



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2016 – 01:58 PM EST

PDB ID : 5KX5
Title : Crystal structure of tubulin-stathmin-TTL-Compound 11 complex
Authors : Parris, K.
Deposited on : 2016-07-20
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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-20028442

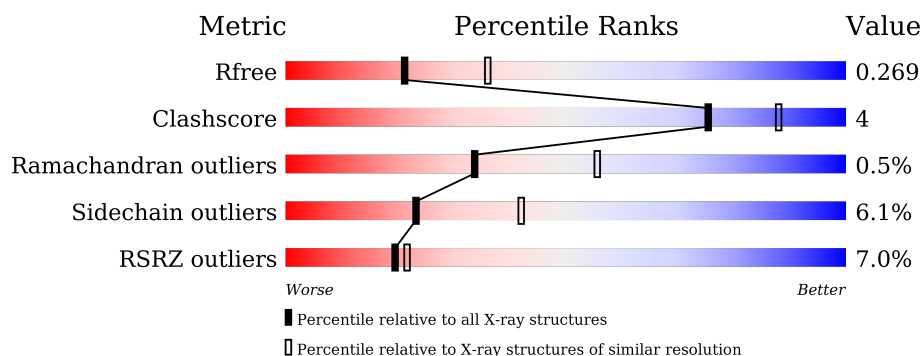
1 Overall quality at a glance ⓘ

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 $\leq 5\%$. 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>6%</div> <div>84% 12% ..</div> </div>
1	C	451	<div> <div>%</div> <div>86% 11% .</div> </div>
2	B	445	<div> <div>%</div> <div>80% 15% . .</div> </div>
2	D	445	<div> <div>8%</div> <div>80% 14% . .</div> </div>
3	E	143	<div> <div>8%</div> <div>67% 17% 15%</div> </div>
4	F	384	<div> <div>19%</div> <div>72% 15% . 12%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	A	502	-	-	-	X
6	MG	C	502	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17802 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3445	2179	585	659	22			
1	C	440	Total	C	N	O	S	0	2	0
			3455	2186	589	658	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	3	0
			3377	2122	578	651	26			
2	D	426	Total	C	N	O	S	0	0	0
			3343	2097	571	650	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			1012	625	185	198	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	conflict	UNP P63043
E	20	TRP	PHE	conflict	UNP P63043

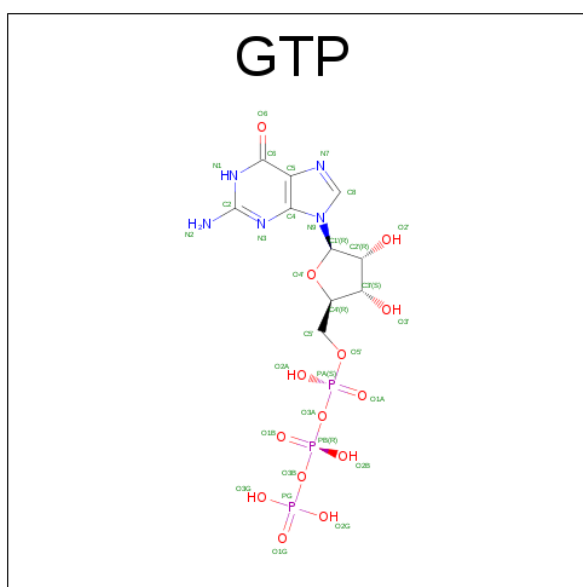
- Molecule 4 is a protein called TTL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	338	Total	C	N	O	S	0	2	0
			2788	1794	474	506	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	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		

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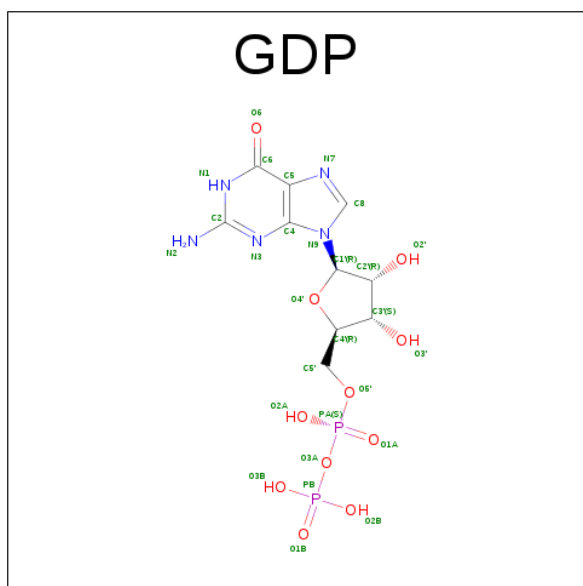
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	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		
7	E	1	Total	Ca	0	0
			1	1		

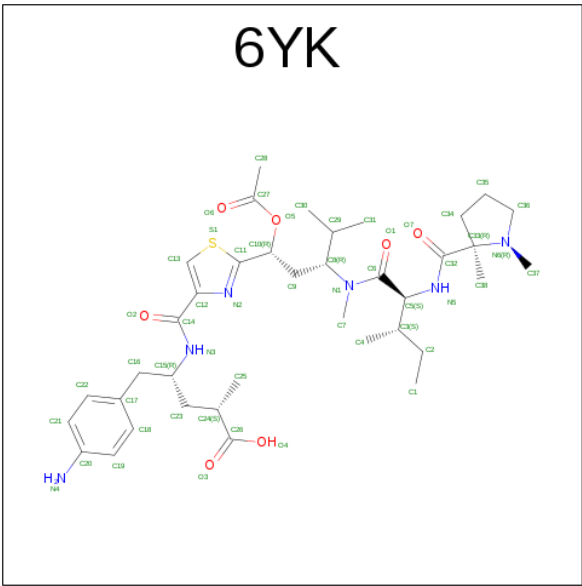
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

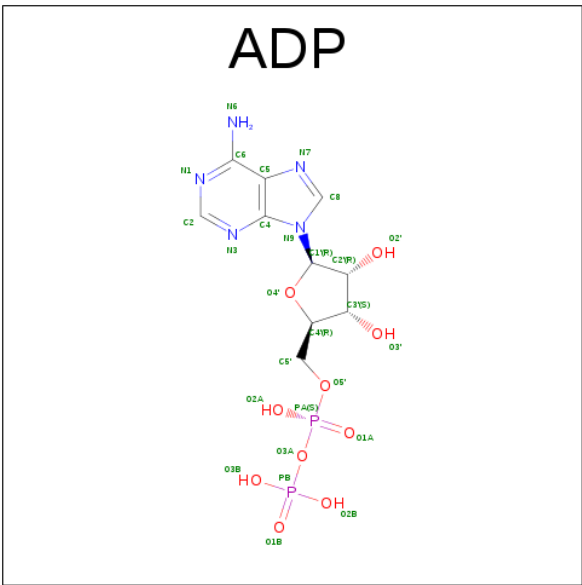
- Molecule 9 is (2 {S},4 {R})-4-[[2-[(1 {R},3 {R})-1-acetyloxy-3-[(2 {S},3 {S})-2-[(2 {R})-1,2-dimethylpyrrolidin-2-yl]carbonylamino]-3-methyl-pentanoyl]-methyl-amino]-4-methyl-pentyl]-1,3-thiazol-4-yl]carbonylamino]-5-(4-aminophenyl)-2-methyl-pentanoic acid (three-letter

code: 6YK) (formula: C₃₈H₅₈N₆O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			52	38	6	7	1		
9	D	1	Total	C	N	O	S	0	0
			52	38	6	7	1		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

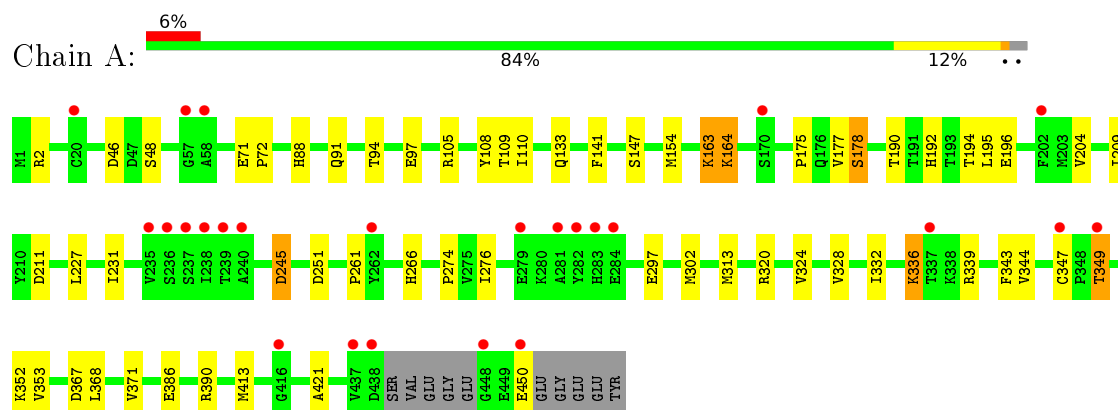
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	22	Total	O	0	0
			22	22		
11	B	33	Total	O	0	0
			33	33		
11	C	41	Total	O	0	0
			41	41		
11	D	7	Total	O	0	0
			7	7		
11	E	4	Total	O	0	0
			4	4		
11	F	14	Total	O	0	0
			14	14		

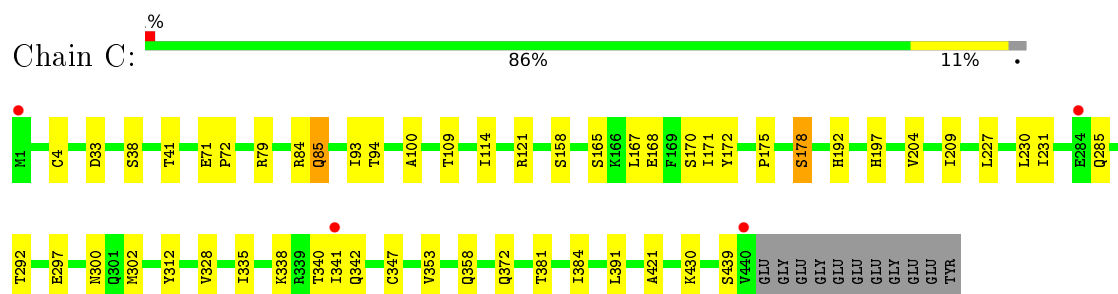
3 Residue-property plots [i](#)

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.

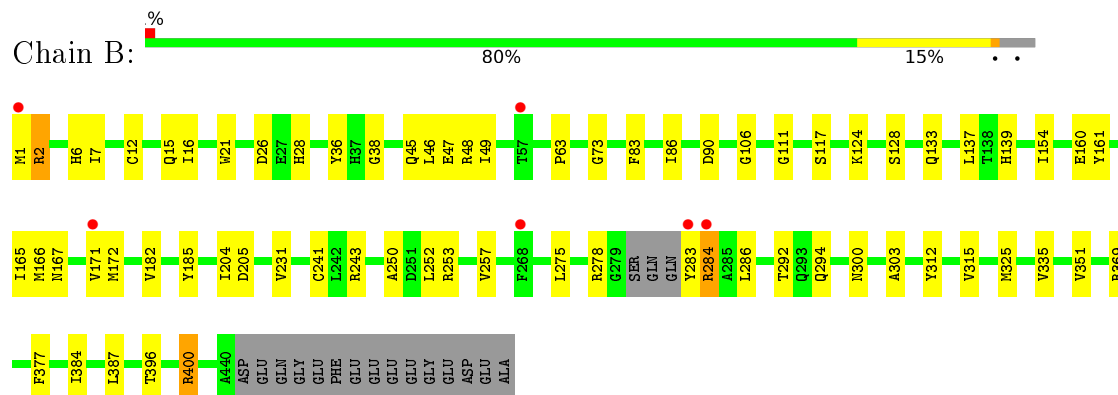
- Molecule 1: Tubulin alpha chain



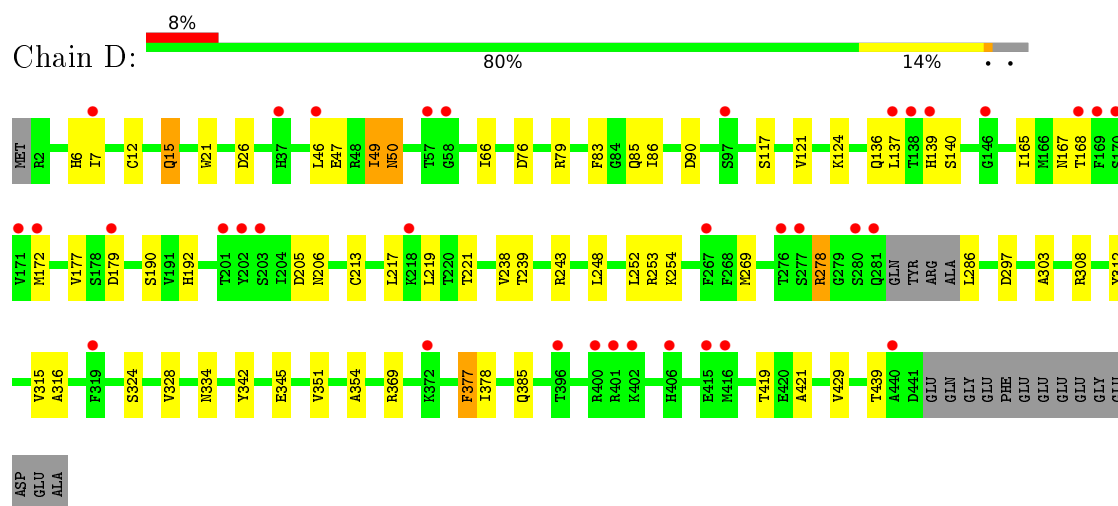
- Molecule 1: Tubulin alpha chain



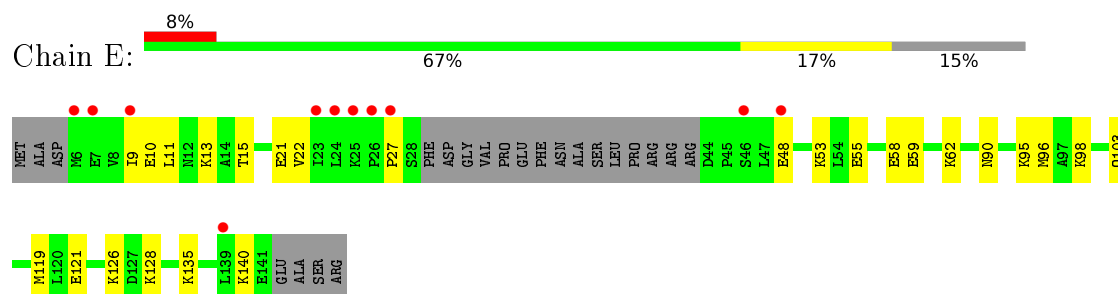
- Molecule 2: Tubulin beta chain



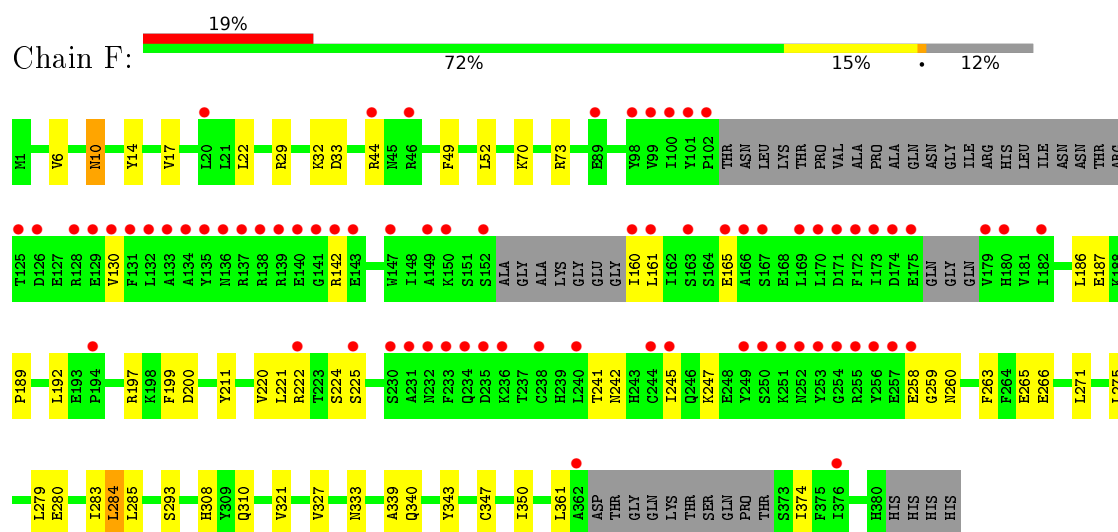
- Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: TTL protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.79 Å 153.90 Å 185.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.47 – 2.50 36.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (38.47-2.50) 97.3 (36.66-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.51 Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.197 , 0.251 0.214 , 0.269	Depositor DCC
R_{free} test set	5070 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17802	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, ADP, CA, GTP, 6YK

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	0.52	0/3522	0.72	0/4779
1	C	0.54	0/3534	0.73	0/4800
2	B	0.54	0/3457	0.73	0/4681
2	D	0.50	0/3416	0.69	0/4627
3	E	0.52	0/1022	0.70	0/1358
4	F	0.49	0/2857	0.70	0/3859
All	All	0.52	0/17808	0.71	0/24104

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3445	0	3349	29	0
1	C	3455	0	3364	23	0
2	B	3377	0	3265	34	0
2	D	3343	0	3216	31	0
3	E	1012	0	1025	5	0
4	F	2788	0	2768	20	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	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
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	0	0
9	B	52	0	0	1	0
9	D	52	0	0	1	0
10	F	27	0	12	0	0
11	A	22	0	0	0	0
11	B	33	0	0	0	0
11	C	41	0	0	0	0
11	D	7	0	0	0	0
11	E	4	0	0	0	0
11	F	14	0	0	0	0
All	All	17802	0	17047	136	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 4.

All (136) 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:B:28:HIS:CE1	2:B:243:ARG:HH11	2.12	0.67
1:A:97:GLU:HG3	2:B:1:MET:HG2	1.76	0.67
2:B:15:GLN:HG2	9:B:504:6YK:C19	2.25	0.66
1:A:195:LEU:HD12	1:A:266:HIS:HE1	1.60	0.66
2:B:28:HIS:HE1	2:B:243:ARG:HH11	1.44	0.66
1:A:245:ASP:OD2	3:E:15:THR:HG22	1.94	0.66
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.78	0.64
4:F:14:TYR:HA	4:F:17:VAL:HB	1.81	0.62
1:C:285:GLN:HE22	1:C:372:GLN:H	1.49	0.61
1:A:175:PRO:HA	1:A:178:SER:HB2	1.83	0.60
1:A:163:LYS:HD3	1:A:163:LYS:H	1.66	0.59
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.86	0.57
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HD11	1:C:302:MET:SD	2.44	0.57
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.85	0.57
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.87	0.56
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.87	0.56
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.87	0.56
2:B:28:HIS:HE1	2:B:243:ARG:HD2	1.70	0.56
2:D:324:SER:O	2:D:328:VAL:HG23	2.06	0.55
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.40	0.55
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.89	0.54
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.88	0.54
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.43	0.54
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.90	0.53
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.89	0.53
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.90	0.53
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.91	0.53
1:A:192:HIS:CG	1:A:421:ALA:HA	2.44	0.52
2:B:2:ARG:H	2:B:133:GLN:HG3	1.74	0.52
2:B:83:PHE:O	2:B:86:ILE:HG22	2.09	0.52
1:A:209:ILE:HD11	1:A:302:MET:SD	2.49	0.52
2:B:182:VAL:O	2:B:185:TYR:HB2	2.10	0.52
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.44	0.52
2:B:241:CYS:O	2:B:250:ALA:HA	2.10	0.51
4:F:347:CYS:HA	4:F:350:ILE:HD12	1.92	0.51
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.92	0.51
2:D:385:GLN:HB2	2:D:429:VAL:HG22	1.93	0.51
1:A:72:PRO:HA	1:A:94:THR:HG21	1.93	0.51
2:D:83:PHE:O	2:D:86:ILE:HG22	2.10	0.51
1:A:154:MET:HG3	1:A:194:THR:HG23	1.93	0.51
1:C:72:PRO:HA	1:C:94:THR:HG21	1.93	0.51
4:F:224:SER:HB2	4:F:241:THR:HG22	1.91	0.50
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.30	0.50
2:D:15:GLN:HG2	9:D:504:6YK:C19	2.43	0.49
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.95	0.49
2:B:283:TYR:HB2	2:B:284:ARG:HG3	1.94	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.49
2:B:396:THR:O	2:B:400[B]:ARG:HB2	2.13	0.49
1:C:100:ALA:HA	2:D:254:LYS:HE2	1.95	0.49
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.95	0.48
2:D:312:TYR:HE1	2:D:377:PHE:HZ	1.59	0.47
1:A:352:LYS:HG2	3:E:21:GLU:HG3	1.96	0.47
1:C:33:ASP:HA	1:C:85:GLN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ASN:ND2	2:D:50:ASN:H	2.12	0.47
2:D:46:LEU:HD23	2:D:49:ILE:HD13	1.97	0.47
3:E:58:GLU:HG2	3:E:62:LYS:HD2	1.96	0.47
1:C:171:ILE:HD13	1:C:204:VAL:HB	1.96	0.47
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.96	0.47
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.46
1:A:88:HIS:HB2	1:A:91:GLN:HG3	1.97	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.45	0.46
1:A:163:LYS:HG2	1:A:164:LYS:HD2	1.97	0.46
2:B:253:ARG:O	2:B:257:VAL:HG23	2.16	0.46
1:A:450:GLU:HG3	4:F:333:ASN:HB3	1.98	0.46
2:B:38:GLY:HA3	2:B:45:GLN:HE22	1.81	0.45
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.81	0.45
2:D:7:ILE:O	2:D:137:LEU:HD12	2.16	0.45
2:D:12:CYS:CB	2:D:140:SER:HB3	2.47	0.45
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.98	0.45
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.52	0.45
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.97	0.45
2:B:160:GLU:HG2	2:B:161:TYR:CE2	2.50	0.45
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.52	0.45
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.45
2:B:48:ARG:HB2	2:B:243:ARG:O	2.16	0.45
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.34	0.45
1:C:79:ARG:O	1:C:84:ARG:HB2	2.16	0.45
2:D:76:ASP:HA	2:D:79:ARG:NH1	2.32	0.45
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.44
4:F:271:LEU:HD23	4:F:275:LEU:HD13	1.99	0.44
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.44
1:C:158:SER:OG	1:C:197:HIS:HD2	2.01	0.44
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.88	0.44
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.98	0.44
2:D:7:ILE:O	2:D:137:LEU:HA	2.18	0.44
4:F:321:VAL:HG22	4:F:327:VAL:HG22	1.99	0.44
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.99	0.44
4:F:187:GLU:O	4:F:189:PRO:HD3	2.18	0.43
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.53	0.43
2:D:316:ALA:HB3	2:D:378:ILE:HB	2.00	0.43
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.01	0.43
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE2	2.53	0.43
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.83	0.43
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:THR:O	2:D:243:ARG:HG3	2.18	0.43
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.99	0.43
1:C:285:GLN:HG3	1:C:372:GLN:HE21	1.82	0.43
2:D:238:VAL:HG12	2:D:378:ILE:HG12	2.01	0.43
4:F:197:ARG:HB2	4:F:224:SER:O	2.19	0.43
1:A:97:GLU:HG2	1:A:105:ARG:HH21	1.84	0.43
2:D:172:MET:HB2	2:D:205:ASP:HA	2.01	0.43
4:F:225:SER:HB3	4:F:260:ASN:HD21	1.83	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.42
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.00	0.42
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.00	0.42
1:C:312:TYR:CD2	1:C:341:ILE:HG23	2.54	0.42
2:B:400[B]:ARG:HB3	2:B:400[B]:ARG:HH11	1.85	0.42
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.02	0.42
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	2.02	0.42
2:B:46:LEU:HA	2:B:49:ILE:HB	2.01	0.42
2:D:165:ILE:HD11	2:D:253:ARG:HG3	2.02	0.41
4:F:6:VAL:HB	4:F:29:ARG:CZ	2.50	0.41
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.02	0.41
1:C:285:GLN:NE2	1:C:372:GLN:H	2.18	0.41
4:F:242:ASN:HB2	4:F:245:ILE:HD12	2.02	0.41
1:C:297:GLU:HB3	1:C:300:ASN:HD22	1.86	0.41
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.01	0.41
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.55	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
4:F:220[A]:VAL:HG11	4:F:339:ALA:HB2	2.02	0.41
4:F:258:GLU:HA	4:F:259:GLY:HA2	1.88	0.41
2:B:172:MET:HG3	2:B:387:LEU:HD21	2.03	0.41
1:C:175:PRO:HA	1:C:178:SER:HB2	2.03	0.41
1:A:332:ILE:HD13	3:E:22:VAL:HG11	2.02	0.41
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.56	0.41
2:B:286:LEU:HD21	2:B:294:GLN:NE2	2.36	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.02	0.40
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.02	0.40
1:A:297:GLU:HG2	1:A:339:ARG:HH22	1.86	0.40
1:C:192:HIS:CG	1:C:421:ALA:HA	2.57	0.40
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.03	0.40
1:A:386:GLU:O	1:A:390:ARG:HG3	2.21	0.40
1:C:209:ILE:CD1	1:C:302:MET:SD	3.10	0.40
2:B:315:VAL:HB	2:B:351:VAL:HG22	2.03	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%)	415 (95%)	20 (5%)	2 (0%)	34	55
1	C	440/451 (98%)	428 (97%)	11 (2%)	1 (0%)	52	75
2	B	426/445 (96%)	413 (97%)	9 (2%)	4 (1%)	21	37
2	D	422/445 (95%)	399 (94%)	22 (5%)	1 (0%)	52	75
3	E	118/143 (82%)	113 (96%)	3 (2%)	2 (2%)	11	19
4	F	330/384 (86%)	310 (94%)	19 (6%)	1 (0%)	46	68
All	All	2173/2319 (94%)	2078 (96%)	84 (4%)	11 (0%)	34	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2	ARG
2	B	73	GLY
3	E	10	GLU
1	C	109	THR
3	E	27	PRO
2	B	128	SER
2	B	278	ARG
1	A	109	THR
1	A	245	ASP
4	F	361	LEU
2	D	278	ARG

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	370/378 (98%)	351 (95%)	19 (5%)	29	52
1	C	372/378 (98%)	352 (95%)	20 (5%)	27	49
2	B	371/383 (97%)	358 (96%)	13 (4%)	43	70
2	D	368/383 (96%)	345 (94%)	23 (6%)	22	40
3	E	109/126 (86%)	92 (84%)	17 (16%)	3	6
4	F	308/342 (90%)	283 (92%)	25 (8%)	15	27
All	All	1898/1990 (95%)	1781 (94%)	117 (6%)	23	41

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	48	SER
1	A	71	GLU
1	A	110	ILE
1	A	141	PHE
1	A	163	LYS
1	A	164	LYS
1	A	177	VAL
1	A	178	SER
1	A	196	GLU
1	A	211	ASP
1	A	251	ASP
1	A	276	ILE
1	A	320	ARG
1	A	324	VAL
1	A	336	LYS
1	A	349	THR
1	A	367	ASP
1	A	368	LEU
2	B	26	ASP
2	B	47	GLU
2	B	90	ASP
2	B	117	SER
2	B	124	LYS
2	B	139	HIS
2	B	167	ASN
2	B	284	ARG

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Mol	Chain	Res	Type
2	B	325	MET
2	B	369	ARG
2	B	384	ILE
2	B	400[A]	ARG
2	B	400[B]	ARG
1	C	4	CYS
1	C	38	SER
1	C	41	THR
1	C	71	GLU
1	C	85	GLN
1	C	165	SER
1	C	167	LEU
1	C	168	GLU
1	C	170	SER
1	C	178	SER
1	C	338	LYS
1	C	340	THR
1	C	342	GLN
1	C	347	CYS
1	C	358[A]	GLN
1	C	358[B]	GLN
1	C	381	THR
1	C	384	ILE
1	C	430	LYS
1	C	439	SER
2	D	15	GLN
2	D	26	ASP
2	D	47	GLU
2	D	49	ILE
2	D	50	ASN
2	D	85	GLN
2	D	90	ASP
2	D	117	SER
2	D	124	LYS
2	D	139	HIS
2	D	179	ASP
2	D	190	SER
2	D	219	LEU
2	D	221	THR
2	D	278	ARG
2	D	286	LEU
2	D	297	ASP

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Mol	Chain	Res	Type
2	D	334	ASN
2	D	345	GLU
2	D	369	ARG
2	D	377	PHE
2	D	419	THR
2	D	439	THR
3	E	11	LEU
3	E	13	LYS
3	E	48	GLU
3	E	53	LYS
3	E	55	GLU
3	E	59	GLU
3	E	90	ASN
3	E	95	LYS
3	E	96	MET
3	E	98	LYS
3	E	103	GLN
3	E	119	MET
3	E	121	GLU
3	E	126	LYS
3	E	128	LYS
3	E	135	LYS
3	E	140	LYS
4	F	10	ASN
4	F	22	LEU
4	F	32	LYS
4	F	33	ASP
4	F	70	LYS
4	F	73	ARG
4	F	130	VAL
4	F	142	ARG
4	F	160	ILE
4	F	161	LEU
4	F	165	GLU
4	F	186	LEU
4	F	192	LEU
4	F	200	ASP
4	F	211	TYR
4	F	222	ARG
4	F	247	LYS
4	F	265	GLU
4	F	266	GLU

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Mol	Chain	Res	Type
4	F	284	LEU
4	F	285	LEU
4	F	293	SER
4	F	308	HIS
4	F	310	GLN
4	F	374	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
2	B	28	HIS
2	B	45	GLN
2	B	192	HIS
2	B	229	HIS
1	C	31	GLN
1	C	85	GLN
1	C	101	ASN
1	C	197	HIS
1	C	300	ASN
1	C	372	GLN
1	C	380	ASN
2	D	192	HIS
3	E	115	HIS
4	F	45	ASN
4	F	260	ASN
4	F	310	GLN

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 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	0.98	1 (3%)	29,54,54	2.39	5 (17%)
8	GDP	B	501	-	24,30,30	0.90	1 (4%)	26,47,47	2.50	4 (15%)
9	6YK	B	504	-	48,54,54	1.06	1 (2%)	51,77,77	0.53	0
5	GTP	C	501	6	26,34,34	0.94	2 (7%)	29,54,54	2.51	6 (20%)
8	GDP	D	501	6	24,30,30	0.91	1 (4%)	26,47,47	2.55	4 (15%)
9	6YK	D	504	-	48,54,54	1.13	1 (2%)	51,77,77	0.72	1 (1%)
10	ADP	F	401	-	24,29,29	0.69	0	23,45,45	0.63	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	GDP	B	501	-	-	0/12/32/32	0/3/3/3
9	6YK	B	504	-	-	0/52/77/77	0/3/3/3
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	6YK	D	504	-	-	0/52/77/77	0/3/3/3
10	ADP	F	401	-	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C6-C5	2.12	1.45	1.41
8	B	501	GDP	C6-N1	2.90	1.38	1.33
5	C	501	GTP	C6-N1	3.11	1.38	1.33
8	D	501	GDP	C6-N1	3.16	1.38	1.33
5	A	501	GTP	C6-N1	3.36	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	6YK	C33-C32	6.77	1.61	1.54
9	D	504	6YK	C33-C32	7.43	1.61	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C6-N1	-8.77	112.06	123.52
5	C	501	GTP	C5-C6-N1	-8.70	112.15	123.52
8	B	501	GDP	C5-C6-N1	-8.38	112.56	123.52
5	A	501	GTP	C5-C6-N1	-8.38	112.57	123.52
8	D	501	GDP	N3-C2-N1	-3.10	123.33	127.56
8	B	501	GDP	N3-C2-N1	-3.09	123.36	127.56
5	C	501	GTP	N3-C2-N1	-3.03	123.43	127.56
5	A	501	GTP	N3-C2-N1	-2.89	123.62	127.56
5	C	501	GTP	C6-C5-C4	-2.70	117.77	120.86
5	A	501	GTP	C6-C5-C4	-2.61	117.88	120.86
8	B	501	GDP	C6-C5-C4	-2.39	118.12	120.86
8	D	501	GDP	C6-C5-C4	-2.25	118.28	120.86
5	A	501	GTP	O3G-PG-O1G	2.26	118.01	110.63
9	D	504	6YK	C31-C29-C8	2.29	117.55	111.54
5	C	501	GTP	O5'-PA-O1A	2.50	119.46	109.21
5	C	501	GTP	O3G-PG-O1G	2.72	119.49	110.63
5	A	501	GTP	C6-N1-C2	7.92	125.16	115.88
8	B	501	GDP	C6-N1-C2	8.11	125.39	115.88
5	C	501	GTP	C6-N1-C2	8.12	125.40	115.88
8	D	501	GDP	C6-N1-C2	8.18	125.47	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	1	0
9	B	504	6YK	1	0
9	D	504	6YK	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, 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	441/451 (97%)	0.23	25 (5%) 27 31	38, 61, 92, 146	0
1	C	440/451 (97%)	-0.11	4 (0%) 85 88	35, 51, 76, 106	0
2	B	427/445 (95%)	0.03	6 (1%) 78 80	34, 52, 86, 101	2 (0%)
2	D	426/445 (95%)	0.51	35 (8%) 14 15	48, 73, 97, 126	5 (1%)
3	E	121/143 (84%)	0.45	11 (9%) 11 12	43, 71, 99, 112	0
4	F	338/384 (88%)	1.00	73 (21%) 1 1	50, 84, 142, 164	0
All	All	2193/2319 (94%)	0.31	154 (7%) 19 22	34, 63, 106, 164	7 (0%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	10.7
1	A	282	TYR	7.6
4	F	170	LEU	7.2
1	A	281	ALA	7.1
4	F	234	GLN	7.0
4	F	100	ILE	6.5
4	F	137	ARG	6.4
4	F	161	LEU	6.2
2	D	401	ARG	5.9
4	F	179	VAL	5.8
4	F	173	ILE	5.8
4	F	132	LEU	5.7
4	F	254	GLY	5.6
2	B	283	TYR	5.5
4	F	251	LYS	5.4
4	F	169	LEU	5.2
4	F	102	PRO	5.1
4	F	133	ALA	4.9
4	F	134	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
4	F	256	TYR	4.7
4	F	233	PHE	4.7
4	F	231	ALA	4.5
1	A	438	ASP	4.5
4	F	255	ARG	4.4
4	F	240	LEU	4.4
4	F	141	GLY	4.3
4	F	236	LYS	4.3
4	F	147	TRP	4.2
3	E	25	LYS	4.2
4	F	249	TYR	4.2
1	A	235	VAL	4.2
4	F	139	ARG	4.1
2	D	277	SER	4.1
2	D	280	SER	4.1
4	F	140	GLU	3.8
4	F	258	GLU	3.8
4	F	250	SER	3.8
2	D	57	THR	3.7
2	D	170	SER	3.6
4	F	152	SER	3.6
4	F	252	ASN	3.6
4	F	230	SER	3.6
4	F	130	VAL	3.6
4	F	128	ARG	3.6
4	F	131	PHE	3.5
2	B	1	MET	3.5
4	F	238	CYS	3.5
4	F	171	ASP	3.5
3	E	9	ILE	3.4
4	F	362	ALA	3.4
2	D	202	TYR	3.4
4	F	167	SER	3.4
4	F	136	ASN	3.3
2	D	37	HIS	3.3
2	D	179	ASP	3.3
2	D	139	HIS	3.2
4	F	165	GLU	3.2
4	F	89	GLU	3.2
1	A	279	GLU	3.2
2	D	169	PHE	3.1
4	F	129	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	440	VAL	3.1
2	D	281	GLN	3.1
4	F	182	ILE	3.1
4	F	126	ASP	3.1
2	D	168	THR	3.0
3	E	6	MET	3.0
1	A	236	SER	3.0
4	F	142	ARG	3.0
4	F	175	GLU	2.9
1	C	1	MET	2.9
4	F	20	LEU	2.9
3	E	23	ILE	2.9
4	F	101	TYR	2.9
4	F	253	TYR	2.9
2	B	57	THR	2.8
2	D	400	ARG	2.8
4	F	235	ASP	2.8
2	D	415	GLU	2.7
2	D	146	GLY	2.7
4	F	160	ILE	2.7
3	E	26	PRO	2.7
1	A	450	GLU	2.7
4	F	135	TYR	2.7
1	A	448	GLY	2.6
4	F	174	ASP	2.6
4	F	194	PRO	2.6
3	E	48	GLU	2.6
4	F	44	ARG	2.6
1	A	416	GLY	2.6
1	A	437	VAL	2.6
2	D	276	THR	2.6
4	F	149	ALA	2.6
1	A	237	SER	2.5
4	F	257	GLU	2.5
2	D	402	LYS	2.5
1	A	349	THR	2.5
2	D	201	THR	2.5
4	F	180	HIS	2.5
4	F	172	PHE	2.5
2	D	440	ALA	2.5
4	F	99	VAL	2.4
2	D	203	SER	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	46	ARG	2.4
4	F	244	CYS	2.4
2	D	137	LEU	2.4
1	A	284	GLU	2.4
2	D	58	GLY	2.4
2	D	138	THR	2.4
1	A	283	HIS	2.3
2	D	7	ILE	2.3
1	A	170	SER	2.3
4	F	138	ARG	2.3
2	D	406	HIS	2.3
1	A	20	CYS	2.3
1	A	238	ILE	2.3
2	D	267	PHE	2.3
1	A	347	CYS	2.3
1	A	262	TYR	2.3
4	F	125	THR	2.3
2	D	416	MET	2.3
2	D	218	LYS	2.3
3	E	139	LEU	2.3
2	B	284	ARG	2.3
4	F	245	ILE	2.3
4	F	232	ASN	2.2
2	D	396	THR	2.2
4	F	225	SER	2.2
1	A	58	ALA	2.2
1	C	284	GLU	2.2
3	E	46	SER	2.2
2	D	172	MET	2.2
1	A	57	GLY	2.2
1	A	337	THR	2.2
2	B	268	PHE	2.2
4	F	222	ARG	2.2
4	F	163	SER	2.2
4	F	98	TYR	2.1
1	A	239	THR	2.1
2	D	97	SER	2.1
2	D	319	PHE	2.1
3	E	24	LEU	2.1
1	A	240	ALA	2.1
2	B	171	VAL	2.1
2	D	171	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	2.1
2	D	46	LEU	2.1
4	F	150	LYS	2.1
4	F	376	ILE	2.1
1	C	341	ILE	2.1
1	A	202	PHE	2.1
3	E	7	GLU	2.0
2	D	372	LYS	2.0
4	F	143	GLU	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(Å ²)	Q<0.9
6	MG	C	502	1/1	0.96	0.34	10.05	47,47,47,47	0
6	MG	A	502	1/1	0.85	0.33	9.16	50,50,50,50	0
9	6YK	D	504	52/52	0.84	0.32	1.75	86,102,117,119	0
9	6YK	B	504	52/52	0.96	0.15	0.77	35,49,65,76	0
8	GDP	B	501	28/28	0.98	0.20	0.20	31,40,43,47	0
5	GTP	A	501	32/32	0.97	0.17	0.08	40,47,51,53	0
5	GTP	C	501	32/32	0.98	0.16	0.00	37,44,49,54	0
7	CA	E	201	1/1	0.92	0.17	0.00	113,113,113,113	0
10	ADP	F	401	27/27	0.87	0.21	-0.65	91,103,121,122	0
8	GDP	D	501	28/28	0.96	0.16	-0.69	58,62,67,74	0
7	CA	B	503	1/1	0.83	0.12	-1.14	101,101,101,101	0
7	CA	A	503	1/1	0.96	0.07	-2.71	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CA	C	503	1/1	0.97	0.05	-3.91	71,71,71,71	0
6	MG	B	502	1/1	0.68	0.41	-	57,57,57,57	0
6	MG	B	505	1/1	0.87	0.15	-	78,78,78,78	0
6	MG	D	503	1/1	0.72	0.13	-	61,61,61,61	0
6	MG	D	502	1/1	0.91	0.12	-	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.