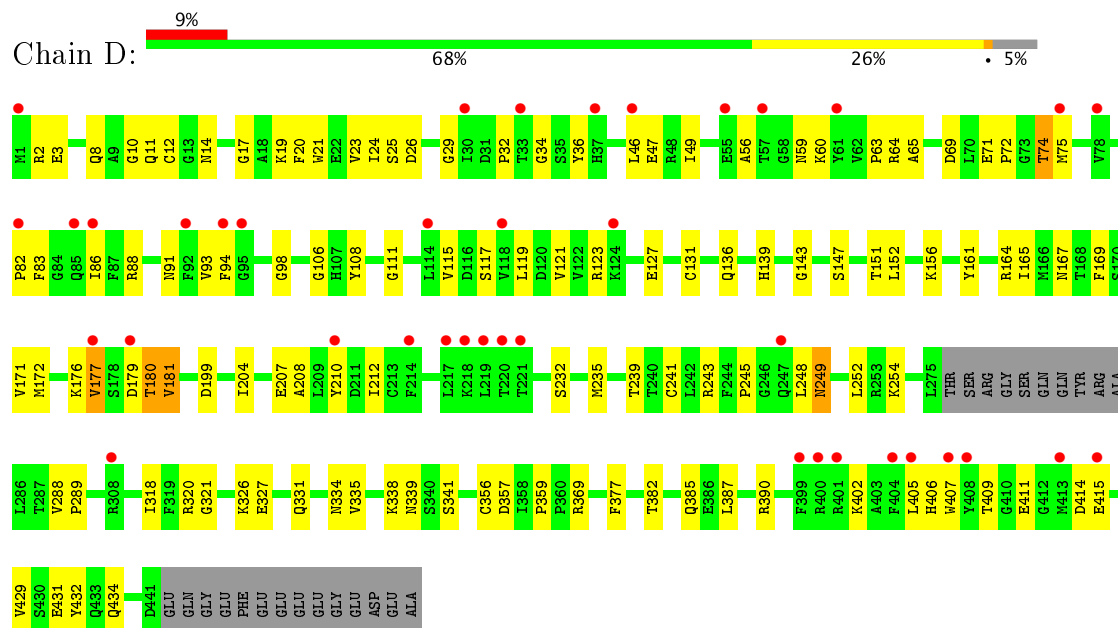


#### • Molecule 2: Tubulin beta-2B chain

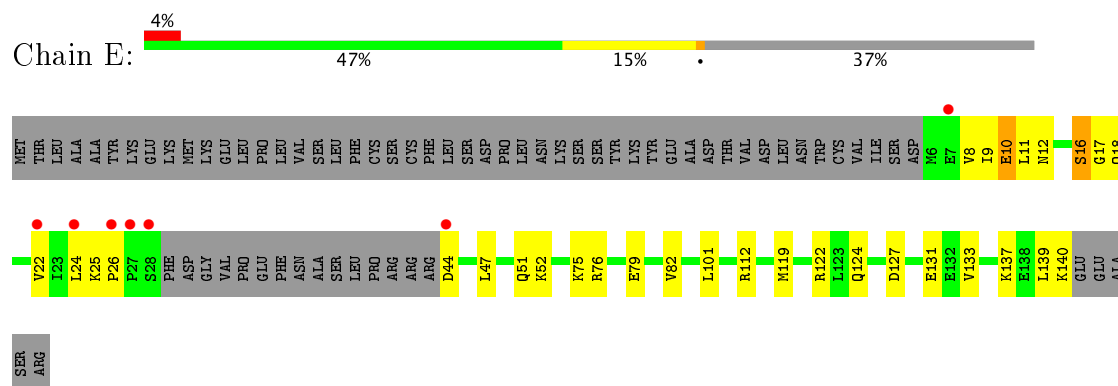




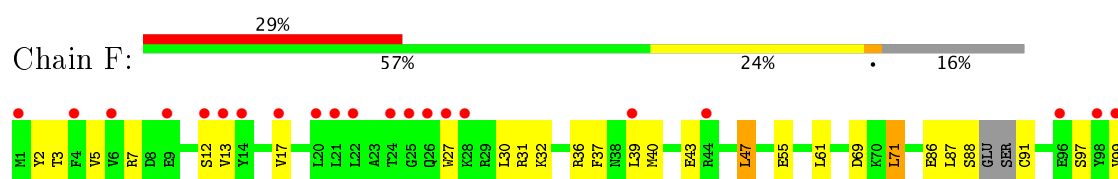
• Molecule 2: Tubulin beta-2B chain

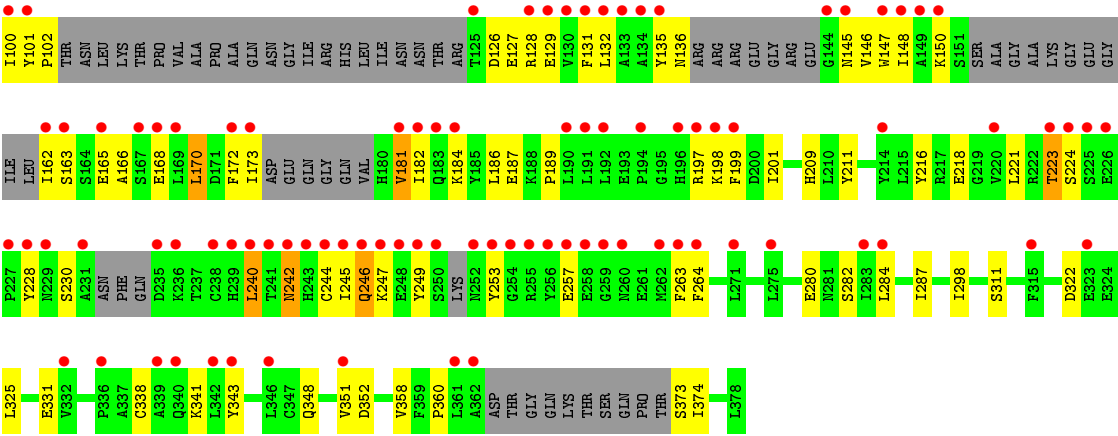


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.27Å 156.12Å 182.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.56 47.92 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.56) 99.9 (47.92-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.211 , 0.255 0.204 , 0.252	Depositor DCC
$R_{free}$ test set	1991 reflections (2.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, GOL, MG, IMD, CA, GTP, 93X, MES, ACP

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	0.43	0/3584	0.60	0/4865
1	C	0.52	1/3584 (0.0%)	0.66	0/4867
2	B	0.46	0/3474	0.62	1/4706 (0.0%)
2	D	0.42	0/3403	0.57	0/4611
3	E	0.50	0/1008	0.56	0/1337
4	F	0.41	1/2674 (0.0%)	0.57	0/3609
All	All	0.46	2/17727 (0.0%)	0.60	1/23995 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	47	LEU	C-N	7.58	1.48	1.34
1	C	20	CYS	CB-SG	-5.15	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	LEU	CA-CB-CG	-5.21	103.31	115.30

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	3476	0	3417	55	0
1	C	3482	0	3401	49	1
2	B	3376	0	3265	63	1
2	D	3321	0	3210	74	0
3	E	997	0	1020	22	0
4	F	2609	0	2599	72	0
5	A	32	0	12	2	0
5	C	32	0	12	2	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	18	0	24	1	0
7	B	18	0	24	6	0
7	C	24	0	32	2	0
7	D	12	0	15	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	12	0	12	0	0
11	B	28	0	0	0	0
11	D	28	0	0	1	0
12	C	10	0	10	3	0
12	E	5	0	4	2	0
13	F	31	0	14	1	0
14	A	20	0	0	3	0
14	B	20	0	0	2	0
14	C	48	0	0	0	0
14	D	9	0	0	4	0
14	E	15	0	0	1	0
14	F	18	0	0	9	0
All	All	17705	0	17095	321	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 9.

All (321) 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:411:GLU:HA	3:E:137:LYS:HD2	1.61	0.82
4:F:145:ASN:HB3	4:F:147:TRP:HE1	1.45	0.82
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.13	0.81
4:F:31:ARG:HE	4:F:32:LYS:H	1.28	0.81
2:B:217:LEU:HD22	2:B:277:SER:HB3	1.63	0.81
2:D:180:THR:OG1	2:D:181:VAL:N	2.08	0.79
2:B:320:ARG:HH11	7:B:505:GOL:H11	1.49	0.77
2:D:17:GLY:O	14:D:601:HOH:O	2.02	0.77
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.19	0.75
4:F:373:SER:N	14:F:505:HOH:O	2.19	0.75
5:A:501:GTP:O3G	14:A:601:HOH:O	2.05	0.74
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.22	0.73
1:C:199:ASP:OD1	7:C:506:GOL:H31	1.90	0.72
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.23	0.71
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.73	0.71
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.26	0.71
4:F:150:LYS:O	14:F:501:HOH:O	2.08	0.70
4:F:135:TYR:OH	14:F:502:HOH:O	2.09	0.70
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.73	0.69
2:D:334:ASN:HD21	2:D:338:LYS:HE2	1.57	0.69
2:D:10:GLY:O	2:D:14:ASN:ND2	2.21	0.67
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.78	0.66
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.29	0.66
1:A:241:SER:HB2	1:A:249:ASN:O	1.95	0.66
2:D:321:GLY:HA2	2:D:359:PRO:HG3	1.78	0.65
2:B:2:ARG:HA	2:B:131:CYS:O	1.96	0.65
2:D:11:GLN:HB3	9:D:501:GDP:O2A	1.95	0.65
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.29	0.65
2:D:21:TRP:O	2:D:25:SER:OG	2.09	0.65
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.62	0.65
3:E:112:ARG:HE	12:E:201:IMD:H5	1.61	0.65
2:D:123:ARG:O	2:D:127:GLU:HG2	1.97	0.65
4:F:187:GLU:OE2	14:F:503:HOH:O	2.16	0.63
4:F:373:SER:OG	4:F:374:ILE:N	2.30	0.63
4:F:162:ILE:HD11	4:F:240:LEU:HD13	1.80	0.63
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.72	0.62
2:B:376:THR:OG1	7:B:505:GOL:H31	1.99	0.62
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.82	0.62
2:D:406:HIS:HA	2:D:409:THR:HG22	1.81	0.62
4:F:184:LYS:NZ	4:F:187:GLU:OE2	2.33	0.62
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.82	0.61
2:B:106:GLY:O	2:B:111:GLY:HA3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:44:ASP:N	14:E:301:HOH:O	2.33	0.61
2:B:155[B]:SER:OG	3:E:76:ARG:NH2	2.32	0.61
2:B:76:ASP:N	14:B:604:HOH:O	2.34	0.61
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.82	0.61
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.81	0.61
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.18	0.60
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.84	0.60
7:A:506:GOL:O2	3:E:44:ASP:OD2	2.20	0.60
1:C:39:ASP:OD2	1:C:41:THR:OG1	2.18	0.60
4:F:166:ALA:N	14:F:502:HOH:O	2.34	0.60
3:E:9:ILE:HG22	3:E:10:GLU:H	1.67	0.59
1:C:179:THR:HG23	5:C:502:GTP:H3'	1.85	0.59
1:C:241:SER:HA	1:C:249:ASN:HD21	1.67	0.59
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.85	0.58
2:D:171:VAL:HA	2:D:204:ILE:O	2.04	0.58
2:B:320:ARG:NH1	7:B:505:GOL:H11	2.18	0.57
4:F:163:SER:OG	4:F:168:GLU:OE1	2.20	0.57
4:F:7:ARG:NH2	4:F:43:GLU:OE2	2.30	0.57
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.86	0.57
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.19	0.57
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.85	0.57
2:D:19:LYS:O	2:D:23:VAL:HG23	2.05	0.57
1:C:253:THR:HB	7:C:501:GOL:H11	1.87	0.57
2:D:93:VAL:HG21	2:D:121:VAL:HG21	1.86	0.57
4:F:40:MET:HE2	4:F:47:LEU:HG	1.86	0.57
2:D:369:ARG:NH1	14:D:603:HOH:O	2.38	0.56
4:F:136:ASN:O	4:F:145:ASN:ND2	2.38	0.56
2:D:46:LEU:HA	2:D:49:ILE:HB	1.86	0.56
2:B:217:LEU:HD11	2:B:230:LEU:HD21	1.88	0.56
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.88	0.56
2:D:249:ASN:HB3	2:D:254:LYS:NZ	2.20	0.56
4:F:36:ARG:NH1	4:F:55:GLU:OE1	2.36	0.56
3:E:112:ARG:HH21	12:E:201:IMD:C5	2.19	0.55
2:D:136:GLN:HA	2:D:167:ASN:O	2.06	0.55
2:D:177:VAL:HG13	7:D:503:GOL:H2	1.87	0.55
1:A:214:ARG:NH1	1:A:220:GLU:O	2.40	0.55
4:F:31:ARG:HE	4:F:32:LYS:HG3	1.72	0.54
2:B:237:GLY:CA	7:B:505:GOL:H12	2.38	0.54
2:D:179:ASP:N	2:D:179:ASP:OD1	2.40	0.54
1:A:245:ASP:HB3	3:E:16:SER:HB2	1.90	0.54
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LEU:HD11	2:B:431[B]:GLU:HG2	1.91	0.53
2:D:382:THR:HA	2:D:432:TYR:CD1	2.43	0.53
1:A:70:LEU:HG	1:A:145:THR:HG23	1.90	0.53
1:C:210:TYR:OH	1:C:221:ARG:NH2	2.41	0.53
4:F:186:LEU:HB3	13:F:402:ACP:H2	1.91	0.53
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.44	0.53
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.43	0.52
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.44	0.52
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.44	0.52
4:F:101:TYR:CD2	4:F:126:ASP:HB3	2.45	0.52
2:B:221:THR:HG21	1:C:326:LYS:HA	1.91	0.52
4:F:39:LEU:HD13	4:F:61:LEU:HD23	1.90	0.52
2:D:176:LYS:HD2	2:D:210:TYR:CD2	2.44	0.52
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.90	0.52
2:B:19:LYS:HB3	2:B:232:SER:OG	2.10	0.51
2:B:69:ASP:O	2:B:94:PHE:HA	2.10	0.51
2:D:71:GLU:HB3	2:D:98:GLY:HA2	1.90	0.51
4:F:263:PHE:CG	4:F:341:LYS:HE2	2.45	0.51
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.51
4:F:88:SER:HG	4:F:91:CYS:N	2.08	0.51
1:A:339:ARG:O	14:A:602:HOH:O	2.19	0.51
4:F:181:VAL:O	14:F:501:HOH:O	2.19	0.51
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.92	0.51
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.92	0.51
2:B:132:LEU:O	2:B:164:ARG:NH1	2.43	0.51
2:B:320:ARG:HD3	7:B:505:GOL:H2	1.93	0.51
2:B:181:VAL:HG22	1:C:258:ASN:OD1	2.10	0.50
2:B:326:LYS:NZ	2:B:330:GLU:OE2	2.40	0.50
4:F:100:ILE:HG23	4:F:128:ARG:HG3	1.93	0.50
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.25	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.46	0.50
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.47	0.50
2:D:431:GLU:OE2	14:D:602:HOH:O	2.20	0.50
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.46	0.50
4:F:128:ARG:HH21	4:F:170:LEU:HD21	1.76	0.50
4:F:12:SER:OG	14:F:504:HOH:O	2.18	0.50
4:F:5:VAL:HG13	4:F:37:PHE:HB3	1.94	0.50
1:A:102:ASN:HB3	1:A:105:ARG:HB3	1.94	0.49
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.47	0.49
4:F:43:GLU:OE1	4:F:43:GLU:N	2.36	0.49
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:PRO:HB3	2:D:94:PHE:CD2	2.47	0.49
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.77	0.49
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.95	0.49
1:A:68[A]:VAL:HG11	1:A:149:PHE:CE2	2.47	0.49
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.94	0.49
2:D:208:ALA:O	2:D:212:ILE:HG13	2.12	0.49
4:F:99:VAL:O	4:F:126:ASP:HB2	2.13	0.49
4:F:247:LYS:HG3	4:F:253:TYR:CE2	2.48	0.49
2:B:360:PRO:HG3	7:B:505:GOL:O2	2.13	0.49
2:D:152:LEU:O	2:D:156:LYS:HG2	2.13	0.49
2:D:357:ASP:O	2:D:359:PRO:HD3	2.13	0.49
2:D:3:GLU:N	2:D:3:GLU:OE2	2.45	0.49
4:F:145:ASN:HB3	4:F:147:TRP:NE1	2.19	0.49
4:F:100:ILE:HG13	4:F:182:ILE:HD12	1.94	0.49
4:F:71:LEU:HD13	4:F:298:ILE:HD13	1.94	0.49
1:A:338:LYS:HE2	1:A:339:ARG:HG3	1.95	0.49
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.93	0.49
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.13	0.48
1:A:230:LEU:O	1:A:234:ILE:HD12	2.14	0.48
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.45	0.48
4:F:224:SER:HA	4:F:246:GLN:HE22	1.78	0.48
2:B:195:VAL:HG13	2:B:264:ARG:HG2	1.95	0.48
4:F:189:PRO:HA	4:F:322:ASP:HA	1.95	0.48
4:F:86:GLU:O	4:F:87:LEU:HD23	2.14	0.48
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.78	0.48
4:F:91:CYS:N	14:F:507:HOH:O	2.46	0.48
2:D:327:GLU:O	2:D:331:GLN:HG2	2.14	0.48
4:F:102:PRO:HA	4:F:173:ILE:HG12	1.95	0.48
2:B:415:GLU:HG3	14:B:616:HOH:O	2.14	0.48
4:F:358:VAL:O	4:F:360:PRO:HD3	2.14	0.48
1:A:297:GLU:OE2	1:A:339:ARG:NH1	2.44	0.47
2:D:402:LYS:HB3	2:D:405:LEU:HD13	1.96	0.47
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.47
3:E:8:VAL:HG22	3:E:22:VAL:HG22	1.96	0.47
3:E:47:LEU:O	3:E:51:GLN:HG2	2.14	0.47
2:B:210:TYR:CE1	2:B:222:PRO:HD2	2.49	0.47
2:B:318:ILE:HD11	2:B:376:THR:HB	1.97	0.47
2:D:161:TYR:HB3	2:D:164:ARG:HG2	1.96	0.47
4:F:128:ARG:O	4:F:131:PHE:HB3	2.15	0.47
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:263:PHE:CD2	4:F:341:LYS:HE2	2.49	0.47
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.97	0.47
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.97	0.47
1:C:166:LYS:HE2	1:C:197:HIS:O	2.15	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
3:E:127:ASP:O	3:E:131:GLU:HG2	2.15	0.47
4:F:2:TYR:OH	4:F:360:PRO:O	2.19	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.47
1:C:21:TRP:CZ2	1:C:65:ALA:HB2	2.50	0.47
1:C:1:MET:O	1:C:2:ARG:HG2	2.14	0.47
1:C:333:ALA:O	1:C:337:THR:HG23	2.15	0.46
2:B:282:GLN:N	2:B:282:GLN:HE21	2.12	0.46
2:D:63:PRO:O	2:D:65:ALA:N	2.48	0.46
4:F:146:VAL:HG13	14:F:503:HOH:O	2.15	0.46
4:F:131:PHE:HD1	4:F:132:LEU:HG	1.80	0.46
1:C:141:PHE:O	1:C:147:SER:HB3	2.15	0.46
1:C:175:PRO:HD2	1:C:207:GLU:OE2	2.16	0.46
1:C:174:ALA:HB2	1:C:207:GLU:N	2.31	0.46
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.33	0.46
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.98	0.46
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.46
2:D:414:ASP:OD1	2:D:415:GLU:N	2.47	0.46
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.16	0.46
2:B:19:LYS:HA	2:B:19:LYS:HD3	1.77	0.46
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.51	0.46
1:A:415:GLU:O	1:A:418:PHE:HB2	2.16	0.46
1:C:174:ALA:O	1:C:178:SER:HB3	2.15	0.46
2:D:239:THR:O	2:D:243:ARG:HG3	2.15	0.46
1:A:217:LEU:HA	1:A:277:SER:HB2	1.98	0.45
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.51	0.45
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.45
2:D:59:ASN:N	14:D:606:HOH:O	2.48	0.45
2:B:298:SER:H	2:B:308:ARG:HH12	1.65	0.45
4:F:3:THR:CG2	4:F:37:PHE:HA	2.46	0.45
2:D:335:VAL:O	2:D:339:ASN:HB2	2.16	0.45
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.99	0.45
4:F:3:THR:HG23	4:F:30:LEU:CD1	2.47	0.45
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.56	0.45
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.80	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:SER:O	2:D:151:THR:HG23	2.16	0.45
4:F:284[A]:LEU:HD12	4:F:287:ILE:HB	1.98	0.45
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.50	0.45
2:B:325:MET:HB3	2:B:325:MET:HE2	1.86	0.45
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.98	0.45
2:D:177:VAL:HA	7:D:503:GOL:H32	1.98	0.45
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.98	0.45
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.51	0.45
4:F:31:ARG:NE	4:F:32:LYS:H	2.04	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.45
1:A:196:GLU:HG3	1:A:197:HIS:CD2	2.52	0.45
4:F:245:ILE:HG23	4:F:249:TYR:HD2	1.80	0.45
1:A:401:LYS:HE3	2:B:438:ALA:HB1	1.99	0.44
1:C:262:TYR:CB	12:C:508:IMD:H5	2.47	0.44
4:F:201:ILE:HG12	4:F:221:LEU:CD2	2.47	0.44
1:A:337:THR:OG1	1:A:338:LYS:N	2.50	0.44
1:C:220:GLU:CD	2:D:326:LYS:HD3	2.38	0.44
1:C:296:PHE:O	1:C:298:PRO:HD3	2.18	0.44
1:C:262:TYR:CG	12:C:508:IMD:H5	2.52	0.44
4:F:3:THR:HG23	4:F:30:LEU:HD11	1.99	0.44
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.18	0.44
2:B:295:MET:SD	2:B:375:ALA:HB1	2.58	0.44
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.57	0.44
4:F:189:PRO:HG3	4:F:198:LYS:HD3	1.99	0.44
1:C:6:SER:O	1:C:65:ALA:HA	2.18	0.44
1:A:154:MET:HG3	1:A:194:THR:HG23	1.99	0.44
1:C:248:LEU:HB3	1:C:355:ILE:HB	2.00	0.44
1:C:209:ILE:HD11	1:C:302:MET:SD	2.57	0.43
2:D:75:MET:SD	2:D:94:PHE:HB3	2.58	0.43
2:D:249:ASN:HB3	2:D:254:LYS:HZ2	1.82	0.43
2:D:82:PRO:O	2:D:83:PHE:HB2	2.19	0.43
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.01	0.43
2:D:108:TYR:CG	3:E:133:VAL:HG11	2.54	0.43
2:B:136:GLN:HG3	2:B:169:PHE:HE1	1.83	0.43
3:E:119:MET:HA	3:E:122:ARG:NH2	2.33	0.43
3:E:139:LEU:N	3:E:139:LEU:HD23	2.33	0.43
1:C:141:PHE:HE1	1:C:191:THR:OG1	2.02	0.43
2:B:359:PRO:HB2	2:B:371:LEU:O	2.19	0.43
3:E:101:LEU:HD12	3:E:101:LEU:HA	1.86	0.43
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.54	0.43
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:HD2	2:B:371:LEU:HD13	2.00	0.43
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.43
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.43
4:F:198:LYS:HG3	4:F:228:TYR:CD1	2.54	0.43
2:B:176:LYS:HD2	2:B:207:GLU:HG3	2.01	0.43
2:B:158:ARG:NH1	2:B:196:GLU:O	2.52	0.43
2:D:248:LEU:HB3	11:D:505:93X:O50	2.19	0.43
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.84	0.42
1:A:2:ARG:HB3	1:A:133:GLN:HG3	2.00	0.42
1:A:285:GLN:NE2	1:A:285:GLN:HA	2.34	0.42
1:A:72:PRO:HA	1:A:94:THR:HG21	2.02	0.42
1:A:401:LYS:HE2	2:B:346:TRP:CD2	2.55	0.42
2:B:431[B]:GLU:O	2:B:434:GLN:HG2	2.19	0.42
4:F:209:HIS:HA	4:F:311:SER:O	2.20	0.42
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.55	0.42
2:B:2:ARG:HB3	2:B:133:GLN:HG2	2.00	0.42
2:D:176:LYS:O	2:D:177:VAL:HB	2.20	0.42
2:D:334:ASN:ND2	2:D:338:LYS:HE2	2.30	0.42
1:C:182:VAL:HB	1:C:408:TYR:OH	2.19	0.42
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.55	0.42
4:F:247:LYS:HG3	4:F:253:TYR:HE2	1.85	0.42
1:A:107:HIS:ND1	1:A:152:LEU:HB2	2.35	0.42
4:F:244:CYS:O	4:F:245:ILE:HG12	2.20	0.42
1:A:167:LEU:HD13	1:A:252:LEU:HD22	2.02	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.85	0.41
2:B:234:THR:O	2:B:238:VAL:HB	2.20	0.41
2:D:47:GLU:HG2	2:D:245:PRO:HG3	2.01	0.41
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.54	0.41
2:D:34:GLY:O	2:D:60:LYS:HD3	2.20	0.41
3:E:75:LYS:O	3:E:79:GLU:HG3	2.20	0.41
4:F:97:SER:HA	4:F:182:ILE:O	2.21	0.41
2:B:298:SER:OG	2:B:308:ARG:NH1	2.53	0.41
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.36	0.41
2:D:115:VAL:O	2:D:119:LEU:HG	2.20	0.41
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	0.41
2:B:431[A]:GLU:O	2:B:434:GLN:HG2	2.20	0.41
2:D:29:GLY:O	2:D:36:TYR:HA	2.21	0.41
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.56	0.41
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.85	0.41
1:A:231:ILE:O	1:A:235:VAL:HG23	2.21	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.61	0.41
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.56	0.41
2:B:205:ASP:O	2:B:209:LEU:HG	2.21	0.41
2:D:320:ARG:HG2	2:D:356:CYS:HB3	2.03	0.41
2:D:406:HIS:NE2	2:D:407:TRP:HD1	2.19	0.41
4:F:3:THR:HG22	4:F:37:PHE:HA	2.03	0.41
1:A:264:ARG:HB2	14:A:612:HOH:O	2.21	0.41
1:A:2:ARG:O	1:A:133:GLN:NE2	2.53	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.56	0.41
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.21	0.41
1:C:10:GLY:O	1:C:14:VAL:HG23	2.21	0.40
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	0.40
1:A:90:GLU:O	1:A:121:ARG:HD2	2.21	0.40
1:A:238:ILE:HG12	1:A:378:LEU:HD21	2.02	0.40
2:B:46:LEU:HD23	2:B:49:ILE:HD12	2.04	0.40
1:C:143:GLY:HA3	5:C:502:GTP:O3A	2.21	0.40
1:C:253:THR:HG23	12:C:509:IMD:H4	2.04	0.40
4:F:165:GLU:HB2	4:F:168:GLU:OE2	2.21	0.40
4:F:17:VAL:HG13	4:F:351:VAL:HG22	2.03	0.40
1:A:141:PHE:O	1:A:147:SER:HB3	2.22	0.40
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.56	0.40
1:C:147:SER:OG	1:C:186:ASN:HB3	2.21	0.40
4:F:31:ARG:NE	4:F:32:LYS:HG3	2.36	0.40
1:C:1:MET:HG3	1:C:2:ARG:N	2.36	0.40
2:D:20:PHE:O	2:D:24:ILE:HG23	2.22	0.40
4:F:242:ASN:O	4:F:246:GLN:HB2	2.21	0.40
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.03	0.40
2:D:320:ARG:HB3	2:D:359:PRO:HA	2.03	0.40
3:E:25:LYS:HA	3:E:26:PRO:HD3	1.86	0.40
4:F:284[A]:LEU:HD12	4:F:284[A]:LEU:HA	1.78	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:B:411:GLU:OE1	1:C:282:TYR:OH[4_545]	2.17	0.03



## 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	447/451 (99%)	421 (94%)	22 (5%)	4 (1%)	20	37
1	C	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	51	72
2	B	429/445 (96%)	402 (94%)	24 (6%)	3 (1%)	25	45
2	D	420/445 (94%)	400 (95%)	16 (4%)	4 (1%)	18	34
3	E	117/189 (62%)	105 (90%)	10 (8%)	2 (2%)	11	19
4	F	302/378 (80%)	263 (87%)	37 (12%)	2 (1%)	25	45
All	All	2162/2359 (92%)	2022 (94%)	124 (6%)	16 (1%)	22	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
2	D	177	VAL
3	E	10	GLU
4	F	230	SER
2	D	64	ARG
1	A	366	GLY
2	B	73	GLY
2	B	82	PRO
2	B	216	THR
1	C	176	GLN
1	A	261	PRO
3	E	52	LYS
4	F	242	ASN
1	A	281	ALA
2	D	143	GLY
2	D	181	VAL

### 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	380/379 (100%)	372 (98%)	8 (2%)	59	80
1	C	380/379 (100%)	373 (98%)	7 (2%)	64	83
2	B	375/383 (98%)	357 (95%)	18 (5%)	30	51
2	D	367/383 (96%)	355 (97%)	12 (3%)	43	67
3	E	109/171 (64%)	105 (96%)	4 (4%)	39	62
4	F	289/336 (86%)	275 (95%)	14 (5%)	30	51
All	All	1900/2031 (94%)	1837 (97%)	63 (3%)	43	67

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	178	SER
1	A	179	THR
1	A	207	GLU
1	A	241	SER
1	A	250	VAL
1	A	271	THR
1	A	438	ASP
2	B	2	ARG
2	B	75	MET
2	B	90	ASP
2	B	117	SER
2	B	132	LEU
2	B	139	HIS
2	B	155[A]	SER
2	B	155[B]	SER
2	B	200	GLU
2	B	215	ARG
2	B	220	THR
2	B	238	VAL
2	B	277	SER
2	B	282	GLN

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Mol	Chain	Res	Type
2	B	283	TYR
2	B	298	SER
2	B	318	ILE
2	B	340	SER
1	C	67	PHE
1	C	71	GLU
1	C	179	THR
1	C	181	VAL
1	C	241	SER
1	C	347	CYS
1	C	381	THR
2	D	8	GLN
2	D	26	ASP
2	D	74	THR
2	D	117	SER
2	D	139	HIS
2	D	180	THR
2	D	207	GLU
2	D	249	ASN
2	D	341	SER
2	D	377	PHE
2	D	390	ARG
2	D	434	GLN
3	E	12	ASN
3	E	16	SER
3	E	124	GLN
3	E	140	LYS
4	F	13	VAL
4	F	69	ASP
4	F	71	LEU
4	F	127	GLU
4	F	129	GLU
4	F	170	LEU
4	F	172	PHE
4	F	181	VAL
4	F	211	TYR
4	F	223	THR
4	F	240	LEU
4	F	246	GLN
4	F	264	PHE
4	F	331	GLU

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

sidechains are listed below:

Mol	Chain	Res	Type
1	C	249	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 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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	0.98	1 (3%)	27,54,54	1.78	6 (22%)
7	GOL	A	503	-	5,5,5	0.34	0	5,5,5	0.31	0
7	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.68	0
7	GOL	A	506	-	5,5,5	0.37	0	5,5,5	0.38	0
9	GDP	B	501	6	25,30,30	1.08	2 (8%)	26,47,47	1.97	7 (26%)
7	GOL	B	503	-	5,5,5	0.31	0	5,5,5	0.22	0
7	GOL	B	504	-	5,5,5	0.41	0	5,5,5	0.44	0
7	GOL	B	505	-	5,5,5	0.35	0	5,5,5	0.59	0
10	MES	B	507	-	12,12,12	2.06	1 (8%)	14,16,16	2.49	4 (28%)
11	93X	B	508	-	29,30,30	4.63	8 (27%)	38,43,43	4.12	14 (36%)
7	GOL	C	501	-	5,5,5	0.33	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	C	502	6	27,34,34	1.08	2 (7%)	27,54,54	1.73	5 (18%)
7	GOL	C	504	-	5,5,5	0.29	0	5,5,5	0.46	0
7	GOL	C	505	-	5,5,5	0.39	0	5,5,5	0.12	0
7	GOL	C	506	-	5,5,5	0.52	0	5,5,5	0.53	0
12	IMD	C	508	-	3,5,5	0.59	0	4,5,5	0.52	0
12	IMD	C	509	-	3,5,5	0.56	0	4,5,5	0.54	0
9	GDP	D	501	-	25,30,30	1.29	2 (8%)	26,47,47	2.16	8 (30%)
7	GOL	D	503	-	5,5,5	0.30	0	5,5,5	0.37	0
7	GOL	D	504	12	5,5,5	0.33	0	5,5,5	0.30	0
11	93X	D	505	-	29,30,30	4.84	10 (34%)	38,43,43	3.87	12 (31%)
12	IMD	E	201	7	3,5,5	0.50	0	4,5,5	0.50	0
13	ACP	F	402	-	27,33,33	2.43	9 (33%)	30,52,52	1.94	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
7	GOL	A	503	-	-	0/4/4/4	0/0/0/0
7	GOL	A	504	-	-	0/4/4/4	0/0/0/0
7	GOL	A	506	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
7	GOL	B	503	-	-	0/4/4/4	0/0/0/0
7	GOL	B	504	-	-	0/4/4/4	0/0/0/0
7	GOL	B	505	-	-	0/4/4/4	0/0/0/0
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
11	93X	B	508	-	-	0/18/34/34	0/3/3/3
7	GOL	C	501	-	-	0/4/4/4	0/0/0/0
5	GTP	C	502	6	-	0/18/38/38	0/3/3/3
7	GOL	C	504	-	-	0/4/4/4	0/0/0/0
7	GOL	C	505	-	-	0/4/4/4	0/0/0/0
7	GOL	C	506	-	-	0/4/4/4	0/0/0/0
12	IMD	C	508	-	-	0/0/0/0	0/1/1/1
12	IMD	C	509	-	-	0/0/0/0	0/1/1/1
9	GDP	D	501	-	-	0/12/32/32	0/3/3/3
7	GOL	D	503	-	-	0/4/4/4	0/0/0/0
7	GOL	D	504	12	-	0/4/4/4	0/0/0/0
11	93X	D	505	-	-	0/18/34/34	0/3/3/3
12	IMD	E	201	7	-	0/0/0/0	0/1/1/1
13	ACP	F	402	-	-	0/15/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	507	MES	C8-S	-6.84	1.67	1.77
13	F	402	ACP	C2'-C1'	-3.53	1.48	1.53
13	F	402	ACP	C4-N3	-2.91	1.31	1.35
13	F	402	ACP	C2'-C3'	-2.75	1.46	1.53
13	F	402	ACP	PB-O2B	-2.43	1.50	1.56
13	F	402	ACP	O2'-C2'	2.01	1.47	1.43
11	B	508	93X	O23-C10	2.03	1.40	1.37
11	D	505	93X	O21-C9	2.16	1.42	1.38
11	B	508	93X	O25-C8	2.18	1.40	1.37
5	C	502	GTP	C2-N1	2.29	1.39	1.35
11	D	505	93X	O18-C16	2.33	1.41	1.36
9	B	501	GDP	C5-C4	2.42	1.46	1.40
11	D	505	93X	C6-N1	2.53	1.47	1.43
13	F	402	ACP	C5-N7	2.56	1.48	1.39
11	B	508	93X	O19-C15	2.65	1.41	1.37
11	B	508	93X	O21-C9	2.76	1.43	1.38
11	D	505	93X	O25-C8	2.85	1.41	1.37
11	D	505	93X	C2-N1	2.89	1.51	1.48
9	B	501	GDP	C6-C5	2.98	1.47	1.41
9	D	501	GDP	C5-C4	3.01	1.47	1.40
5	C	502	GTP	C6-N1	3.03	1.38	1.33
11	B	508	93X	O18-C16	3.06	1.42	1.36
11	D	505	93X	O23-C10	3.06	1.41	1.37
5	A	501	GTP	C6-N1	3.07	1.38	1.33
13	F	402	ACP	C6-N6	3.12	1.46	1.34
11	B	508	93X	C12-C2	3.40	1.56	1.51
11	D	505	93X	O19-C15	3.69	1.42	1.37
9	D	501	GDP	C6-C5	4.31	1.49	1.41
11	B	508	93X	C29-C3	4.87	1.60	1.53
11	D	505	93X	C12-C2	5.10	1.59	1.51
13	F	402	ACP	O4'-C1'	5.30	1.48	1.41
11	D	505	93X	C29-C3	5.67	1.61	1.53
13	F	402	ACP	PB-O3A	7.54	1.66	1.58
11	B	508	93X	C4-N1	23.16	1.74	1.37
11	D	505	93X	C4-N1	23.53	1.75	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	93X	C2-N1-C4	-12.48	82.45	95.27
11	D	505	93X	C2-N1-C4	-12.15	82.79	95.27
13	F	402	ACP	N3-C2-N1	-7.67	122.18	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	GTP	N3-C2-N1	-5.24	119.80	127.46
11	B	508	93X	C26-O25-C8	-5.23	110.02	117.54
5	A	501	GTP	N3-C2-N1	-4.58	120.77	127.46
9	D	501	GDP	C6-C5-C4	-4.47	116.40	120.84
11	D	505	93X	O23-C10-C11	-4.43	116.70	124.17
11	D	505	93X	O25-C8-C7	-4.31	116.91	124.17
11	B	508	93X	O23-C10-C11	-3.97	117.48	124.17
9	B	501	GDP	C6-C5-C4	-3.97	116.90	120.84
11	B	508	93X	O25-C8-C7	-3.83	117.72	124.17
9	B	501	GDP	N3-C2-N1	-3.68	122.09	127.46
9	D	501	GDP	C4-C5-N7	-3.48	106.05	109.41
9	D	501	GDP	C5-C6-N1	-3.47	118.54	123.48
11	B	508	93X	C24-O23-C10	-3.30	112.79	117.54
13	F	402	ACP	C4'-O4'-C1'	-3.23	106.33	109.77
9	D	501	GDP	N3-C2-N1	-3.20	122.79	127.46
10	B	507	MES	C6-C5-N4	-3.13	105.72	110.11
5	A	501	GTP	C5-C6-N1	-3.05	119.14	123.48
13	F	402	ACP	C4-C5-N7	-2.69	106.81	109.41
9	B	501	GDP	C4-C5-N7	-2.60	106.90	109.41
9	B	501	GDP	C5-C6-N1	-2.60	119.78	123.48
11	B	508	93X	C14-C13-C12	-2.47	118.69	121.20
5	A	501	GTP	O3'-C3'-C2'	-2.20	104.78	111.83
11	D	505	93X	C24-O23-C10	-2.02	114.62	117.54
9	B	501	GDP	C1'-N9-C4	-2.02	123.14	126.64
5	C	502	GTP	C5-C6-N1	-2.00	120.63	123.48
5	A	501	GTP	N2-C2-N1	2.01	120.45	117.24
9	D	501	GDP	C2'-C3'-C4'	2.21	106.93	102.62
5	C	502	GTP	N2-C2-N1	2.22	120.79	117.24
5	C	502	GTP	C6-N1-C2	2.27	119.33	116.06
13	F	402	ACP	C2'-C3'-C4'	2.31	107.13	102.62
11	D	505	93X	O19-C15-C16	2.42	117.50	114.55
11	B	508	93X	C7-C6-N1	2.55	121.83	119.40
11	B	508	93X	O21-C9-C10	2.68	123.95	120.12
5	A	501	GTP	C6-N1-C2	2.72	119.97	116.06
11	B	508	93X	O5-C4-N1	2.83	135.93	131.76
9	D	501	GDP	C4'-O4'-C1'	2.83	112.78	109.77
11	B	508	93X	O25-C8-C9	2.86	120.26	115.22
11	D	505	93X	O5-C4-N1	2.86	135.99	131.76
11	D	505	93X	C7-C6-N1	2.89	122.15	119.40
9	B	501	GDP	C6-N1-C2	3.45	121.02	116.06
10	B	507	MES	O1S-S-C8	3.53	109.82	106.79
13	F	402	ACP	O3'-C3'-C4'	3.85	122.35	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	505	93X	O25-C8-C9	4.16	122.55	115.22
9	D	501	GDP	C6-N1-C2	4.26	122.19	116.06
5	C	502	GTP	C2-N3-C4	4.28	120.15	115.16
5	A	501	GTP	C2-N3-C4	4.29	120.17	115.16
11	B	508	93X	O23-C10-C9	4.56	123.25	115.22
11	D	505	93X	O23-C10-C9	4.78	123.64	115.22
9	D	501	GDP	C2-N3-C4	5.04	121.04	115.16
10	B	507	MES	C5-N4-C3	5.09	120.39	108.87
10	B	507	MES	O3S-S-C8	5.26	112.52	106.06
9	B	501	GDP	C2-N3-C4	5.32	121.37	115.16
11	D	505	93X	C6-N1-C2	7.00	141.94	130.31
11	B	508	93X	O5-C4-C3	7.44	141.84	135.61
11	D	505	93X	O5-C4-C3	7.64	142.01	135.61
11	B	508	93X	C6-N1-C2	7.89	143.41	130.31
11	D	505	93X	C3-C2-N1	13.80	97.28	86.40
11	B	508	93X	C3-C2-N1	14.73	98.01	86.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	2	0
7	A	506	GOL	1	0
9	B	501	GDP	1	0
7	B	505	GOL	6	0
7	C	501	GOL	1	0
5	C	502	GTP	2	0
7	C	506	GOL	1	0
12	C	508	IMD	2	0
12	C	509	IMD	1	0
9	D	501	GDP	2	0
7	D	503	GOL	2	0
11	D	505	93X	1	0
12	E	201	IMD	2	0
13	F	402	ACP	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	439/451 (97%)	0.34	15 (3%) 46 43	48, 71, 104, 153	0
1	C	440/451 (97%)	0.02	8 (1%) 69 67	40, 55, 82, 106	0
2	B	424/445 (95%)	0.27	20 (4%) 32 30	38, 64, 102, 176	0
2	D	421/445 (94%)	0.59	39 (9%) 9 8	48, 85, 122, 181	4 (0%)
3	E	120/189 (63%)	0.35	7 (5%) 24 21	50, 80, 115, 154	0
4	F	317/378 (83%)	1.55	111 (35%) 0 0	55, 100, 170, 220	0
All	All	2161/2359 (91%)	0.49	200 (9%) 9 8	38, 73, 124, 220	4 (0%)

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	15.4
4	F	245	ILE	10.9
4	F	133	ALA	9.2
4	F	249	TYR	8.4
4	F	248	GLU	7.6
4	F	256	TYR	7.2
4	F	225	SER	7.1
4	F	239	HIS	6.6
4	F	17	VAL	6.5
4	F	253	TYR	6.3
4	F	240	LEU	5.9
4	F	224	SER	5.9
2	B	59	ASN	5.9
1	A	439	SER	5.7
2	D	219	LEU	5.6
4	F	231	ALA	5.6
4	F	132	LEU	5.6
4	F	134	ALA	5.4
4	F	100	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
4	F	255	ARG	5.3
2	B	62	VAL	5.3
4	F	21	LEU	5.1
3	E	27	PRO	5.0
4	F	257	GLU	4.9
4	F	130	VAL	4.9
2	B	1	MET	4.9
4	F	147	TRP	4.8
4	F	131	PHE	4.7
4	F	236	LYS	4.5
4	F	9	GLU	4.5
2	D	94	PHE	4.5
2	D	1	MET	4.4
2	D	177	VAL	4.4
4	F	14	TYR	4.3
4	F	252	ASN	4.3
4	F	235	ASP	4.3
4	F	346	LEU	4.2
4	F	199	PHE	4.2
4	F	144	GLY	4.2
2	B	50[A]	ASN	4.1
4	F	182	ILE	4.0
4	F	241	THR	3.9
2	D	401	ARG	3.9
4	F	190	LEU	3.9
4	F	27	TRP	3.9
4	F	259	GLY	3.8
4	F	250	SER	3.8
2	D	218	LYS	3.7
4	F	238	CYS	3.7
2	B	60	LYS	3.7
4	F	227	PRO	3.7
4	F	13	VAL	3.7
4	F	361	LEU	3.6
2	B	37	HIS	3.6
4	F	339	ALA	3.5
4	F	242	ASN	3.5
2	B	249	ASN	3.5
4	F	315	PHE	3.4
4	F	150	LYS	3.4
2	B	36	TYR	3.4
2	D	400	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	254	GLY	3.4
4	F	228	TYR	3.4
2	D	57	THR	3.3
4	F	24	THR	3.3
4	F	99	VAL	3.3
4	F	135	TYR	3.3
4	F	243	HIS	3.3
2	D	404	PHE	3.3
4	F	263	PHE	3.3
2	D	95	GLY	3.3
4	F	169	LEU	3.3
4	F	264	PHE	3.3
1	A	262	TYR	3.2
2	D	220	THR	3.2
4	F	283	ILE	3.2
4	F	128	ARG	3.2
2	D	37	HIS	3.2
2	B	61	TYR	3.2
4	F	198	LYS	3.2
4	F	163	SER	3.1
2	D	179	ASP	3.1
1	C	1	MET	3.1
3	E	28	SER	3.1
4	F	148	ILE	3.1
2	D	407	TRP	3.1
4	F	129	GLU	3.0
4	F	172	PHE	3.0
4	F	197	ARG	3.0
1	A	349	THR	3.0
4	F	20	LEU	3.0
3	E	7	GLU	3.0
2	D	75	MET	3.0
4	F	168	GLU	3.0
4	F	101	TYR	3.0
1	A	179	THR	3.0
1	C	241	SER	3.0
4	F	125	THR	2.9
4	F	247	LYS	2.9
2	D	408	TYR	2.9
4	F	1	MET	2.9
2	D	210	TYR	2.9
4	F	96	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	399	PHE	2.9
2	B	57	THR	2.9
2	D	92	PHE	2.8
3	E	22	VAL	2.8
4	F	323	GLU	2.8
2	D	308	ARG	2.7
4	F	258	GLU	2.7
4	F	220	VAL	2.7
4	F	167	SER	2.7
4	F	22	LEU	2.7
4	F	271	LEU	2.7
2	D	124	LYS	2.7
4	F	149	ALA	2.7
2	D	405	LEU	2.7
4	F	260	ASN	2.7
1	A	438	ASP	2.7
4	F	165	GLU	2.6
2	B	283	TYR	2.6
1	A	141	PHE	2.6
2	B	247	GLN	2.6
1	A	350	GLY	2.6
4	F	28	LYS	2.6
2	D	61	TYR	2.6
1	A	347	CYS	2.6
3	E	24	LEU	2.6
4	F	192	LEU	2.6
4	F	262	MET	2.6
4	F	362	ALA	2.5
2	D	118	VAL	2.5
3	E	26	PRO	2.5
4	F	145	ASN	2.5
2	D	30	ILE	2.5
4	F	4	PHE	2.5
2	D	82	PRO	2.5
2	D	78	VAL	2.4
4	F	214	TYR	2.4
2	B	30	ILE	2.4
4	F	25	GLY	2.4
4	F	226	GLU	2.4
2	D	33	THR	2.4
1	A	346	TRP	2.4
4	F	183	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	49	ILE	2.4
1	C	251	ASP	2.4
2	D	85	GLN	2.4
2	D	413	MET	2.3
4	F	336	PRO	2.3
2	D	247	GLN	2.3
2	B	83	PHE	2.3
4	F	229	ASN	2.3
4	F	223	THR	2.3
4	F	26	GLN	2.3
4	F	194	PRO	2.3
4	F	162	ILE	2.3
1	C	253	THR	2.3
1	A	282	TYR	2.2
1	A	42	ILE	2.2
4	F	184	LYS	2.2
2	D	86	ILE	2.2
2	D	114	LEU	2.2
4	F	342	LEU	2.2
4	F	181	VAL	2.2
4	F	196	HIS	2.2
4	F	39	LEU	2.2
2	D	415	GLU	2.2
4	F	173	ILE	2.2
4	F	44	ARG	2.2
2	D	46	LEU	2.1
4	F	351	VAL	2.1
2	D	214	PHE	2.1
3	E	44	ASP	2.1
1	A	78	VAL	2.1
4	F	98	TYR	2.1
1	A	178	SER	2.1
2	B	88	ARG	2.1
4	F	12	SER	2.1
2	B	318	ILE	2.1
1	C	252	LEU	2.1
4	F	340	GLN	2.1
4	F	332	VAL	2.1
2	D	217	LEU	2.1
4	F	284[A]	LEU	2.1
2	B	58	GLY	2.1
1	C	440	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	82	PRO	2.1
1	C	357	TYR	2.1
4	F	275[A]	LEU	2.1
2	B	2	ARG	2.1
1	A	201	ALA	2.0
2	D	221[A]	THR	2.0
1	C	2	ARG	2.0
4	F	343	TYR	2.0
2	D	55	GLU	2.0
1	A	56	THR	2.0
4	F	246	GLN	2.0
4	F	6	VAL	2.0
4	F	191	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
7	GOL	B	505	6/6	0.57	0.77	14.01	100,107,115,123	0
7	GOL	C	505	6/6	0.74	0.74	12.72	108,114,117,119	0
7	GOL	A	504	6/6	0.50	0.45	7.69	111,113,114,115	0
7	GOL	B	503	6/6	0.71	0.37	6.36	82,96,105,110	0
12	IMD	E	201	5/5	0.86	0.33	4.11	123,124,128,129	0
7	GOL	B	504	6/6	0.70	0.38	3.83	77,95,99,102	0
7	GOL	D	504	6/6	0.82	0.31	3.66	101,109,113,118	0
7	GOL	C	501	6/6	0.80	0.36	3.58	78,88,91,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	IMD	C	509	5/5	0.82	0.36	3.24	110,112,113,114	0
6	MG	C	503	1/1	0.96	0.28	2.97	52,52,52,52	0
7	GOL	C	506	6/6	0.86	0.23	2.86	79,86,88,88	0
12	IMD	C	508	5/5	0.91	0.18	2.36	66,73,74,78	0
7	GOL	A	506	6/6	0.74	0.26	0.99	86,93,98,101	0
7	GOL	A	503	6/6	0.89	0.21	0.80	89,92,95,99	0
9	GDP	B	501	28/28	0.97	0.22	0.67	36,46,54,66	0
5	GTP	C	502	32/32	0.98	0.20	0.65	43,51,57,60	0
11	93X	B	508	28/28	0.95	0.24	0.60	34,62,74,83	0
7	GOL	C	504	6/6	0.85	0.23	0.44	91,98,99,101	0
5	GTP	A	501	32/32	0.98	0.23	0.37	49,55,60,62	0
13	ACP	F	402	31/31	0.70	0.33	0.17	86,147,176,178	0
10	MES	B	507	12/12	0.96	0.15	0.17	52,69,81,85	0
9	GDP	D	501	28/28	0.90	0.17	-0.28	79,90,101,102	0
11	93X	D	505	28/28	0.96	0.19	-0.60	55,66,75,83	0
8	CA	A	505	1/1	0.92	0.08	-1.34	97,97,97,97	0
8	CA	B	506	1/1	0.98	0.08	-1.88	118,118,118,118	0
7	GOL	D	503	6/6	0.66	0.57	-	139,142,144,145	0
6	MG	B	502	1/1	0.95	0.41	-	51,51,51,51	0
6	MG	A	502	1/1	0.98	0.26	-	80,80,80,80	0
6	MG	D	502	1/1	0.69	0.13	-	95,95,95,95	0
6	MG	F	401	1/1	0.92	0.23	-	119,119,119,119	0
8	CA	C	507	1/1	0.96	0.07	-	112,112,112,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.