Full wwPDB X-ray Structure Validation Report (i)

Jul 19, 2016 – 05:46 AM EDT

PDB ID	:	4ZOL
Title	:	Crystal Structure of Tubulin-Stathmin-TTL-Tubulysin M Complex
Authors	:	Wang, Y.; Zhang, R.
Deposited on	:	2015-05-06
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

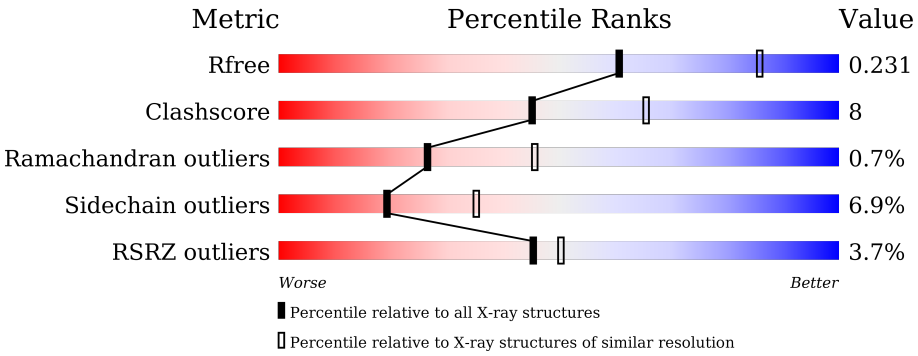
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 >=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 <=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	2% 82% 14%
1	C	451	2% 83% 13%
2	B	445	81% 14%
2	D	445	6% 72% 21%
3	E	143	6% 66% 16% 15%
4	F	384	9% 70% 17% 9%

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
11	55Q	B	507	-	-	-	X
11	55Q	D	503	-	-	-	X
8	GOL	A	506	-	-	X	X
8	GOL	F	402	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18159 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	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3376	2120	579	651	26			
2	D	427	Total	C	N	O	S	0	0	0
			3343	2099	571	647	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	3	0
			1033	637	190	201	5			

There are 2 discrepancies between the modelled and reference sequences:

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

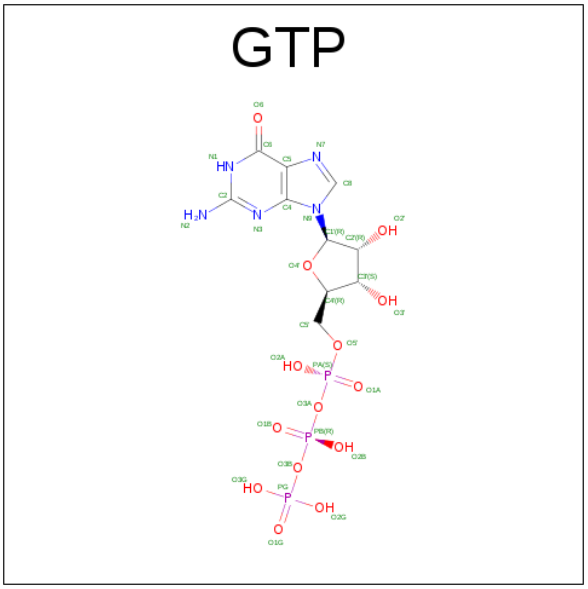
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	348	Total	C	N	O	S	0	0	0
			2862	1832	494	522	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

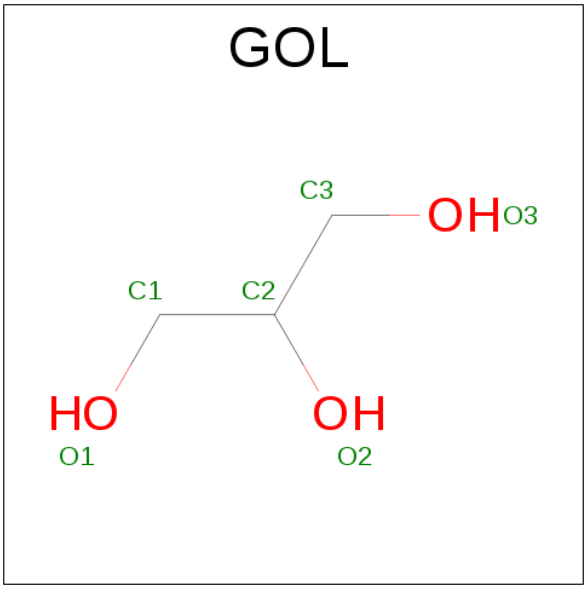
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

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

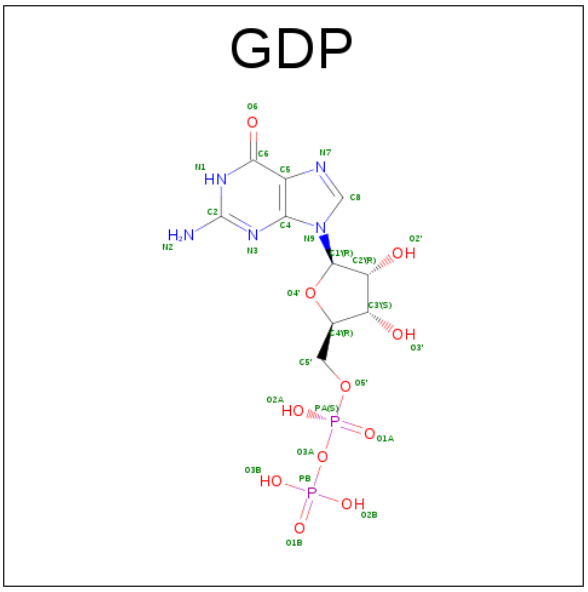
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



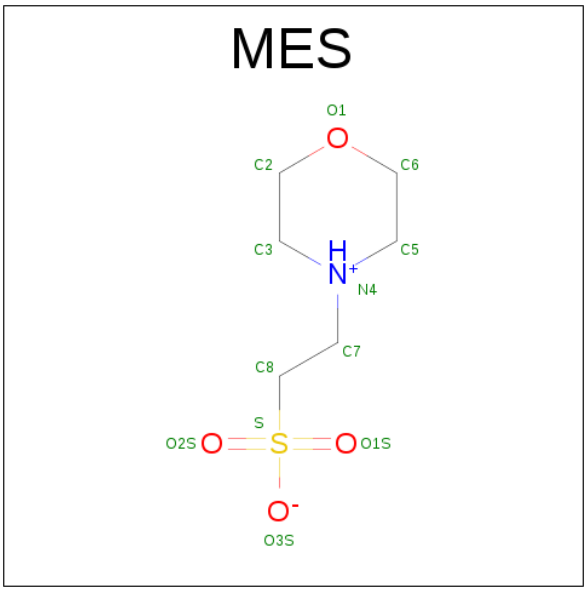
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0

- 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
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

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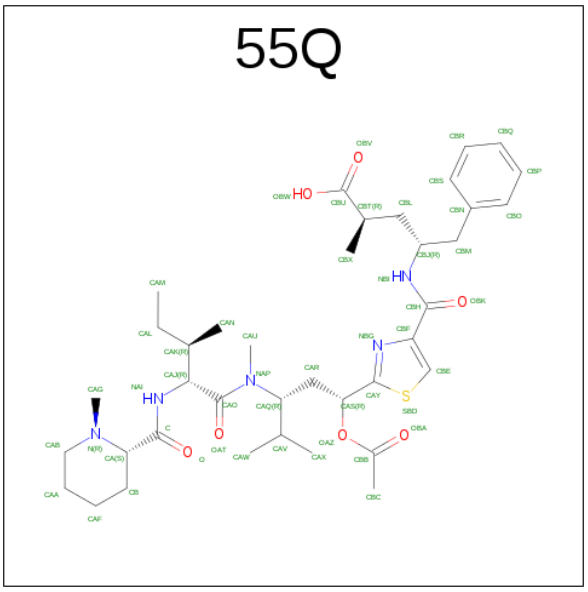
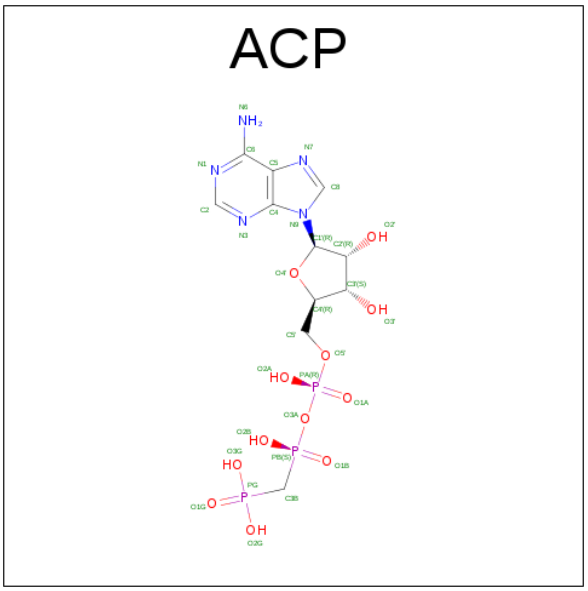
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (2R,4R)-4-{[(2-{(1R,3R)-1-(acetyloxy)-4-methyl-3-[methyl(N-{[(2S)-1-methylpiperidin-2-yl]carbonyl}-D-isoleucyl)amino]pentyl}-1,3-thiazol-4-yl)carbonyl]amino}-2-methyl-5-phenylpentanoic acid (three-letter code: 55Q) (formula: $C_{38}H_{57}N_5O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			51	38	5	7	1		
11	D	1	Total	C	N	O	S	0	0
			51	38	5	7	1		

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

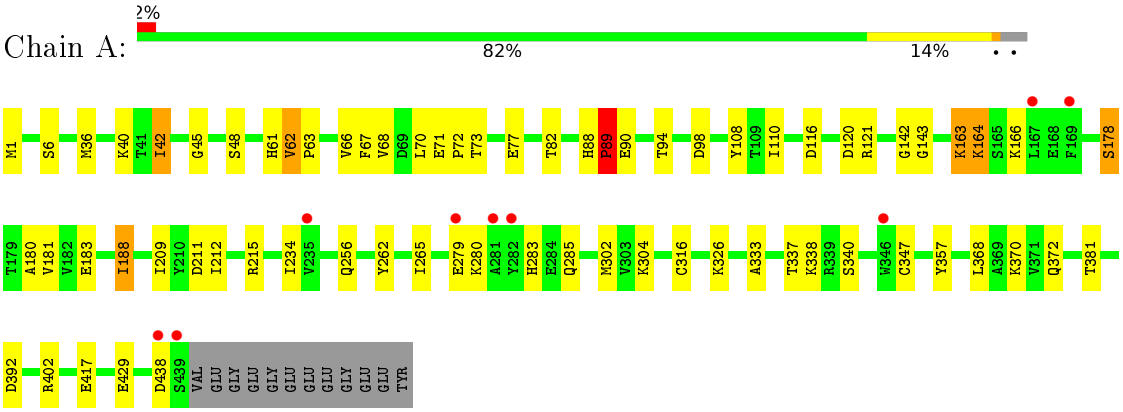
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	80	Total	O	0	0
			80	80		
13	B	63	Total	O	0	0
			63	63		
13	C	123	Total	O	0	0
			123	123		
13	D	34	Total	O	0	0
			34	34		
13	E	9	Total	O	0	0
			9	9		
13	F	44	Total	O	0	0
			44	44		

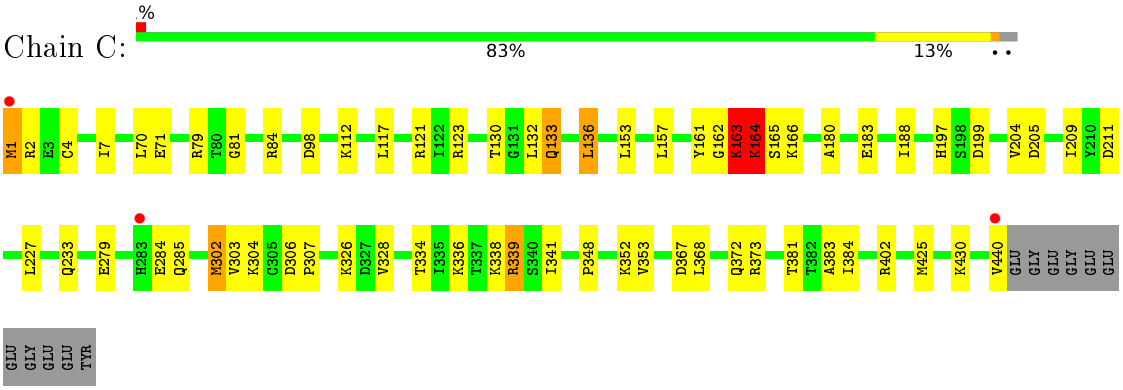
3 Residue-property plots (i)

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.

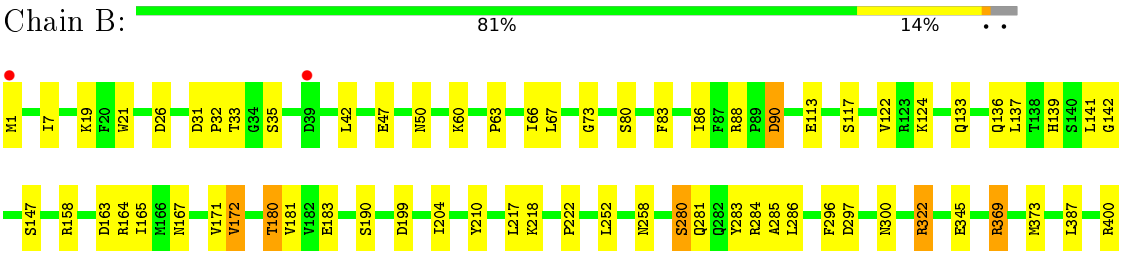
- Molecule 1: Tubulin alpha-1B chain



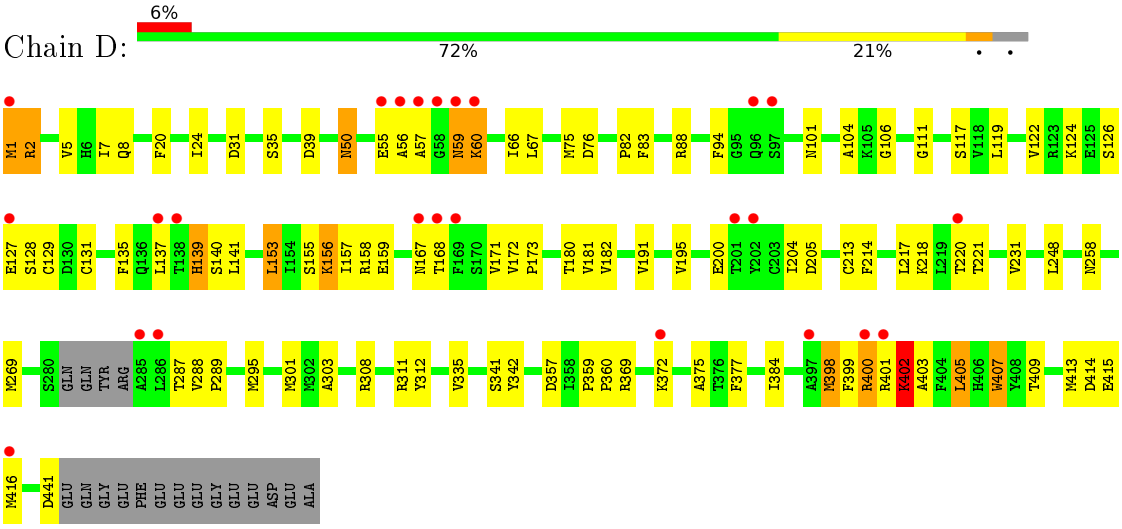
- Molecule 1: Tubulin alpha-1B chain



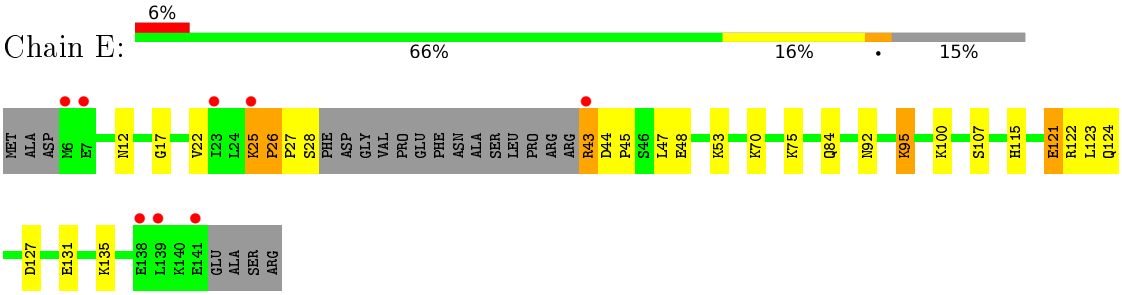
- Molecule 2: Tubulin beta chain



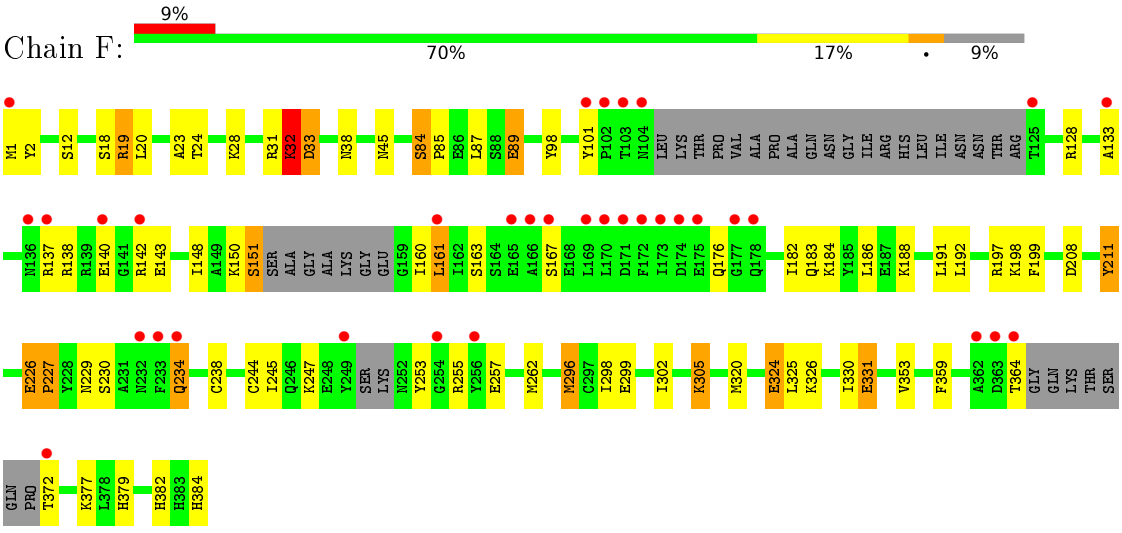
- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin-tyrosine ligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.13Å 154.82Å 186.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.63 – 2.50 40.14 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.63-2.50) 99.9 (40.14-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.232 0.176 , 0.231	Depositor DCC
R_{free} test set	5201 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18159	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CA, 55Q, GTP, ACP, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.79	0/3508	0.89	2/4762 (0.0%)
1	C	0.86	0/3515	0.95	6/4772 (0.1%)
2	B	0.85	0/3451	0.90	2/4676 (0.0%)
2	D	0.76	1/3416 (0.0%)	0.87	5/4628 (0.1%)
3	E	0.78	0/1049	0.87	2/1393 (0.1%)
4	F	0.67	0/2929	0.84	2/3958 (0.1%)
All	All	0.79	1/17868 (0.0%)	0.89	19/24189 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	173	PRO	N-CD	5.06	1.54	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	136	LEU	CA-CB-CG	7.19	131.83	115.30
1	A	402	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	316	CYS	CB-CA-C	-6.11	98.18	110.40
2	D	359	PRO	C-N-CD	6.06	141.12	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	402	ARG	NE-CZ-NH2	5.93	123.26	120.30
4	F	161	LEU	CA-CB-CG	-5.92	101.68	115.30
3	E	26	PRO	C-N-CD	5.81	140.60	128.40
3	E	25	LYS	C-N-CD	5.81	140.60	128.40
1	C	373	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	B	163	ASP	CB-CG-OD1	5.65	123.39	118.30
2	D	172	VAL	C-N-CD	5.53	140.01	128.40
2	D	2	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	D	248	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	C	302	MET	CB-CG-SD	-5.26	96.61	112.40
1	C	402	ARG	NE-CZ-NH1	-5.18	117.71	120.30
2	B	172	VAL	C-N-CD	5.17	139.26	128.40
4	F	305	LYS	C-N-CA	-5.12	108.91	121.70
1	C	123	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	D	407	TRP	CA-CB-CG	5.08	123.35	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	280	SER	Peptide
3	E	115[B]	HIS	Mainchain

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	3430	0	3340	45	0
1	C	3437	0	3348	54	0
2	B	3376	0	3258	40	0
2	D	3343	0	3223	75	0
3	E	1033	0	1048	12	0
4	F	2862	0	2808	49	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	13	0
8	B	12	0	16	1	0
8	C	6	0	8	0	0
8	F	6	0	8	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	B	51	0	0	0	0
11	D	51	0	0	0	0
12	F	31	0	14	4	0
13	A	80	0	0	4	0
13	B	63	0	0	4	0
13	C	123	0	0	6	0
13	D	34	0	0	1	0
13	E	9	0	0	0	0
13	F	44	0	0	3	0
All	All	18159	0	17169	271	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 8.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:CYS:HB3	13:C:719:HOH:O	1.12	1.24
1:C:161:TYR:O	1:C:163:LYS:CD	1.86	1.23
2:D:57:ALA:O	2:D:60:LYS:HD2	1.33	1.22
1:C:1:MET:CE	1:C:130:THR:OG1	1.87	1.22
4:F:296:MET:HE1	13:F:540:HOH:O	1.47	1.15
1:C:161:TYR:O	1:C:163:LYS:HD3	1.40	1.12
4:F:138:ARG:NH2	4:F:184:LYS:HE2	1.75	0.99
1:C:161:TYR:O	1:C:163:LYS:HD2	1.63	0.98
1:C:1:MET:HE2	1:C:130:THR:OG1	1.69	0.92
2:D:57:ALA:O	2:D:60:LYS:CD	2.18	0.89
4:F:31:ARG:HD3	4:F:32:LYS:H	1.39	0.88
1:A:304:LYS:HE3	8:A:506:GOL:H2	1.57	0.86
2:B:199:ASP:OD2	10:B:504:MES:H52	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:HE2	1:C:164:LYS:HD2	1.54	0.86
4:F:150:LYS:HG2	4:F:151:SER:H	1.39	0.86
1:C:381:THR:HG23	13:C:672:HOH:O	1.76	0.86
1:C:1:MET:HE1	1:C:130:THR:OG1	1.74	0.85
1:A:178:SER:HB2	1:A:183:GLU:OE1	1.77	0.83
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.62	0.82
1:A:211:ASP:HB2	8:A:506:GOL:H31	1.64	0.80
1:C:2:ARG:HD2	13:C:714:HOH:O	1.82	0.79
9:B:501:GDP:O3B	13:B:601:HOH:O	2.00	0.78
1:C:204:VAL:HG22	1:C:302:MET:CE	2.16	0.76
2:B:172:VAL:HG11	2:B:387:LEU:HD11	1.66	0.76
2:D:56:ALA:HB3	2:D:60:LYS:O	1.85	0.76
1:A:304:LYS:HE3	8:A:506:GOL:C2	2.16	0.75
4:F:234:GLN:HA	4:F:234:GLN:NE2	2.01	0.74
4:F:89:GLU:CD	4:F:89:GLU:H	1.91	0.74
2:D:400:ARG:NH1	2:D:400:ARG:HB3	2.03	0.74
4:F:382:HIS:ND1	4:F:384:HIS:HD2	1.85	0.73
8:A:504:GOL:H12	3:E:44[A]:ASP:OD2	1.89	0.72
2:D:220:THR:HG23	2:D:221:THR:H	1.54	0.72
2:D:398:MET:O	2:D:400:ARG:N	2.23	0.71
4:F:234:GLN:HA	4:F:234:GLN:HE21	1.54	0.71
1:C:1:MET:HG3	1:C:1:MET:O	1.90	0.71
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.72	0.71
1:C:336:LYS:HD2	13:C:656:HOH:O	1.91	0.70
2:D:400:ARG:CG	2:D:400:ARG:HH11	2.04	0.70
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.73	0.69
4:F:244:CYS:SG	4:F:245:ILE:N	2.65	0.69
2:D:400:ARG:HG2	2:D:400:ARG:HH11	1.58	0.69
12:F:401:ACP:O1A	12:F:401:ACP:O3G	2.11	0.68
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.25	0.68
2:D:180:THR:CG2	2:D:182:VAL:HG12	2.25	0.67
2:D:269:MET:CE	2:D:301:MET:HG3	2.24	0.67
2:D:31:ASP:OD2	2:D:35:SER:HB2	1.95	0.66
1:C:367:ASP:O	13:C:601:HOH:O	2.13	0.66
9:D:501:GDP:O3B	13:D:601:HOH:O	2.13	0.66
2:D:1:MET:HG3	2:D:50:ASN:CB	2.26	0.65
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.77	0.65
2:D:56:ALA:CB	2:D:60:LYS:O	2.43	0.65
1:A:211:ASP:HB3	8:A:506:GOL:O3	1.96	0.65
1:C:163:LYS:HD3	1:C:164:LYS:H	1.62	0.65
4:F:150:LYS:HE3	12:F:401:ACP:O2B	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:MET:SD	2:D:375:ALA:HB1	2.37	0.65
4:F:320:MET:HB2	4:F:330:ILE:HD11	1.77	0.65
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.79	0.65
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.33	0.64
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.78	0.64
4:F:150:LYS:HG2	4:F:151:SER:N	2.11	0.64
1:A:209:ILE:HD11	1:A:302:MET:SD	2.39	0.63
4:F:31:ARG:HD3	4:F:32:LYS:N	2.11	0.63
1:A:215:ARG:HH21	8:A:506:GOL:C3	2.12	0.62
2:D:59:ASN:N	2:D:59:ASN:OD1	2.33	0.62
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.82	0.61
2:B:26:ASP:OD2	2:B:369:ARG:NH1	2.34	0.61
1:A:215:ARG:HH21	8:A:506:GOL:H32	1.65	0.61
2:D:153:LEU:O	2:D:157:ILE:HG13	2.00	0.61
2:D:101:ASN:HD22	2:D:180:THR:HG21	1.65	0.61
2:D:55:GLU:OE2	2:D:55:GLU:HA	2.00	0.60
4:F:138:ARG:HH21	4:F:184:LYS:HE2	1.66	0.60
4:F:324:GLU:O	4:F:325:LEU:HB2	2.01	0.60
1:C:163:LYS:HE2	1:C:164:LYS:CD	2.29	0.60
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.37	0.60
4:F:138:ARG:HH22	4:F:184:LYS:HE2	1.61	0.60
1:C:279:GLU:N	1:C:279:GLU:OE1	2.34	0.59
1:A:108:TYR:OH	1:A:417:GLU:OE1	2.19	0.59
4:F:191:LEU:HA	4:F:197:ARG:O	2.03	0.59
1:A:265:ILE:O	1:A:265:ILE:HG22	2.03	0.59
2:D:220:THR:CG2	2:D:221:THR:H	2.16	0.59
2:D:180:THR:HG22	2:D:182:VAL:HG12	1.85	0.59
1:A:211:ASP:CB	8:A:506:GOL:H31	2.33	0.59
1:A:211:ASP:HB2	8:A:506:GOL:C3	2.31	0.58
2:D:400:ARG:HH11	2:D:400:ARG:CB	2.15	0.58
1:C:204:VAL:HG22	1:C:302:MET:HE3	1.85	0.58
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.04	0.58
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.87	0.57
1:C:1:MET:HE1	1:C:130:THR:CB	2.33	0.57
1:C:1:MET:HE2	1:C:130:THR:HG1	1.67	0.57
1:C:163:LYS:CE	1:C:164:LYS:HD2	2.29	0.57
2:D:39:ASP:N	2:D:39:ASP:OD1	2.35	0.57
2:D:400:ARG:HB3	2:D:400:ARG:HH11	1.70	0.56
2:D:287:THR:HB	2:D:289:PRO:HD2	1.86	0.56
1:C:1:MET:HE3	1:C:130:THR:OG1	1.97	0.55
1:A:45:GLY:HA3	13:A:603:HOH:O	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:THR:HG23	2:D:221:THR:N	2.20	0.55
4:F:31:ARG:NE	4:F:31:ARG:HA	2.21	0.55
1:A:42:ILE:N	1:A:42:ILE:HD13	2.21	0.55
4:F:382:HIS:ND1	4:F:384:HIS:CD2	2.73	0.55
2:D:7:ILE:O	2:D:137:LEU:HD12	2.07	0.54
2:D:191:VAL:O	2:D:195:VAL:HG12	2.07	0.54
3:E:43:ARG:HB2	3:E:43:ARG:CZ	2.36	0.54
2:B:284:ARG:HH12	2:B:286:LEU:HA	1.71	0.54
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.89	0.54
4:F:140:GLU:C	4:F:142:ARG:H	2.11	0.54
4:F:1:MET:SD	4:F:28:LYS:HG2	2.48	0.54
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.25	0.54
4:F:377:LYS:HG2	4:F:379:HIS:HD2	1.73	0.54
2:D:180:THR:HG22	2:D:182:VAL:H	1.73	0.54
2:B:164:ARG:NE	13:B:603:HOH:O	2.41	0.53
4:F:160:ILE:HG22	4:F:161:LEU:N	2.22	0.53
1:A:98:ASP:OD1	1:A:98:ASP:C	2.47	0.53
2:D:56:ALA:CB	2:D:60:LYS:HB2	2.38	0.53
2:D:204:ILE:HG21	2:D:231:VAL:HG22	1.91	0.53
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.23	0.53
2:D:66:ILE:HD13	2:D:122:VAL:HG22	1.89	0.53
2:B:297:ASP:HB3	2:B:300:ASN:HD22	1.74	0.52
1:A:212:ILE:HG13	8:A:506:GOL:H32	1.91	0.52
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.44	0.52
2:B:284:ARG:NH1	2:B:285:ALA:O	2.42	0.52
2:B:1:MET:N	2:B:50:ASN:HB2	2.25	0.52
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.92	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.45	0.52
2:B:401:ARG:HE	8:B:506:GOL:H11	1.75	0.52
3:E:27:PRO:O	3:E:27:PRO:HG2	2.10	0.52
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.10	0.52
1:C:163:LYS:N	1:C:163:LYS:CD	2.72	0.51
1:A:211:ASP:CB	8:A:506:GOL:O3	2.58	0.51
2:B:345:GLU:OE1	2:B:345:GLU:N	2.37	0.51
1:C:180:ALA:O	1:C:183:GLU:HG3	2.10	0.51
2:D:401:ARG:O	2:D:403:ALA:N	2.43	0.51
4:F:192:LEU:HD13	4:F:262:MET:CE	2.41	0.51
3:E:121:GLU:HG3	3:E:122:ARG:N	2.25	0.51
3:E:43:ARG:HB2	3:E:43:ARG:NH1	2.25	0.51
2:D:398:MET:O	2:D:401:ARG:N	2.43	0.50
2:D:167:ASN:OD1	2:D:200:GLU:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:CB	8:A:506:GOL:C3	2.89	0.50
1:C:381:THR:HG22	1:C:383:ALA:H	1.76	0.50
1:C:163:LYS:H	1:C:163:LYS:CD	2.24	0.50
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.50
2:D:126:SER:O	2:D:129:CYS:HB2	2.11	0.50
4:F:331:GLU:OE2	12:F:401:ACP:O1B	2.30	0.50
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.12	0.49
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.93	0.49
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.47	0.49
2:D:414:ASP:OD1	2:D:415:GLU:N	2.46	0.49
2:B:158:ARG:CZ	10:B:504:MES:H21	2.43	0.49
1:C:161:TYR:C	1:C:163:LYS:HD2	2.31	0.49
1:A:234:ILE:HD13	1:A:302:MET:SD	2.52	0.49
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.94	0.49
4:F:160:ILE:CG2	4:F:161:LEU:N	2.76	0.49
2:B:88:ARG:HH21	2:B:124:LYS:HE3	1.77	0.49
1:C:381:THR:CG2	13:C:672:HOH:O	2.48	0.49
2:B:141:LEU:HD22	2:B:190:SER:HB3	1.95	0.49
2:D:56:ALA:HB3	2:D:60:LYS:CB	2.42	0.49
1:A:304:LYS:HE3	8:A:506:GOL:O2	2.13	0.48
1:C:81:GLY:O	1:C:84:ARG:NH2	2.45	0.48
2:D:409:THR:HA	2:D:413:MET:O	2.13	0.48
12:F:401:ACP:O1B	13:F:501:HOH:O	2.20	0.48
2:D:1:MET:O	2:D:131:CYS:HB3	2.14	0.47
3:E:47:LEU:HD12	3:E:47:LEU:O	2.14	0.47
4:F:32:LYS:HB3	4:F:33:ASP:OD1	2.14	0.47
4:F:84:SER:HA	4:F:85:PRO:HD2	1.72	0.47
2:D:311:ARG:NH1	2:D:341:SER:O	2.46	0.47
2:B:297:ASP:HB3	2:B:300:ASN:ND2	2.29	0.47
2:D:402:LYS:HE3	2:D:415:GLU:OE2	2.15	0.47
2:B:90:ASP:OD1	2:B:90:ASP:N	2.47	0.47
1:C:161:TYR:O	1:C:163:LYS:N	2.48	0.47
2:D:400:ARG:CG	2:D:400:ARG:NH1	2.72	0.47
2:D:180:THR:HG21	2:D:182:VAL:HG12	1.97	0.46
2:D:67:LEU:N	2:D:67:LEU:HD12	2.31	0.46
1:A:188:ILE:HD13	1:A:188:ILE:N	2.31	0.46
1:A:285:GLN:NE2	1:A:372:GLN:H	2.14	0.46
2:B:35:SER:OG	2:B:60:LYS:HE3	2.15	0.46
4:F:101:TYR:O	4:F:128:ARG:NH2	2.48	0.46
2:B:322:ARG:O	2:B:373:MET:HE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:VAL:HA	2:D:204:ILE:O	2.15	0.46
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.46	0.46
2:B:164:ARG:HD2	13:B:603:HOH:O	2.14	0.46
4:F:20:LEU:O	4:F:24:THR:HG23	2.16	0.46
2:B:296:PHE:O	10:B:503:MES:H81	2.16	0.45
2:B:83:PHE:O	2:B:86:ILE:HG22	2.17	0.45
4:F:192:LEU:HD13	4:F:262:MET:HE3	1.97	0.45
2:B:218:LYS:HA	2:B:218:LYS:HD2	1.69	0.45
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.45
2:B:142:GLY:O	2:B:183:GLU:HG2	2.16	0.45
2:D:398:MET:C	2:D:400:ARG:H	2.20	0.45
1:C:372:GLN:OE1	1:C:372:GLN:HA	2.17	0.45
2:D:269:MET:HE3	2:D:301:MET:HG3	1.98	0.45
2:B:33:THR:O	2:B:60:LYS:HE2	2.18	0.44
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.98	0.44
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.99	0.44
2:D:104:ALA:HB2	2:D:413:MET:SD	2.57	0.44
2:D:5:VAL:HB	2:D:135:PHE:CD1	2.52	0.44
4:F:208:ASP:OD1	4:F:208:ASP:C	2.56	0.44
1:A:88:HIS:O	1:A:89:PRO:C	2.56	0.44
2:D:119:LEU:HD11	2:D:156:LYS:HG2	2.00	0.44
4:F:19:ARG:HD3	13:F:532:HOH:O	2.17	0.44
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.00	0.44
4:F:148:ILE:HG22	4:F:183:GLN:O	2.18	0.44
2:B:210:TYR:CE2	2:B:222:PRO:HG2	2.52	0.44
1:A:333:ALA:O	1:A:337:THR:HG23	2.17	0.43
1:C:70:LEU:HA	1:C:70:LEU:HD23	1.73	0.43
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.53	0.43
1:A:347:CYS:C	3:E:27:PRO:HB3	2.38	0.43
1:A:116:ASP:HB2	13:A:656:HOH:O	2.18	0.43
4:F:140:GLU:C	4:F:142:ARG:N	2.72	0.43
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.52	0.43
3:E:127:ASP:O	3:E:131:GLU:HG2	2.19	0.43
1:A:72:PRO:HA	1:A:94:THR:HG21	2.01	0.43
3:E:95:LYS:HB3	3:E:95:LYS:HE2	1.68	0.43
1:A:280:LYS:HD3	1:A:283:HIS:HB2	1.99	0.43
1:A:164:LYS:HD3	1:A:164:LYS:N	2.32	0.43
2:B:281:GLN:HB3	2:B:283:TYR:CZ	2.52	0.42
1:C:306:ASP:HA	1:C:307:PRO:HD3	1.88	0.42
2:D:398:MET:C	2:D:400:ARG:N	2.73	0.42
2:B:415:GLU:O	2:B:418:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:247:LYS:HA	4:F:253:TYR:CD2	2.54	0.42
1:A:392:ASP:OD2	1:A:429:GLU:OE1	2.37	0.42
1:A:68:VAL:O	1:A:68:VAL:HG13	2.19	0.42
2:B:180:THR:HG22	1:C:352:LYS:NZ	2.35	0.42
2:D:405:LEU:HA	2:D:405:LEU:HD13	1.88	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.42
2:B:199:ASP:OD1	10:B:504:MES:H32	2.19	0.42
1:C:233:GLN:HG3	1:C:368:LEU:HD11	2.02	0.42
2:D:56:ALA:N	2:D:60:LYS:O	2.52	0.42
1:A:256:GLN:HG3	13:A:666:HOH:O	2.20	0.42
4:F:226:GLU:HA	4:F:227:PRO:HD2	1.88	0.42
1:A:1:MET:C	1:A:1:MET:SD	2.98	0.42
1:C:132:LEU:O	1:C:164:LYS:HE2	2.20	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.42
1:C:334:THR:O	1:C:338:LYS:HB2	2.20	0.42
4:F:143:GLU:HG2	4:F:143:GLU:H	1.69	0.42
1:A:90:GLU:O	1:A:121:ARG:HD2	2.20	0.42
4:F:133:ALA:O	4:F:137:ARG:HB2	2.19	0.42
2:D:398:MET:O	2:D:401:ARG:HG2	2.20	0.41
2:D:56:ALA:HB1	2:D:60:LYS:HD3	2.02	0.41
1:A:40:LYS:HA	1:A:40:LYS:HD3	1.57	0.41
4:F:199:PHE:O	4:F:320:MET:CE	2.67	0.41
2:D:205:ASP:HB2	2:D:303:ALA:HA	2.02	0.41
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.55	0.41
4:F:31:ARG:HA	4:F:31:ARG:HE	1.85	0.41
4:F:98:TYR:HB2	4:F:182:ILE:HG23	2.02	0.41
1:A:163:LYS:HB2	13:A:679:HOH:O	2.20	0.41
2:D:441:ASP:N	2:D:441:ASP:OD1	2.54	0.41
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.95	0.41
4:F:211:TYR:CE2	4:F:299:GLU:HB2	2.56	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.51	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41
2:D:156:LYS:O	2:D:159:GLU:HB2	2.21	0.41
2:B:67:LEU:HD12	2:B:67:LEU:N	2.36	0.41
1:C:166:LYS:HE2	1:C:197:HIS:O	2.21	0.41
2:D:1:MET:SD	2:D:1:MET:N	2.84	0.41
1:A:67:PHE:N	1:A:67:PHE:CD1	2.89	0.40
2:D:220:THR:CG2	2:D:221:THR:N	2.81	0.40
2:B:181:VAL:HG23	1:C:348:PRO:CG	2.51	0.40
2:D:139:HIS:CE1	2:D:141:LEU:CD2	3.04	0.40
2:D:158:ARG:HG2	3:E:123:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.56	0.40
1:C:2:ARG:HB3	1:C:133:GLN:HB2	2.03	0.40
4:F:198:LYS:HG3	4:F:199:PHE:N	2.37	0.40
2:B:7:ILE:O	2:B:137:LEU:HA	2.21	0.40
2:B:164:ARG:CD	13:B:603:HOH:O	2.70	0.40
1:C:153:LEU:O	1:C:157:LEU:HG	2.21	0.40
2:D:106:GLY:O	2:D:111:GLY:HA3	2.20	0.40
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.40
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.03	0.40
1:C:79:ARG:O	1:C:84:ARG:HB2	2.21	0.40
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.40
2:D:400:ARG:CZ	2:D:400:ARG:HB3	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	437/451 (97%)	416 (95%)	20 (5%)	1 (0%)	52	75
1	C	438/451 (97%)	419 (96%)	15 (3%)	4 (1%)	21	37
2	B	428/445 (96%)	415 (97%)	12 (3%)	1 (0%)	52	75
2	D	423/445 (95%)	401 (95%)	18 (4%)	4 (1%)	21	37
3	E	121/143 (85%)	114 (94%)	6 (5%)	1 (1%)	24	41
4	F	338/384 (88%)	313 (93%)	21 (6%)	4 (1%)	16	29
All	All	2185/2319 (94%)	2078 (95%)	92 (4%)	15 (1%)	26	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLY

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Mol	Chain	Res	Type
1	C	339	ARG
2	D	399	PHE
2	D	402	LYS
4	F	32	LYS
2	B	73	GLY
4	F	23	ALA
1	C	164	LYS
2	D	214	PHE
4	F	230	SER
2	D	360	PRO
4	F	227	PRO
1	A	89	PRO
1	C	163	LYS
3	E	45	PRO

5.3.2 Protein sidechains (i)

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	370/379 (98%)	344 (93%)	26 (7%)	19 34
1	C	371/379 (98%)	357 (96%)	14 (4%)	40 67
2	B	369/381 (97%)	353 (96%)	16 (4%)	35 61
2	D	366/381 (96%)	336 (92%)	30 (8%)	14 27
3	E	113/127 (89%)	95 (84%)	18 (16%)	3 5
4	F	314/342 (92%)	286 (91%)	28 (9%)	12 23
All	All	1903/1989 (96%)	1771 (93%)	132 (7%)	19 35

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	42	ILE
1	A	48	SER
1	A	62	VAL

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Mol	Chain	Res	Type
1	A	66	VAL
1	A	71	GLU
1	A	73	THR
1	A	77	GLU
1	A	82	THR
1	A	89	PRO
1	A	120	ASP
1	A	163	LYS
1	A	164	LYS
1	A	166	LYS
1	A	178	SER
1	A	181	VAL
1	A	188	ILE
1	A	262	TYR
1	A	279	GLU
1	A	326	LYS
1	A	338	LYS
1	A	340	SER
1	A	368	LEU
1	A	370	LYS
1	A	381	THR
1	A	438	ASP
2	B	19	LYS
2	B	42	LEU
2	B	47	GLU
2	B	80	SER
2	B	90	ASP
2	B	113	GLU
2	B	117	SER
2	B	133	GLN
2	B	139	HIS
2	B	147	SER
2	B	180	THR
2	B	217	LEU
2	B	280	SER
2	B	322	ARG
2	B	369	ARG
2	B	400	ARG
1	C	1	MET
1	C	112	LYS
1	C	133	GLN
1	C	136	LEU

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Mol	Chain	Res	Type
1	C	163	LYS
1	C	164	LYS
1	C	284	GLU
1	C	285	GLN
1	C	326	LYS
1	C	339	ARG
1	C	341	ILE
1	C	384	ILE
1	C	430	LYS
1	C	440	VAL
2	D	1	MET
2	D	2	ARG
2	D	8	GLN
2	D	50	ASN
2	D	59	ASN
2	D	60	LYS
2	D	76	ASP
2	D	88	ARG
2	D	117	SER
2	D	124	LYS
2	D	127	GLU
2	D	128	SER
2	D	139	HIS
2	D	140	SER
2	D	153	LEU
2	D	155	SER
2	D	156	LYS
2	D	181	VAL
2	D	218	LYS
2	D	335	VAL
2	D	357	ASP
2	D	369	ARG
2	D	372	LYS
2	D	384	ILE
2	D	398	MET
2	D	400	ARG
2	D	402	LYS
2	D	405	LEU
2	D	407	TRP
2	D	416	MET
3	E	12	ASN
3	E	22	VAL

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Mol	Chain	Res	Type
3	E	25	LYS
3	E	26	PRO
3	E	28	SER
3	E	43	ARG
3	E	48	GLU
3	E	53	LYS
3	E	70	LYS
3	E	75	LYS
3	E	84	GLN
3	E	92	ASN
3	E	95	LYS
3	E	100	LYS
3	E	107	SER
3	E	121	GLU
3	E	124	GLN
3	E	135	LYS
4	F	12	SER
4	F	18	SER
4	F	19	ARG
4	F	32	LYS
4	F	33	ASP
4	F	45	ASN
4	F	84	SER
4	F	87	LEU
4	F	89	GLU
4	F	151	SER
4	F	163	SER
4	F	167	SER
4	F	176	GLN
4	F	188	LYS
4	F	211	TYR
4	F	226	GLU
4	F	229	ASN
4	F	234	GLN
4	F	238	CYS
4	F	255	ARG
4	F	296	MET
4	F	305	LYS
4	F	324	GLU
4	F	326	LYS
4	F	331	GLU
4	F	353	VAL

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Mol	Chain	Res	Type
4	F	364	THR
4	F	372	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	300	ASN
2	B	15	GLN
2	B	85	GLN
2	B	167	ASN
2	B	300	ASN
1	C	11	GLN
1	C	285	GLN
1	C	293	ASN
2	D	101	ASN
2	D	247	GLN
4	F	45	ASN
4	F	234	GLN
4	F	260	ASN
4	F	379	HIS
4	F	384	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 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	26,34,34	1.43	4 (15%)	29,54,54	1.97	6 (20%)
8	GOL	A	504	-	5,5,5	0.33	0	5,5,5	0.42	0
8	GOL	A	505	-	5,5,5	0.17	0	5,5,5	0.83	0
8	GOL	A	506	-	5,5,5	0.45	0	5,5,5	0.52	0
9	GDP	B	501	6	24,30,30	1.36	3 (12%)	26,47,47	2.11	7 (26%)
10	MES	B	503	-	12,12,12	1.95	1 (8%)	15,16,16	3.16	8 (53%)
10	MES	B	504	-	12,12,12	1.98	1 (8%)	15,16,16	8.57	10 (66%)
8	GOL	B	505	-	5,5,5	0.30	0	5,5,5	0.42	0
8	GOL	B	506	-	5,5,5	0.33	0	5,5,5	0.36	0
11	55Q	B	507	-	47,53,53	1.87	11 (23%)	56,73,73	2.02	17 (30%)
5	GTP	C	501	6	26,34,34	1.16	3 (11%)	29,54,54	2.34	8 (27%)
8	GOL	C	504	-	5,5,5	0.43	0	5,5,5	1.08	0
9	GDP	D	501	6	24,30,30	1.02	1 (4%)	26,47,47	2.71	8 (30%)
11	55Q	D	503	-	47,53,53	1.90	8 (17%)	56,73,73	1.72	13 (23%)
12	ACP	F	401	-	29,33,33	1.87	7 (24%)	29,52,52	1.68	3 (10%)
8	GOL	F	402	-	5,5,5	0.55	0	5,5,5	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
8	GOL	A	504	-	-	0/4/4/4	0/0/0/0
8	GOL	A	505	-	-	0/4/4/4	0/0/0/0
8	GOL	A	506	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
8	GOL	B	505	-	-	0/4/4/4	0/0/0/0
8	GOL	B	506	-	-	0/4/4/4	0/0/0/0
11	55Q	B	507	-	-	0/50/73/73	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GOL	C	504	-	-	0/4/4/4	0/0/0/0
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
11	55Q	D	503	-	-	0/50/73/73	0/3/3/3
12	ACP	F	401	-	-	0/15/38/38	0/3/3/3
8	GOL	F	402	-	-	0/4/4/4	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	55Q	CBF-CBH	-7.61	1.32	1.50
11	B	507	55Q	CBF-CBH	-6.81	1.34	1.50
10	B	504	MES	C8-S	-6.12	1.68	1.77
10	B	503	MES	C8-S	-6.10	1.68	1.77
11	D	503	55Q	CBM-CBN	-4.51	1.40	1.51
11	B	507	55Q	CBM-CBN	-3.12	1.43	1.51
5	A	501	GTP	C2'-C1'	-2.42	1.49	1.53
12	F	401	ACP	PG-O2G	-2.41	1.49	1.54
12	F	401	ACP	C2'-C1'	-2.05	1.50	1.53
11	B	507	55Q	CAK-CAJ	-2.02	1.48	1.54
11	B	507	55Q	CA-C	2.01	1.57	1.52
5	C	501	GTP	C5-C4	2.04	1.45	1.40
11	B	507	55Q	CBC-CBB	2.16	1.57	1.49
11	D	503	55Q	CAO-NAP	2.23	1.40	1.35
11	D	503	55Q	CB-CA	2.24	1.57	1.52
11	B	507	55Q	CAO-NAP	2.26	1.40	1.35
9	B	501	GDP	O4'-C1'	2.27	1.44	1.41
5	C	501	GTP	C8-N7	2.41	1.39	1.34
12	F	401	ACP	PB-O2B	2.52	1.62	1.56
11	B	507	55Q	CAV-CAQ	2.53	1.57	1.53
11	D	503	55Q	CBE-SBD	2.56	1.74	1.70
5	A	501	GTP	O4'-C1'	2.66	1.45	1.41
11	B	507	55Q	CAB-N	2.69	1.52	1.47
9	D	501	GDP	C5-C4	2.75	1.46	1.40
5	C	501	GTP	C6-C5	2.76	1.46	1.41
12	F	401	ACP	PG-O3G	2.77	1.61	1.54
5	A	501	GTP	C5-C4	2.93	1.47	1.40
5	A	501	GTP	C6-C5	3.02	1.47	1.41
11	B	507	55Q	CA-N	3.20	1.52	1.48
9	B	501	GDP	C6-C5	3.24	1.47	1.41
12	F	401	ACP	C5-C4	3.43	1.48	1.40
11	B	507	55Q	OAZ-CBB	3.51	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	55Q	OAZ-CBB	3.52	1.43	1.35
9	B	501	GDP	C5-C4	3.59	1.48	1.40
11	D	503	55Q	OAZ-CAS	3.61	1.51	1.46
11	D	503	55Q	CAV-CAQ	3.71	1.58	1.53
11	B	507	55Q	CBE-SBD	3.89	1.76	1.70
12	F	401	ACP	PB-O3A	4.35	1.63	1.58
12	F	401	ACP	PG-O1G	5.29	1.62	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	MES	O1S-S-C8	-23.39	90.34	106.87
10	B	504	MES	O3S-S-O1S	-12.82	82.88	111.26
10	B	504	MES	O2S-S-O1S	-12.03	79.99	113.96
12	F	401	ACP	N3-C2-N1	-7.06	123.32	128.87
9	D	501	GDP	O4'-C1'-N9	-6.47	95.88	108.11
5	C	501	GTP	N3-C2-N1	-5.60	119.94	127.56
9	B	501	GDP	C5-C6-N1	-4.99	117.00	123.52
9	D	501	GDP	C5-C6-N1	-4.76	117.30	123.52
11	B	507	55Q	OAT-CAO-CAJ	-4.66	110.93	120.12
5	C	501	GTP	C6-C5-C4	-4.61	115.59	120.86
11	D	503	55Q	OAT-CAO-CAJ	-4.56	111.14	120.12
5	A	501	GTP	C1'-N9-C4	-4.36	121.94	126.81
5	C	501	GTP	C5-C6-N1	-3.97	118.34	123.52
11	B	507	55Q	CAL-CAK-CAJ	-3.91	100.65	111.21
5	A	501	GTP	C6-C5-C4	-3.81	116.50	120.86
9	D	501	GDP	N3-C2-N1	-3.77	122.43	127.56
11	B	507	55Q	CBF-CBE-SBD	-3.69	107.26	111.79
9	B	501	GDP	C6-C5-C4	-3.68	116.66	120.86
11	D	503	55Q	CBN-CBM-CBJ	-3.62	106.61	114.36
5	A	501	GTP	N3-C2-N1	-3.58	122.68	127.56
11	B	507	55Q	CAS-CAR-CAQ	-3.56	105.03	113.11
10	B	503	MES	O1S-S-C8	-3.32	104.52	106.87
11	D	503	55Q	CBF-CBE-SBD	-3.14	107.93	111.79
5	C	501	GTP	C1'-N9-C4	-3.14	123.30	126.81
10	B	504	MES	O1-C6-C5	-3.12	104.62	111.83
9	D	501	GDP	O3'-C3'-C4'	-3.11	101.73	111.01
9	B	501	GDP	N3-C2-N1	-2.98	123.50	127.56
10	B	503	MES	O3S-S-O2S	-2.95	104.74	111.26
5	A	501	GTP	C5-C6-N1	-2.89	119.75	123.52
5	C	501	GTP	C5'-C4'-C3'	-2.71	104.73	115.20
10	B	503	MES	C7-N4-C5	-2.67	105.43	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	MES	C7-N4-C3	-2.66	105.45	111.25
12	F	401	ACP	C1'-N9-C4	-2.41	124.12	126.81
11	B	507	55Q	CBN-CBM-CBJ	-2.34	109.35	114.36
12	F	401	ACP	O2'-C2'-C1'	-2.16	104.85	111.61
9	D	501	GDP	C6-C5-C4	-2.14	118.42	120.86
11	D	503	55Q	OBA-CBB-CBC	-2.13	117.02	124.87
10	B	503	MES	O2S-S-O1S	-2.12	107.96	113.96
9	B	501	GDP	O3'-C3'-C2'	-2.09	105.10	111.86
9	B	501	GDP	O4'-C1'-N9	-2.07	104.20	108.11
11	D	503	55Q	CBM-CBJ-NBI	-2.05	106.01	110.50
11	B	507	55Q	CAK-CAJ-CAO	2.01	115.50	111.12
11	B	507	55Q	CAK-CAJ-NAI	2.05	115.64	111.11
11	D	503	55Q	CBF-CBH-NBI	2.10	119.76	115.07
11	B	507	55Q	CAA-CAB-N	2.11	114.62	111.06
5	C	501	GTP	O3G-PG-O2G	2.11	115.21	107.44
10	B	503	MES	C6-O1-C2	2.12	117.12	109.89
11	B	507	55Q	CBQ-CBR-CBS	2.12	123.15	120.20
11	D	503	55Q	CAL-CAK-CAJ	2.15	117.02	111.21
11	B	507	55Q	CAA-CAF-CB	2.19	115.98	111.44
11	B	507	55Q	CAR-CAQ-CAV	2.21	118.56	113.39
9	D	501	GDP	N2-C2-N3	2.34	122.11	117.72
10	B	504	MES	C5-N4-C3	2.61	114.71	108.87
10	B	503	MES	O3S-S-O1S	2.69	117.21	111.26
11	B	507	55Q	CBP-CBO-CBN	2.69	124.72	120.65
11	B	507	55Q	OAZ-CBB-CBC	2.75	116.33	111.09
10	B	503	MES	C5-N4-C3	2.88	115.32	108.87
5	C	501	GTP	N2-C2-N1	2.93	122.03	117.20
11	D	503	55Q	OAZ-CBB-CBC	2.94	116.68	111.09
5	A	501	GTP	O3G-PG-O2G	3.01	118.48	107.44
9	B	501	GDP	O3B-PB-O1B	3.15	120.89	110.63
11	D	503	55Q	CAK-CAJ-NAI	3.23	118.25	111.11
11	D	503	55Q	OAZ-CAS-CAR	3.36	113.17	106.25
11	D	503	55Q	C-CA-N	3.63	119.50	111.38
11	B	507	55Q	C-CA-N	3.72	119.70	111.38
11	D	503	55Q	CAJ-CAO-NAP	3.72	126.56	118.52
11	B	507	55Q	CAJ-NAI-C	3.74	131.39	121.97
11	B	507	55Q	CAJ-CAO-NAP	3.82	126.77	118.52
11	D	503	55Q	CAO-CAJ-NAI	3.82	117.01	107.89
10	B	504	MES	C2-C3-N4	4.08	116.35	110.11
9	D	501	GDP	O3B-PB-O1B	4.60	125.65	110.63
5	A	501	GTP	C6-N1-C2	5.24	122.03	115.88
11	B	507	55Q	CAO-CAJ-NAI	5.56	121.17	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	MES	O3S-S-C8	5.95	117.36	104.99
5	C	501	GTP	C6-N1-C2	5.97	122.88	115.88
10	B	504	MES	O3S-S-O2S	6.10	124.77	111.26
9	B	501	GDP	C6-N1-C2	6.12	123.05	115.88
9	D	501	GDP	C6-N1-C2	6.64	123.66	115.88
10	B	503	MES	O2S-S-C8	9.50	113.58	106.87
10	B	504	MES	O2S-S-C8	11.28	114.84	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	A	504	GOL	1	0
8	A	506	GOL	12	0
9	B	501	GDP	1	0
10	B	503	MES	1	0
10	B	504	MES	3	0
8	B	506	GOL	1	0
9	D	501	GDP	1	0
12	F	401	ACP	4	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^{th} 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^2)	Q<0.9
1	A	439/451 (97%)	-0.18	9 (2%)	67	71	23, 39, 66, 116	0
1	C	440/451 (97%)	-0.46	3 (0%)	89	90	21, 33, 62, 91	0
2	B	430/445 (96%)	-0.29	2 (0%)	91	92	20, 36, 71, 107	0
2	D	427/445 (95%)	0.06	25 (5%)	26	29	28, 50, 86, 124	0
3	E	122/143 (85%)	0.24	8 (6%)	22	24	30, 55, 87, 114	0
4	F	348/384 (90%)	0.13	34 (9%)	10	10	25, 56, 108, 138	0
All	All	2206/2319 (95%)	-0.14	81 (3%)	45	50	20, 42, 85, 138	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	177	GLY	5.7
1	A	282	TYR	5.0
4	F	372	THR	4.6
1	C	440	VAL	4.3
4	F	166	ALA	4.2
2	D	1	MET	4.2
4	F	104	ASN	4.2
4	F	133	ALA	4.1
4	F	234	GLN	4.1
3	E	43	ARG	3.9
2	D	56	ALA	3.8
4	F	169	LEU	3.7
4	F	103	THR	3.4
2	D	168	THR	3.4
2	D	58	GLY	3.3
4	F	170	LEU	3.3
2	D	55	GLU	3.2
3	E	6	MET	3.2
4	F	173	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	167	SER	3.1
4	F	249	TYR	3.1
1	A	439	SER	3.1
4	F	364	THR	3.0
3	E	138	GLU	3.0
2	D	57	ALA	2.9
4	F	232	ASN	2.8
4	F	142	ARG	2.8
4	F	136	ASN	2.8
2	D	60	LYS	2.8
4	F	140	GLU	2.8
4	F	172	PHE	2.8
2	D	59	ASN	2.7
4	F	171	ASP	2.7
4	F	165	GLU	2.7
4	F	363	ASP	2.7
4	F	161	LEU	2.7
1	A	346	TRP	2.7
2	D	400	ARG	2.6
1	A	235	VAL	2.6
4	F	101	TYR	2.6
2	D	372	LYS	2.6
4	F	178	GLN	2.5
3	E	7	GLU	2.5
1	A	281	ALA	2.5
2	D	286	LEU	2.5
2	D	416	MET	2.5
1	A	279	GLU	2.5
1	A	167	LEU	2.4
4	F	362	ALA	2.4
4	F	256	TYR	2.4
2	D	401	ARG	2.4
3	E	139	LEU	2.4
2	D	285	ALA	2.4
2	B	39	ASP	2.4
2	D	138	THR	2.4
1	A	438	ASP	2.4
2	D	397	ALA	2.4
2	B	1	MET	2.4
4	F	233	PHE	2.4
4	F	175	GLU	2.3
4	F	125	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	137	ARG	2.3
3	E	25	LYS	2.2
2	D	201	THR	2.2
1	C	283	HIS	2.2
2	D	97	SER	2.2
4	F	174	ASP	2.2
2	D	202	TYR	2.1
3	E	23	ILE	2.1
3	E	141	GLU	2.1
4	F	254	GLY	2.1
2	D	137	LEU	2.1
1	A	169	PHE	2.1
2	D	167	ASN	2.1
4	F	102	PRO	2.1
1	C	1	MET	2.1
2	D	127	GLU	2.1
2	D	169	PHE	2.1
4	F	1	MET	2.0
2	D	96	GLN	2.0
2	D	220	THR	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^{th} 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^2)	Q<0.9
8	GOL	A	506	6/6	0.88	0.46	9.78	39,67,99,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	GOL	F	402	6/6	0.83	0.22	3.37	77,80,83,84	0
11	55Q	B	507	51/51	0.96	0.15	3.31	21,36,74,103	0
11	55Q	D	503	51/51	0.89	0.25	2.56	54,70,113,127	0
8	GOL	C	504	6/6	0.93	0.15	1.45	54,58,62,76	0
10	MES	B	503	12/12	0.96	0.15	1.42	50,54,59,60	0
8	GOL	B	506	6/6	0.86	0.18	0.71	60,76,80,93	0
8	GOL	A	504	6/6	0.88	0.18	0.29	61,72,78,87	0
10	MES	B	504	12/12	0.95	0.14	0.13	57,64,73,74	0
5	GTP	A	501	32/32	0.99	0.15	0.05	24,27,30,31	0
8	GOL	A	505	6/6	0.96	0.11	-0.10	50,51,55,58	0
9	GDP	B	501	28/28	0.99	0.14	-0.16	20,27,31,32	0
5	GTP	C	501	32/32	0.99	0.11	-0.57	19,22,26,28	0
9	GDP	D	501	28/28	0.98	0.13	-0.62	33,39,47,52	0
12	ACP	F	401	31/31	0.94	0.14	-0.66	58,72,124,137	0
6	MG	A	502	1/1	0.99	0.08	-1.86	37,37,37,37	0
7	CA	C	503	1/1	0.99	0.02	-2.51	38,38,38,38	0
8	GOL	B	505	6/6	0.92	0.08	-2.69	66,72,74,75	0
7	CA	A	503	1/1	0.99	0.04	-3.66	50,50,50,50	0
6	MG	C	502	1/1	0.97	0.04	-6.82	30,30,30,30	0
6	MG	B	502	1/1	0.96	0.12	-	44,44,44,44	0
6	MG	D	502	1/1	0.93	0.16	-	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.