



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:13 PM GMT

PDB ID : 4O4I
Title : Tubulin-Laulimalide-Epothilone A complex
Authors : Prota, A.E.; Bargsten, K.; Northcote, P.T.; Marsh, M.; Altmann, K.H.; Miller, J.H.; Diaz, J.F.; Steinmetz, M.O.
Deposited on : 2013-12-18
Resolution : 2.40 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

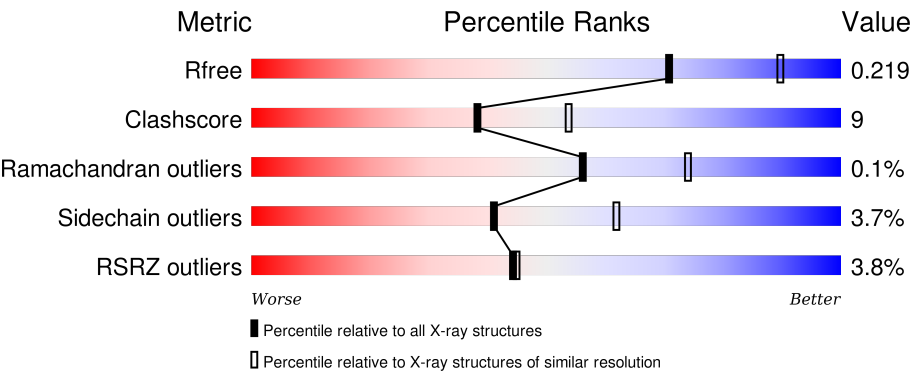
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	<div><div></div><div>76%20%•</div></div>
1	C	451	<div><div></div><div>79%18%••</div></div>
2	B	445	<div><div>2%</div><div>72%22%••</div></div>
2	D	445	<div><div>%</div><div>75%20%••</div></div>
3	E	143	<div><div>%</div><div>52%27%5%15%</div></div>

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	LLM	B	505	-	-	-	X
7	CA	A	503	-	-	-	X
7	CA	C	503	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18304 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	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	1	0
			3440	2177	584	656	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	1	0
			3372	2117	577	651	27			
2	D	431	Total	C	N	O	S	0	1	0
			3381	2120	579	654	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1013	625	184	199	5			

There are 2 discrepancies between the modelled and reference sequences:

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

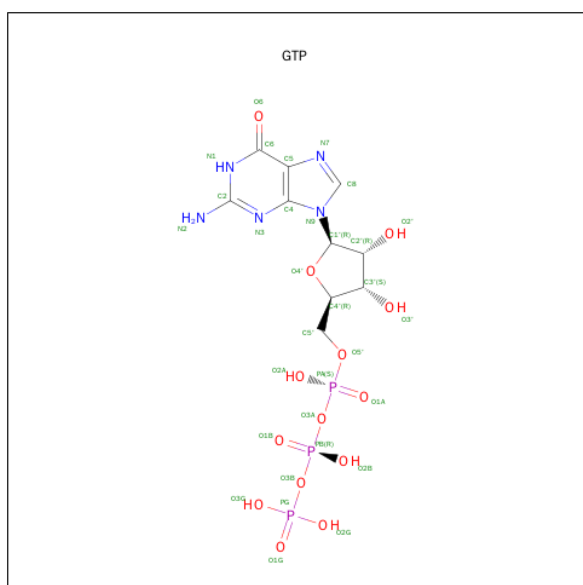
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	0	8	0
			2898	1867	490	527	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: $C_{10}H_{16}N_5O_{14}P_3$).



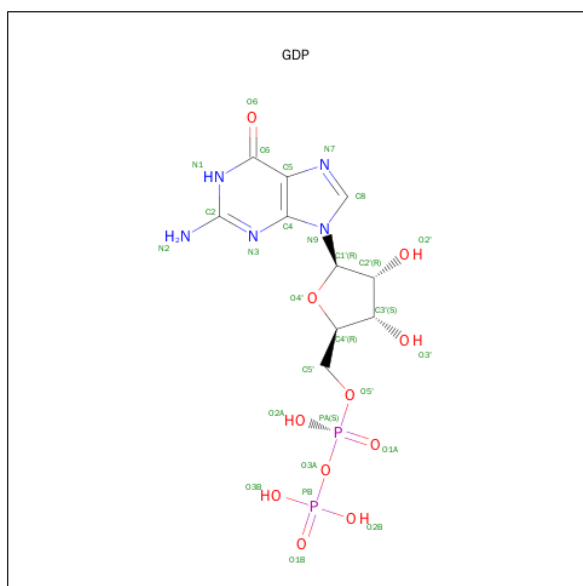
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

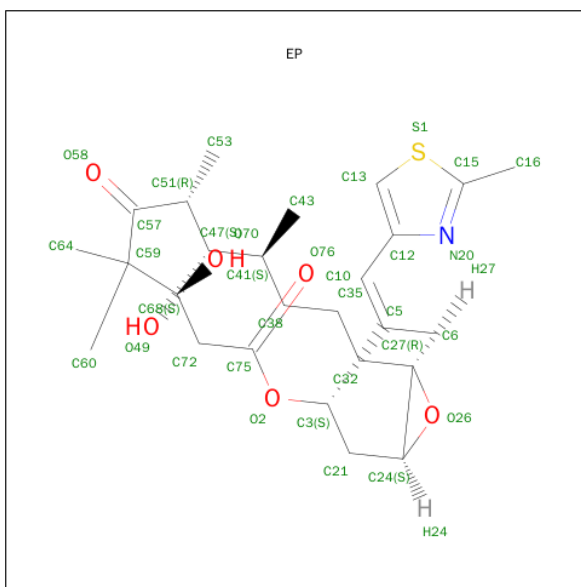
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



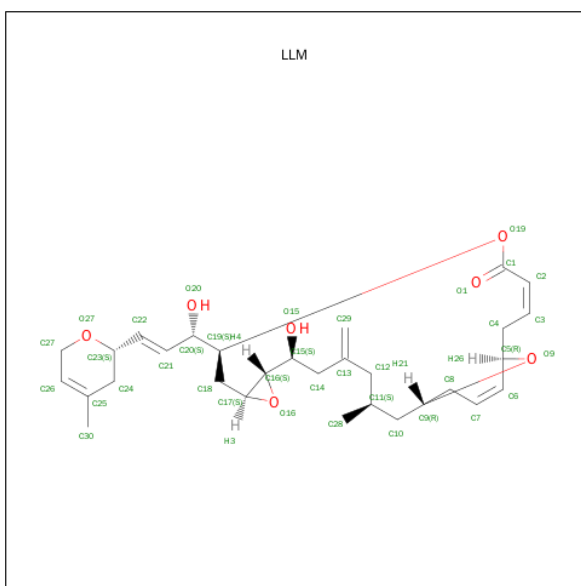
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is EPOTHILONE A (three-letter code: EP) (formula: C₂₆H₃₉NO₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			34	26	1	6	1		
9	D	1	Total	C	N	O	S	0	0
			34	26	1	6	1		

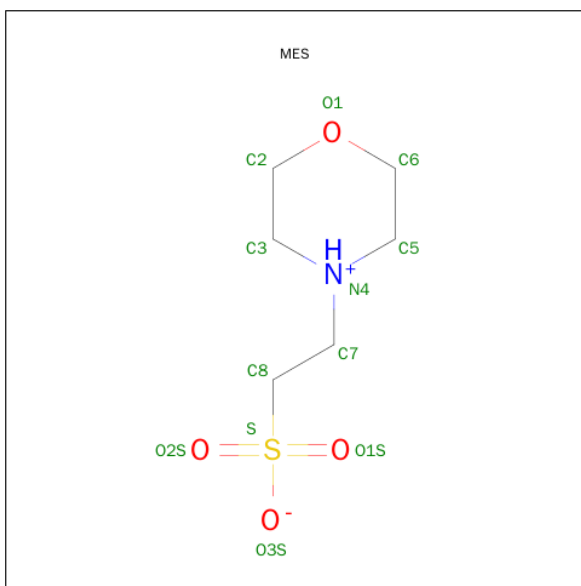
- Molecule 10 is LAULIMALIDE (three-letter code: LLM) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	5	0
			37	30	7		

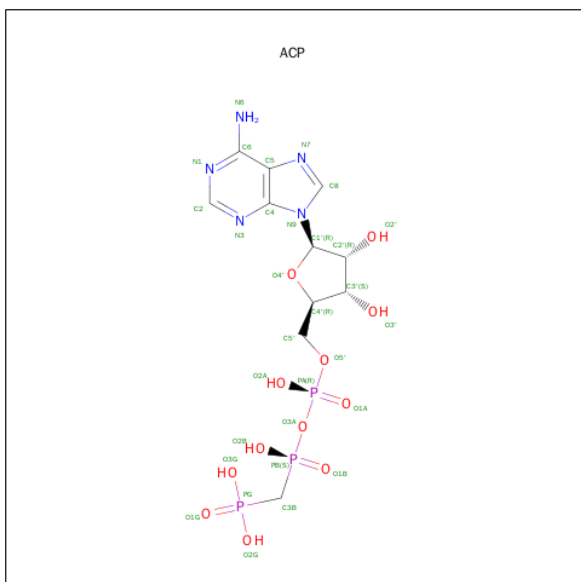
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: $C_6H_{13}NO_4S$).



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

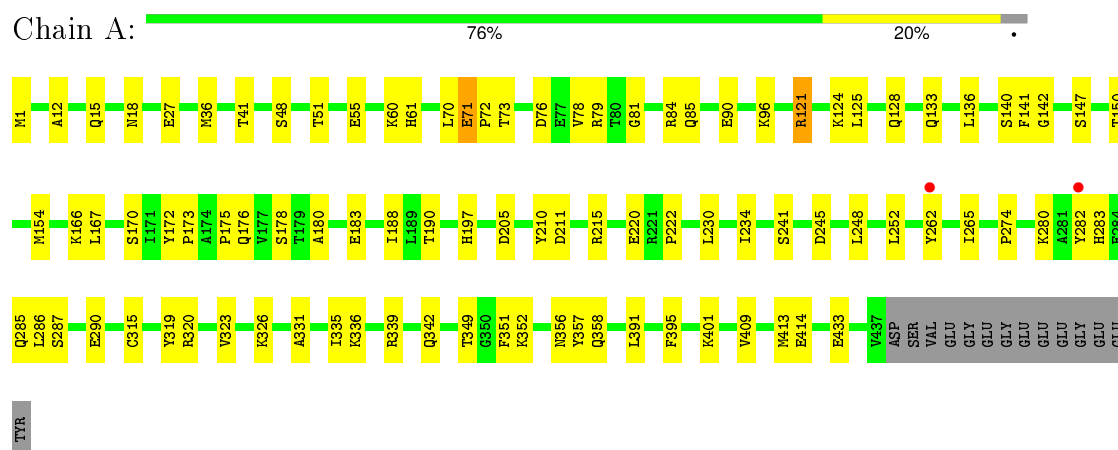
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	112	Total 112	O 112	0	0
13	B	90	Total 90	O 90	0	0
13	C	161	Total 161	O 161	0	0
13	D	63	Total 63	O 63	0	0
13	E	34	Total 34	O 34	0	0
13	F	47	Total 47	O 47	0	0

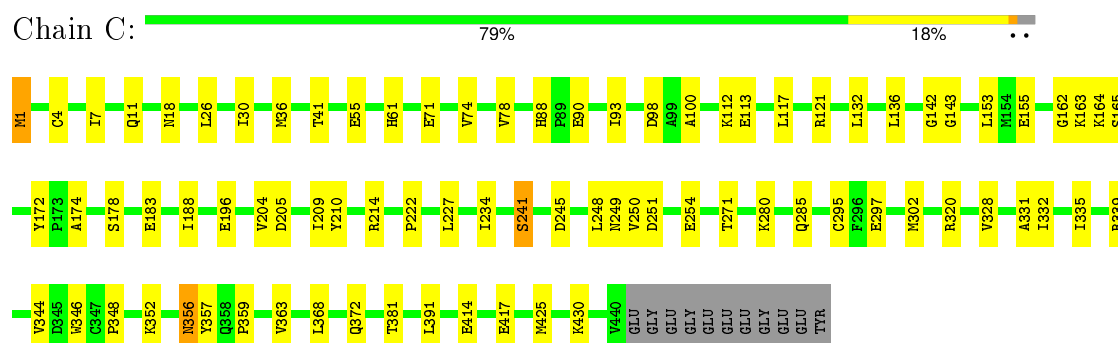
3 Residue-property plots

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.

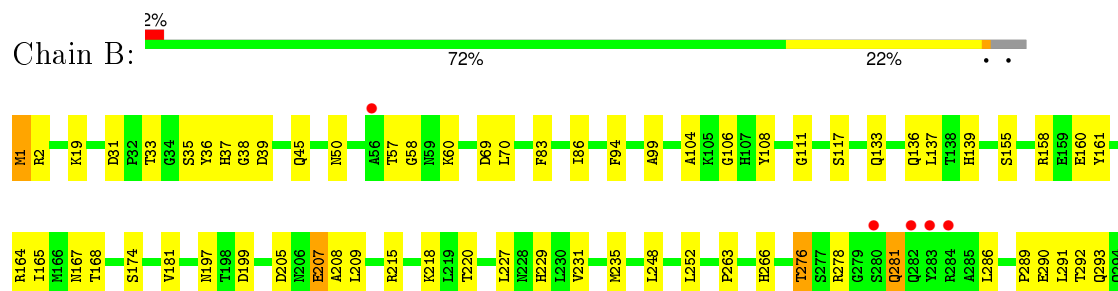
• Molecule 1: Tubulin alpha-1B chain

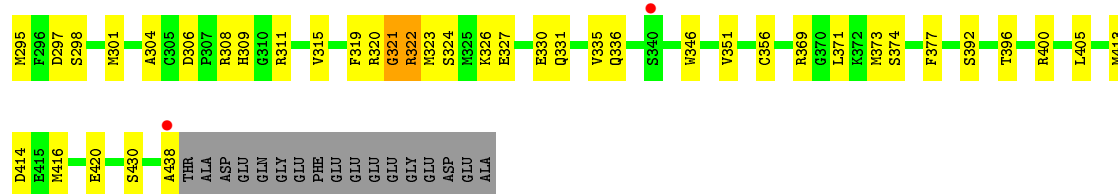


• Molecule 1: Tubulin alpha-1B chain

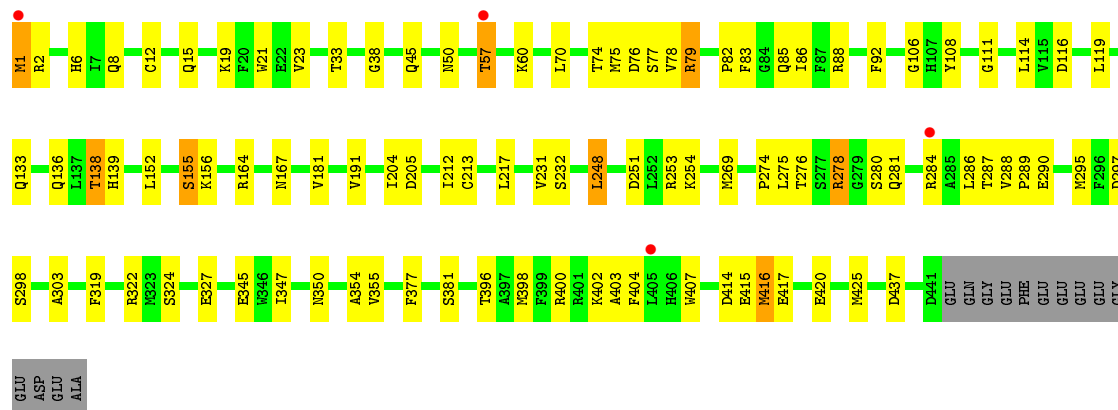
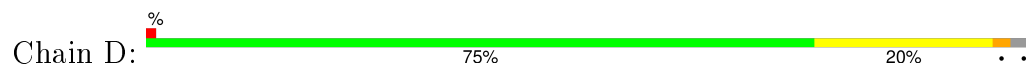


• Molecule 2: Tubulin beta-2B chain

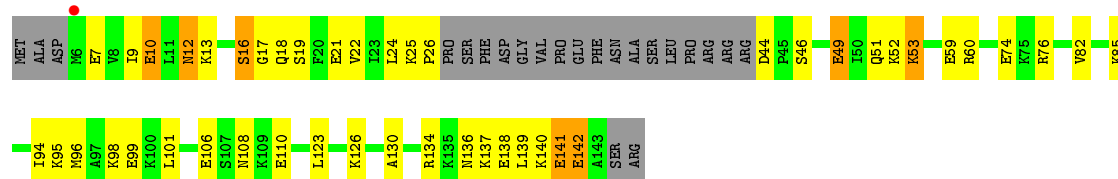




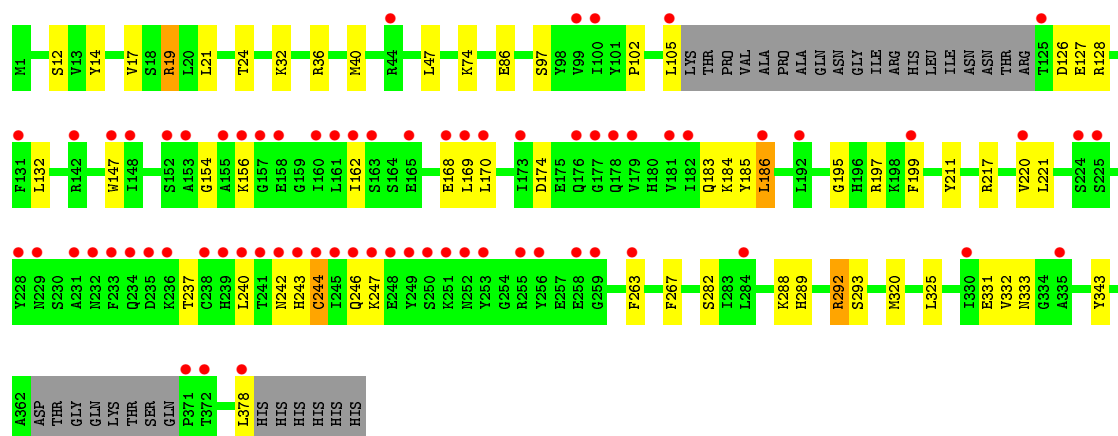
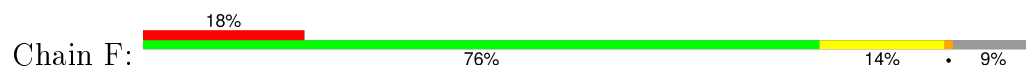
• Molecule 2: Tubulin beta-2B chain



• 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, α , β , γ	105.20Å 158.03Å 180.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.21 – 2.40 78.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (52.21-2.40) 99.7 (78.78-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.188 , 0.214 0.194 , 0.219	Depositor DCC
R_{free} test set	5886 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 117491 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18304	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, MES, CA, GTP, ACP, LLM, EP

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	0.31	0/3494	0.49	0/4743
1	C	0.36	0/3521	0.56	1/4780 (0.0%)
2	B	0.33	0/3450	0.50	0/4672
2	D	0.33	0/3458	0.54	0/4684
3	E	0.32	0/1027	0.46	0/1362
4	F	0.31	0/2985	0.51	0/4032
All	All	0.33	0/17935	0.52	1/24273 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	LEU	CA-CB-CG	-5.00	103.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3331	60	0
1	C	3440	0	3354	53	0
2	B	3372	0	3255	76	0
2	D	3381	0	3258	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1013	0	1030	39	0
4	F	2898	0	2914	41	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	34	0	39	6	0
9	D	34	0	39	1	0
10	B	37	0	42	4	0
11	B	12	0	12	3	0
12	F	31	0	14	4	0
13	A	112	0	0	4	0
13	B	90	0	0	6	0
13	C	161	0	0	10	0
13	D	63	0	0	6	0
13	E	34	0	0	6	0
13	F	47	0	0	4	0
All	All	18304	0	17336	319	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 9.

All (319) 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)
4:F:184:LYS:NZ	4:F:185:TYR:O	2.01	0.94
2:B:276:THR:OG1	9:B:503:EP:N20	2.00	0.92
4:F:74:LYS:NZ	4:F:331:GLU:OE2	2.02	0.92
1:C:163:LYS:NZ	13:C:749:HOH:O	2.03	0.91
3:E:10:GLU:O	3:E:12:ASN:ND2	2.03	0.91
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.04	0.89
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.95	0.85
2:D:33:THR:O	2:D:60:LYS:NZ	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.58	0.84
2:B:36:TYR:O	2:B:37:HIS:ND1	2.11	0.83
2:B:311:ARG:NH1	13:B:602:HOH:O	2.10	0.82
4:F:21:LEU:O	4:F:24:THR:OG1	1.98	0.81
3:E:130:ALA:HB1	3:E:134:ARG:HH12	1.44	0.81
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.13	0.80
2:B:164:ARG:NH1	13:B:689:HOH:O	2.14	0.80
1:C:280:LYS:NZ	13:C:756:HOH:O	2.15	0.79
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.17	0.78
3:E:9:ILE:HG22	3:E:10:GLU:HG2	1.64	0.78
1:A:356:ASN:ND2	13:A:692:HOH:O	2.17	0.77
4:F:331:GLU:OE1	12:F:500:ACP:O2G	2.03	0.77
3:E:46:SER:OG	3:E:49:GLU:OE1	2.03	0.76
2:D:402:LYS:NZ	2:D:415:GLU:OE1	2.13	0.76
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.04	0.75
1:A:280:LYS:HE2	1:A:283:HIS:HB3	1.69	0.73
2:D:181:VAL:O	13:D:657:HOH:O	2.05	0.73
2:B:1:MET:HB3	2:B:50:ASN:OD1	1.88	0.72
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.24	0.72
2:B:215:ARG:NH1	13:B:654:HOH:O	2.09	0.72
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.24	0.71
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.26	0.71
2:D:164:ARG:NH2	13:D:663:HOH:O	2.25	0.70
2:D:85:GLN:N	2:D:85:GLN:OE1	2.22	0.69
3:E:137:LYS:NZ	13:E:214:HOH:O	2.24	0.69
1:C:414:GLU:OE1	13:C:727:HOH:O	2.11	0.68
4:F:168:GLU:OE2	13:F:625:HOH:O	2.11	0.68
1:A:349:THR:OG1	13:A:663:HOH:O	2.11	0.68
2:B:276:THR:O	9:B:503:EP:H722	1.93	0.68
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.35	0.66
1:C:132:LEU:O	1:C:164:LYS:HE3	1.94	0.66
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.29	0.66
2:B:326:LYS:O	2:B:330:GLU:HG3	1.96	0.65
2:D:437:ASP:OD1	13:D:637:HOH:O	2.13	0.65
2:D:287:THR:HB	2:D:289:PRO:HD2	1.79	0.65
4:F:86:GLU:O	13:F:621:HOH:O	2.15	0.64
2:B:324:SER:HB3	2:B:327:GLU:HB2	1.79	0.64
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.07	0.63
3:E:137:LYS:HA	3:E:140:LYS:HD3	1.79	0.63
2:B:33:THR:OG1	2:B:35:SER:OG	2.14	0.63
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:407:TRP:NE1	13:D:618:HOH:O	2.30	0.63
1:A:81:GLY:O	1:A:84:ARG:HD3	1.99	0.62
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.65	0.62
1:A:287:SER:OG	1:A:290:GLU:HG3	2.00	0.62
4:F:292:ARG:HG2	4:F:292:ARG:HH11	1.66	0.61
1:A:133:GLN:OE1	1:A:252:LEU:N	2.26	0.61
2:B:286:LEU:HG	2:B:290:GLU:HB3	1.83	0.60
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.83	0.60
2:D:322:ARG:HG3	2:D:322:ARG:HH21	1.67	0.60
2:B:229:HIS:ND1	9:B:503:EP:H321	2.16	0.60
2:B:276:THR:HG22	2:B:281:GLN:HG3	1.82	0.60
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.36	0.60
2:B:276:THR:CG2	2:B:281:GLN:HG3	2.31	0.60
2:B:289:PRO:O	2:B:293:GLN:HG3	2.02	0.60
2:B:136:GLN:HA	2:B:167:ASN:O	2.01	0.59
2:D:1:MET:SD	2:D:1:MET:N	2.64	0.59
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.84	0.59
1:C:271:THR:HG21	1:C:295:CYS:O	2.03	0.58
2:D:74:THR:O	2:D:78:VAL:HG23	2.04	0.58
1:A:352:LYS:HG3	3:E:21:GLU:HG3	1.85	0.58
1:A:414:GLU:OE1	3:E:60:ARG:NH1	2.36	0.58
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.85	0.58
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.33	0.58
2:B:308:ARG:HD3	10:B:505:LLM:H34	1.86	0.57
1:C:430:LYS:HE2	13:C:673:HOH:O	2.03	0.57
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.86	0.57
2:B:320:ARG:O	2:B:374:SER:N	2.34	0.57
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.86	0.57
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.87	0.57
1:A:166:LYS:HE2	1:A:197:HIS:O	2.05	0.57
1:A:1:MET:HG2	1:A:51:THR:HG22	1.87	0.57
2:D:295:MET:CG	2:D:377:PHE:HB2	2.34	0.56
4:F:40:MET:HE1	4:F:47:LEU:HG	1.86	0.56
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.23	0.56
1:C:234:ILE:HG21	1:C:302:MET:SD	2.45	0.56
2:B:321:GLY:HA2	2:B:356:CYS:O	2.06	0.56
2:B:297:ASP:HA	10:B:505:LLM:O20	2.06	0.56
1:C:204:VAL:HG13	1:C:302:MET:HG2	1.87	0.56
1:C:331:ALA:O	1:C:335:ILE:HD12	2.05	0.56
2:D:274:PRO:HG3	2:D:286:LEU:HD11	1.87	0.56
3:E:44:ASP:HB2	13:E:218:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:HB3	13:A:687:HOH:O	2.05	0.55
3:E:95:LYS:O	3:E:99:GLU:HG3	2.05	0.55
2:D:204:ILE:HG21	2:D:231:VAL:HG22	1.87	0.55
1:A:175:PRO:HA	1:A:178:SER:HB3	1.88	0.55
2:B:323:MET:HB3	2:B:373:MET:CE	2.36	0.55
1:C:1:MET:HG2	1:C:1:MET:O	2.06	0.55
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.88	0.55
4:F:186:LEU:HG	12:F:500:ACP:N1	2.22	0.54
2:B:158:ARG:CZ	11:B:507:MES:H21	2.38	0.54
2:D:106:GLY:O	2:D:111:GLY:HA3	2.08	0.54
2:B:315:VAL:HB	2:B:351:VAL:HG22	1.88	0.53
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.43	0.53
2:B:295:MET:HE1	2:B:319:PHE:CZ	2.43	0.53
9:B:503:EP:H62	9:B:503:EP:H13	1.91	0.53
3:E:137:LYS:O	3:E:141:GLU:HG2	2.09	0.53
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.91	0.53
1:A:60:LYS:NZ	1:A:85:GLN:O	2.24	0.53
1:C:368:LEU:O	13:C:760:HOH:O	2.19	0.53
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.42	0.53
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.43	0.53
1:C:204:VAL:HG22	1:C:302:MET:CE	2.39	0.53
2:B:199:ASP:OD2	11:B:507:MES:H52	2.09	0.53
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.44	0.53
3:E:52:LYS:HG2	3:E:53:LYS:NZ	2.24	0.52
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.91	0.52
4:F:333:ASN:HD21	12:F:500:ACP:PG	2.32	0.52
1:C:196:GLU:OE1	13:C:662:HOH:O	2.18	0.52
2:B:36:TYR:C	2:B:37:HIS:HD1	2.08	0.52
1:A:358:GLN:NE2	13:A:610:HOH:O	2.23	0.52
3:E:16:SER:OG	13:E:201:HOH:O	2.19	0.52
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.92	0.52
4:F:36:ARG:NH1	13:F:635:HOH:O	2.37	0.52
2:B:392:SER:O	2:B:396:THR:HG23	2.09	0.51
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.76	0.51
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.92	0.51
2:D:297:ASP:OD1	2:D:298:SER:N	2.43	0.51
2:D:116:ASP:HA	2:D:119:LEU:HD12	1.92	0.51
2:D:136:GLN:HA	2:D:167:ASN:O	2.10	0.51
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.45	0.51
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.93	0.51
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HD12	1:C:363:VAL:HG12	1.93	0.50
4:F:331:GLU:HG2	4:F:332:VAL:N	2.25	0.50
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.12	0.50
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.93	0.50
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.93	0.50
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.93	0.50
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.93	0.49
4:F:186:LEU:HG	12:F:500:ACP:C2	2.41	0.49
1:A:401:LYS:HE2	2:B:346:TRP:CG	2.46	0.49
1:C:204:VAL:HG22	1:C:302:MET:HE3	1.93	0.49
1:A:336:LYS:HD3	3:E:24:LEU:HD23	1.95	0.49
2:B:336:GLN:OE1	13:B:637:HOH:O	2.20	0.49
2:D:284:ARG:HG2	2:D:290:GLU:OE1	2.13	0.49
2:D:322:ARG:NH2	2:D:322:ARG:HG3	2.27	0.49
3:E:108:ASN:ND2	13:E:229:HOH:O	2.45	0.49
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.94	0.49
1:A:409:VAL:HA	1:A:413:MET:O	2.13	0.49
3:E:44:ASP:N	13:E:221:HOH:O	2.46	0.49
2:D:278:ARG:HH11	2:D:278:ARG:CG	2.26	0.49
2:B:263:PRO:O	2:B:266:HIS:ND1	2.42	0.48
4:F:288:LYS:NZ	13:F:634:HOH:O	2.44	0.48
3:E:106:GLU:O	3:E:110:GLU:HG3	2.13	0.48
1:C:417:GLU:OE1	13:C:717:HOH:O	2.19	0.48
4:F:292:ARG:HG2	4:F:292:ARG:NH1	2.28	0.48
2:D:155:SER:OG	3:E:126:LYS:HE2	2.14	0.48
3:E:140:LYS:HB3	3:E:140:LYS:HZ2	1.79	0.48
1:A:180:ALA:O	1:A:183:GLU:HG3	2.14	0.48
4:F:12:SER:HG	4:F:343:TYR:HH	1.62	0.48
1:A:150:THR:O	1:A:154:MET:HG2	2.13	0.48
2:D:213:CYS:HA	2:D:217:LEU:HD12	1.96	0.47
4:F:243:HIS:C	4:F:243:HIS:HD1	2.18	0.47
2:B:83:PHE:O	2:B:86:ILE:HG22	2.14	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.47
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.97	0.47
2:B:331:GLN:O	2:B:335:VAL:HG23	2.14	0.47
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.15	0.47
3:E:123:LEU:O	3:E:126:LYS:HB2	2.15	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.50	0.47
2:D:398:MET:HE2	2:D:398:MET:HB3	1.77	0.47
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.97	0.47
2:B:39:ASP:OD1	2:B:39:ASP:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:25:LYS:HG3	3:E:26:PRO:HD2	1.97	0.47
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.97	0.47
2:D:152:LEU:O	2:D:156:LYS:HG2	2.15	0.47
2:D:276:THR:HG22	2:D:280:SER:HB2	1.97	0.46
4:F:247:LYS:O	4:F:247:LYS:HG2	2.14	0.46
2:B:231:VAL:O	2:B:235:MET:HG3	2.16	0.46
2:D:19:LYS:O	2:D:23:VAL:HG23	2.15	0.46
2:B:293:GLN:O	10:B:505:LLM:H30	2.15	0.46
1:A:331:ALA:O	1:A:335:ILE:HG12	2.15	0.46
1:A:262:TYR:CD1	1:A:265:ILE:HD12	2.51	0.46
1:A:90:GLU:O	1:A:121:ARG:HG2	2.16	0.46
1:A:280:LYS:CE	1:A:283:HIS:HB3	2.44	0.46
4:F:292:ARG:HD3	4:F:378[B]:LEU:HB3	1.97	0.46
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.51	0.46
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.46
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.98	0.45
2:B:2:ARG:HB3	2:B:133:GLN:HG3	1.98	0.45
1:C:30:ILE:HG12	1:C:36:MET:HB2	1.98	0.45
3:E:136:ASN:O	3:E:140:LYS:HD3	2.15	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.45
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.45
3:E:138:GLU:HA	3:E:138:GLU:OE1	2.17	0.45
2:B:158:ARG:NH1	2:B:197:ASN:OD1	2.43	0.45
2:D:286:LEU:HD13	9:D:503:EP:H163	1.98	0.45
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.97	0.45
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE2	2.52	0.45
4:F:186:LEU:HD11	4:F:320:MET:CE	2.46	0.45
2:B:286:LEU:HG	2:B:290:GLU:CB	2.45	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.45
2:B:174:SER:OG	2:B:207:GLU:HB2	2.17	0.45
2:B:286:LEU:HD12	2:B:286:LEU:HA	1.74	0.44
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.99	0.44
2:D:74:THR:O	2:D:77:SER:OG	2.21	0.44
3:E:142:GLU:HG3	3:E:142:GLU:H	1.67	0.44
2:D:57:THR:HA	13:D:650:HOH:O	2.17	0.44
1:C:359:PRO:HB3	13:C:658:HOH:O	2.17	0.44
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.98	0.44
2:D:416:MET:O	2:D:420:GLU:HG3	2.17	0.44
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.85	0.44
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.32	0.44
3:E:53:LYS:HA	3:E:53:LYS:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:ILE:HG21	2:D:275:LEU:HD13	1.99	0.44
3:E:85:LYS:NZ	13:E:207:HOH:O	2.27	0.44
1:A:230:LEU:O	1:A:234:ILE:HD13	2.17	0.44
2:B:438:ALA:O	13:B:602:HOH:O	2.21	0.44
2:D:83:PHE:O	2:D:86:ILE:HG22	2.17	0.44
2:B:218:LYS:HA	2:B:218:LYS:HD3	1.73	0.44
1:A:315:CYS:HG	1:A:351:PHE:HE2	1.65	0.44
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.17	0.44
4:F:97:SER:OG	4:F:183:GLN:NE2	2.48	0.44
2:B:323:MET:HB3	2:B:373:MET:HE1	1.99	0.44
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.83	0.44
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.21	0.44
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.53	0.44
2:B:322:ARG:HB2	13:B:627:HOH:O	2.17	0.44
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.18	0.43
1:A:319:TYR:HB3	1:A:323:VAL:HG21	2.00	0.43
4:F:156:LYS:HB3	4:F:244:CYS:SG	2.58	0.43
3:E:134:ARG:HG3	3:E:134:ARG:HH11	1.83	0.43
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.33	0.43
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.18	0.43
2:D:79:ARG:HB2	2:D:79:ARG:HH11	1.82	0.43
3:E:13:LYS:HG2	3:E:18:GLN:CG	2.48	0.43
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.43
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.54	0.43
2:B:174:SER:CB	2:B:207:GLU:HB2	2.49	0.43
3:E:51:GLN:OE1	3:E:51:GLN:HA	2.18	0.43
2:D:396:THR:O	2:D:400:ARG:HG2	2.18	0.43
1:A:245:ASP:HB3	3:E:16:SER:OG	2.19	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.43
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.43
4:F:186:LEU:HD11	4:F:320:MET:HE3	2.00	0.42
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.48	0.42
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.54	0.42
2:B:301:MET:CE	2:B:301:MET:HA	2.49	0.42
1:C:372:GLN:O	13:C:658:HOH:O	2.21	0.42
2:B:57:THR:HG22	2:B:58:GLY:N	2.34	0.42
1:C:155:GLU:HB3	3:E:101:LEU:HD22	2.00	0.42
3:E:9:ILE:HG22	3:E:10:GLU:N	2.34	0.42
2:B:320:ARG:HA	2:B:321:GLY:HA2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:CB	1:A:140:SER:HB3	2.49	0.42
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.02	0.42
2:D:8:GLN:HB3	2:D:138:THR:CG2	2.50	0.42
2:D:276:THR:HB	2:D:281:GLN:HG2	2.01	0.42
2:D:75:MET:N	13:D:606:HOH:O	2.25	0.42
4:F:156:LYS:HD2	4:F:156:LYS:HA	1.88	0.42
2:D:403:ALA:HB1	2:D:404:PHE:CE2	2.55	0.42
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.82	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.55	0.42
2:B:160:GLU:HB3	2:B:161:TYR:CE1	2.54	0.42
2:D:269:MET:HE3	2:D:381:SER:HB3	2.01	0.42
4:F:14:TYR:HA	4:F:17:VAL:HB	2.01	0.42
2:B:371:LEU:HD21	9:B:503:EP:C13	2.50	0.42
2:D:295:MET:HE1	2:D:319:PHE:CZ	2.55	0.42
2:D:19:LYS:HD3	2:D:19:LYS:HA	1.61	0.42
4:F:237:THR:O	4:F:246:GLN:NE2	2.50	0.42
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.19	0.42
2:D:70:LEU:HD23	2:D:114:LEU:HD22	2.01	0.41
4:F:126:ASP:OD1	4:F:127:GLU:N	2.53	0.41
4:F:292:ARG:HD3	4:F:378[A]:LEU:HB3	2.01	0.41
1:A:188:ILE:HD13	1:A:395:PHE:HB2	2.03	0.41
1:C:174:ALA:O	1:C:178:SER:HB3	2.20	0.41
1:A:211:ASP:O	1:A:215:ARG:HB2	2.21	0.41
2:B:276:THR:N	9:B:503:EP:O76	2.33	0.41
1:A:336:LYS:HD3	3:E:24:LEU:CD2	2.51	0.41
2:D:8:GLN:HB3	2:D:138:THR:HG23	2.01	0.41
4:F:289:HIS:O	4:F:293:SER:OG	2.33	0.41
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.55	0.41
2:B:298:SER:N	10:B:505:LLM:O20	2.41	0.41
2:B:295:MET:CG	2:B:377:PHE:HB2	2.51	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.41
2:D:82:PRO:O	2:D:83:PHE:HB2	2.20	0.41
1:A:136:LEU:CD2	1:A:167:LEU:HB2	2.50	0.41
2:B:158:ARG:HG3	11:B:507:MES:H62	2.03	0.41
1:A:241:SER:HB2	1:A:248:LEU:O	2.21	0.41
2:D:205:ASP:HB3	2:D:303:ALA:HA	2.03	0.41
1:A:283:HIS:CD2	1:A:285:GLN:HE21	2.38	0.41
2:B:2:ARG:HB3	2:B:133:GLN:HG2	2.02	0.41
1:A:125:LEU:O	1:A:128:GLN:HB2	2.21	0.41
2:D:251:ASP:OD1	2:D:253:ARG:N	2.52	0.41
1:A:220:GLU:OE1	2:B:326:LYS:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.56	0.41
2:B:396:THR:O	2:B:400:ARG:HG3	2.21	0.41
2:D:76:ASP:HA	2:D:79:ARG:HH12	1.86	0.41
3:E:7:GLU:O	3:E:22:VAL:HA	2.21	0.41
4:F:221:LEU:HD11	4:F:267:PHE:CD2	2.55	0.41
1:C:143:GLY:HA3	5:C:501:GTP:O3A	2.21	0.41
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.41
4:F:162:ILE:HD11	4:F:240:LEU:HD21	2.03	0.41
1:C:241:SER:HB3	1:C:250:VAL:O	2.20	0.40
1:C:339:ARG:NE	13:C:686:HOH:O	2.31	0.40
2:D:414:ASP:N	2:D:414:ASP:OD1	2.55	0.40
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.85	0.40
2:B:292:THR:HA	2:B:295:MET:CE	2.51	0.40
1:C:328:VAL:O	1:C:332:ILE:HG13	2.22	0.40
4:F:19:ARG:CG	4:F:19:ARG:HH11	2.34	0.40
3:E:134:ARG:HG3	3:E:134:ARG:NH1	2.36	0.40
2:D:319:PHE:HB2	2:D:355:VAL:HG22	2.03	0.40
1:A:71:GLU:HG2	1:A:72:PRO:N	2.37	0.40
2:D:79:ARG:HB2	2:D:79:ARG:NH1	2.37	0.40
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.53	0.40
1:A:265:ILE:O	1:A:265:ILE:HG22	2.21	0.40
2:D:324:SER:HB3	2:D:327:GLU:HB2	2.03	0.40
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.86	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	435/451 (96%)	426 (98%)	9 (2%)	0	100	100
1	C	439/451 (97%)	431 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	427/445 (96%)	412 (96%)	14 (3%)	1 (0%)	52	69
2	D	430/445 (97%)	421 (98%)	9 (2%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	352/384 (92%)	341 (97%)	10 (3%)	1 (0%)	46	63
All	All	2202/2319 (95%)	2150 (98%)	50 (2%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	321	GLY
4	F	154	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	358 (97%)	10 (3%)	52	73
1	C	372/379 (98%)	363 (98%)	9 (2%)	57	76
2	B	371/383 (97%)	353 (95%)	18 (5%)	31	48
2	D	371/383 (97%)	358 (96%)	13 (4%)	43	64
3	E	110/127 (87%)	97 (88%)	13 (12%)	6	8
4	F	321/342 (94%)	313 (98%)	8 (2%)	55	76
All	All	1913/1993 (96%)	1842 (96%)	71 (4%)	41	62

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	71	GLU
1	A	96	LYS
1	A	121	ARG

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Mol	Chain	Res	Type
1	A	124	LYS
1	A	176	GLN
1	A	326	LYS
1	A	342	GLN
1	A	433	GLU
2	B	1	MET
2	B	19	LYS
2	B	60	LYS
2	B	117	SER
2	B	139	HIS
2	B	207	GLU
2	B	220	THR
2	B	248	LEU
2	B	276	THR
2	B	278	ARG
2	B	281	GLN
2	B	322	ARG
2	B	369	ARG
2	B	405	LEU
2	B	414	ASP
2	B	416	MET
2	B	420	GLU
2	B	430	SER
1	C	1	MET
1	C	41	THR
1	C	165	SER
1	C	241	SER
1	C	245	ASP
1	C	251	ASP
1	C	297	GLU
1	C	356	ASN
1	C	381	THR
2	D	1	MET
2	D	15	GLN
2	D	50	ASN
2	D	57	THR
2	D	79	ARG
2	D	88	ARG
2	D	138	THR
2	D	139	HIS
2	D	155	SER
2	D	248	LEU

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Mol	Chain	Res	Type
2	D	278	ARG
2	D	345	GLU
2	D	416	MET
3	E	10	GLU
3	E	12	ASN
3	E	16	SER
3	E	19	SER
3	E	49	GLU
3	E	53	LYS
3	E	59	GLU
3	E	74	GLU
3	E	96	MET
3	E	98	LYS
3	E	139	LEU
3	E	141	GLU
3	E	142	GLU
4	F	19	ARG
4	F	32	LYS
4	F	186	LEU
4	F	211	TYR
4	F	217	ARG
4	F	242	ASN
4	F	244	CYS
4	F	292	ARG

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

Mol	Chain	Res	Type
2	B	339	ASN
3	E	12	ASN
3	E	108	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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	6	25,34,34	0.96	1 (4%)	34,54,54	1.71	7 (20%)
8	GDP	B	501	6	23,30,30	1.14	2 (8%)	30,47,47	1.85	7 (23%)
9	EP	B	503	-	32,36,36	1.23	3 (9%)	35,53,53	2.44	11 (31%)
10	LLM	B	505	-	37,40,40	2.30	12 (32%)	33,55,55	1.81	4 (12%)
11	MES	B	507	-	11,12,12	0.59	0	14,16,16	2.31	5 (35%)
5	GTP	C	501	6	25,34,34	0.95	1 (4%)	34,54,54	1.67	8 (23%)
8	GDP	D	501	6	23,30,30	1.14	2 (8%)	30,47,47	1.93	7 (23%)
9	EP	D	503	-	32,36,36	1.41	4 (12%)	35,53,53	2.12	9 (25%)
12	ACP	F	500	6	25,33,33	1.39	5 (20%)	31,52,52	1.93	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
8	GDP	B	501	6	-	0/12/32/32	0/3/3/3
9	EP	B	503	-	-	1/49/55/55	0/1/3/3
10	LLM	B	505	-	-	0/39/64/64	0/1/4/4
11	MES	B	507	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	6	-	0/12/32/32	0/3/3/3
9	EP	D	503	-	-	1/49/55/55	0/1/3/3
12	ACP	F	500	6	-	0/15/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	LLM	C30-C25	-5.20	1.38	1.50
10	B	505	LLM	C5-C6	-4.92	1.40	1.50
10	B	505	LLM	C2-C1	-3.83	1.39	1.48
10	B	505	LLM	C8-C7	-3.68	1.41	1.49
10	B	505	LLM	C4-C3	-3.37	1.39	1.50
10	B	505	LLM	C27-C26	-3.34	1.40	1.48
10	B	505	LLM	C24-C25	-2.84	1.41	1.50
9	D	503	EP	O2-C3	-2.59	1.40	1.45
9	B	503	EP	C59-C57	-2.09	1.51	1.54
12	F	500	ACP	PB-O2B	2.09	1.61	1.56
12	F	500	ACP	PG-O3G	2.29	1.60	1.54
10	B	505	LLM	C2-C3	2.67	1.39	1.31
10	B	505	LLM	C16-C17	2.70	1.50	1.46
9	D	503	EP	C13-S1	2.71	1.74	1.70
10	B	505	LLM	C6-C7	2.73	1.40	1.32
8	D	501	GDP	C5-C4	2.77	1.46	1.40
10	B	505	LLM	C29-C13	2.78	1.39	1.32
8	B	501	GDP	C5-C4	2.84	1.46	1.40
12	F	500	ACP	PB-O3A	2.84	1.61	1.58
12	F	500	ACP	PG-O2G	2.87	1.61	1.54
5	C	501	GTP	C6-N1	2.93	1.38	1.33
5	A	501	GTP	C6-N1	2.94	1.38	1.33
12	F	500	ACP	C5-C4	3.22	1.47	1.40
8	B	501	GDP	C6-C5	3.45	1.48	1.41
8	D	501	GDP	C6-C5	3.45	1.48	1.41
9	B	503	EP	O2-C75	3.64	1.45	1.34
9	D	503	EP	O2-C75	3.66	1.45	1.34
9	B	503	EP	C27-C24	4.11	1.53	1.46
9	D	503	EP	C27-C24	4.82	1.54	1.46
10	B	505	LLM	C21-C22	6.28	1.52	1.32

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	EP	C32-C27-C24	-7.01	113.93	123.40
12	F	500	ACP	N3-C2-N1	-6.79	123.70	128.89
10	B	505	LLM	C23-C22-C21	-6.54	114.27	125.55
5	A	501	GTP	N3-C2-N1	-5.15	119.60	127.44
9	B	503	EP	O26-C27-C32	-4.90	109.20	116.59
5	C	501	GTP	N3-C2-N1	-4.89	119.99	127.44
12	F	500	ACP	PA-O3A-PB	-4.57	119.89	132.73
9	D	503	EP	O26-C24-C27	-4.35	57.28	59.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C6-N1	-4.31	117.70	123.59
9	D	503	EP	O26-C27-C32	-4.16	110.32	116.59
10	B	505	LLM	C18-C17-C16	-4.01	115.85	124.52
9	B	503	EP	O26-C27-C24	-3.97	57.49	59.66
8	B	501	GDP	C5-C6-N1	-3.92	118.23	123.59
8	B	501	GDP	C6-C5-C4	-3.87	116.27	120.90
9	D	503	EP	O26-C27-C24	-3.68	57.65	59.66
9	B	503	EP	O26-C24-C27	-3.68	57.65	59.66
8	D	501	GDP	C6-C5-C4	-3.55	116.65	120.90
9	B	503	EP	O26-C24-C21	-3.42	108.43	116.36
9	D	503	EP	C32-C27-C24	-3.36	118.86	123.40
12	F	500	ACP	C2'-C1'-N9	-3.35	109.17	114.29
8	D	501	GDP	N3-C2-N1	-3.31	122.41	127.44
5	C	501	GTP	C5-C6-N1	-3.30	119.08	123.59
8	D	501	GDP	PA-O3A-PB	-3.26	121.72	132.67
8	B	501	GDP	N3-C2-N1	-3.25	122.49	127.44
9	B	503	EP	C21-C3-C5	-3.20	109.14	113.72
9	D	503	EP	O26-C24-C21	-3.08	109.21	116.36
5	A	501	GTP	C5-C6-N1	-3.07	119.39	123.59
5	A	501	GTP	PA-O3A-PB	-2.98	124.37	132.73
8	B	501	GDP	C4-C5-N7	-2.94	106.77	109.48
9	D	503	EP	C53-C51-C47	-2.91	107.25	112.37
8	D	501	GDP	C4-C5-N7	-2.91	106.80	109.48
10	B	505	LLM	C11-C10-C9	-2.90	110.17	115.46
8	D	501	GDP	C1'-N9-C4	-2.78	122.74	126.94
8	B	501	GDP	C1'-N9-C4	-2.78	122.75	126.94
9	B	503	EP	C53-C51-C47	-2.61	107.77	112.37
5	C	501	GTP	C2'-C1'-N9	-2.54	110.41	114.29
12	F	500	ACP	C4-C5-N7	-2.39	107.28	109.48
5	C	501	GTP	C1'-N9-C4	-2.35	123.39	126.94
5	A	501	GTP	C4-C5-N7	-2.33	107.34	109.48
5	A	501	GTP	C1'-N9-C4	-2.32	123.44	126.94
9	D	503	EP	C21-C3-C5	-2.32	110.40	113.72
5	C	501	GTP	C4-C5-N7	-2.32	107.35	109.48
11	B	507	MES	C7-C8-S	-2.20	105.71	112.51
8	B	501	GDP	O3A-PA-O5'	-2.13	97.30	102.94
5	C	501	GTP	O2A-PA-O3A	2.00	114.17	105.09
9	B	503	EP	C64-C59-C68	2.16	113.24	109.38
5	C	501	GTP	N2-C2-N1	2.18	120.80	117.20
12	F	500	ACP	C2-N1-C6	2.19	122.68	118.77
11	B	507	MES	C2-C3-N4	2.19	113.45	110.12
5	A	501	GTP	N2-C2-N1	2.56	121.44	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	500	ACP	O2G-PG-C3B	2.57	112.64	106.40
11	B	507	MES	O1S-S-C8	2.58	109.11	106.91
9	B	503	EP	O2-C75-C72	2.74	116.84	111.54
11	B	507	MES	O2S-S-C8	3.05	109.50	106.91
9	D	503	EP	C16-C15-N20	3.11	132.06	123.88
5	A	501	GTP	C6-N1-C2	3.21	120.40	115.94
5	C	501	GTP	C6-N1-C2	3.23	120.42	115.94
9	B	503	EP	C16-C15-N20	3.24	132.40	123.88
10	B	505	LLM	C16-O16-C17	3.63	62.66	60.59
8	B	501	GDP	C6-N1-C2	4.91	122.76	115.94
8	D	501	GDP	C6-N1-C2	4.97	122.83	115.94
9	B	503	EP	C27-O26-C24	6.21	64.85	60.69
11	B	507	MES	C5-N4-C3	6.41	122.78	108.90
9	D	503	EP	C27-O26-C24	6.53	65.07	60.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	503	EP	C5-C10-C12-N20
9	D	503	EP	C5-C10-C12-N20

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	B	503	EP	6	0
10	B	505	LLM	4	0
11	B	507	MES	3	0
5	C	501	GTP	1	0
8	D	501	GDP	1	0
9	D	503	EP	1	0
12	F	500	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, 95th 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	437/451 (96%)	-0.13	2 (0%) 91 91	24, 40, 68, 119	0
1	C	440/451 (97%)	-0.16	0 100 100	19, 32, 59, 84	0
2	B	428/445 (96%)	0.02	7 (1%) 74 74	23, 43, 81, 115	2 (0%)
2	D	431/445 (96%)	-0.12	4 (0%) 85 85	25, 47, 79, 107	6 (1%)
3	E	121/143 (84%)	0.04	1 (0%) 87 87	30, 53, 100, 118	0
4	F	351/384 (91%)	0.95	71 (20%) 1 1	36, 65, 136, 154	0
All	All	2208/2319 (95%)	0.08	85 (3%) 44 45	19, 44, 99, 154	8 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	240	LEU	7.6
4	F	173	ILE	7.0
4	F	234	GLN	6.6
4	F	249	TYR	5.5
4	F	152	SER	4.8
4	F	236	LYS	4.7
4	F	233	PHE	4.7
4	F	157	GLY	4.6
4	F	232	ASN	4.6
4	F	244	CYS	4.5
4	F	156	LYS	4.4
4	F	162	ILE	4.2
4	F	177	GLY	4.2
4	F	186	LEU	4.1
4	F	179	VAL	4.0
4	F	131	PHE	3.9
4	F	161	LEU	3.9
4	F	243	HIS	3.8
4	F	238	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
4	F	258	GLU	3.8
4	F	259	GLY	3.7
4	F	242	ASN	3.7
4	F	225	SER	3.7
4	F	170	LEU	3.6
4	F	253	TYR	3.5
4	F	168	GLU	3.5
4	F	220[A]	VAL	3.4
4	F	245	ILE	3.4
4	F	169	LEU	3.3
4	F	231	ALA	3.3
2	B	438	ALA	3.3
2	B	56	ALA	3.3
4	F	372	THR	3.2
4	F	224	SER	3.2
2	B	280	SER	3.2
2	B	284	ARG	3.1
4	F	163	SER	3.1
4	F	239	HIS	3.1
2	B	283	TYR	3.1
4	F	176	GLN	3.1
2	B	282	GLN	3.0
4	F	241	THR	2.9
4	F	255[A]	ARG	2.9
4	F	182	ILE	2.9
4	F	158	GLU	2.8
4	F	125	THR	2.8
4	F	371	PRO	2.8
4	F	229	ASN	2.8
2	B	340	SER	2.7
4	F	142	ARG	2.6
4	F	199	PHE	2.6
4	F	284[A]	LEU	2.6
1	A	262	TYR	2.5
4	F	99	VAL	2.5
4	F	178	GLN	2.5
2	D	1	MET	2.5
3	E	6	MET	2.5
4	F	247	LYS	2.5
4	F	330	ILE	2.5
4	F	378[A]	LEU	2.4
4	F	100	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	147	TRP	2.4
4	F	44	ARG	2.4
4	F	155	ALA	2.4
4	F	335	ALA	2.4
4	F	105	LEU	2.3
4	F	165	GLU	2.3
4	F	181	VAL	2.3
4	F	252	ASN	2.3
4	F	153	ALA	2.3
1	A	282	TYR	2.3
4	F	251	LYS	2.2
2	D	405	LEU	2.2
2	D	57	THR	2.2
4	F	250	SER	2.1
4	F	148	ILE	2.1
4	F	248	GLU	2.1
4	F	160	ILE	2.1
4	F	228	TYR	2.1
4	F	256	TYR	2.1
4	F	235	ASP	2.1
4	F	246	GLN	2.1
2	D	284	ARG	2.1
4	F	192	LEU	2.0
4	F	263	PHE	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, 95th 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(\AA^2)	Q<0.9
7	CA	A	503	1/1	0.95	0.18	3.65	64,64,64,64	0
10	LLM	B	505	37/37	0.78	0.26	3.34	72,99,120,123	5
7	CA	C	503	1/1	0.91	0.19	2.29	68,68,68,68	0
5	GTP	A	501	32/32	0.98	0.17	0.83	19,26,34,42	0
9	EP	B	503	34/34	0.85	0.27	0.83	54,67,75,82	0
5	GTP	C	501	32/32	0.98	0.16	0.79	16,22,27,42	0
8	GDP	B	501	28/28	0.98	0.17	0.51	18,27,32,35	0
9	EP	D	503	34/34	0.96	0.16	0.09	35,46,60,63	0
8	GDP	D	501	28/28	0.98	0.12	-0.29	29,34,46,51	0
11	MES	B	507	12/12	0.93	0.13	-0.46	48,55,71,74	0
12	ACP	F	500	31/31	0.90	0.20	-0.83	69,83,158,200	0
6	MG	F	501	1/1	0.79	0.14	-2.19	77,77,77,77	0
6	MG	B	502	1/1	0.80	0.24	-	54,54,54,54	0
6	MG	D	502	1/1	0.86	0.12	-	62,62,62,62	0
6	MG	A	502	1/1	0.97	0.35	-	30,30,30,30	0
7	CA	B	506	1/1	0.94	0.20	-	80,80,80,80	0
6	MG	C	502	1/1	0.85	0.32	-	29,29,29,29	0
6	MG	B	504	1/1	0.99	0.29	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.