



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:17 PM GMT

PDB ID : 4EB6  
Title : Tubulin-Vinblastine: Stathmin-like complex  
Authors : Ranaivoson, F.M.; Gigant, B.; Knossow, M.  
Deposited on : 2012-03-23  
Resolution : 3.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

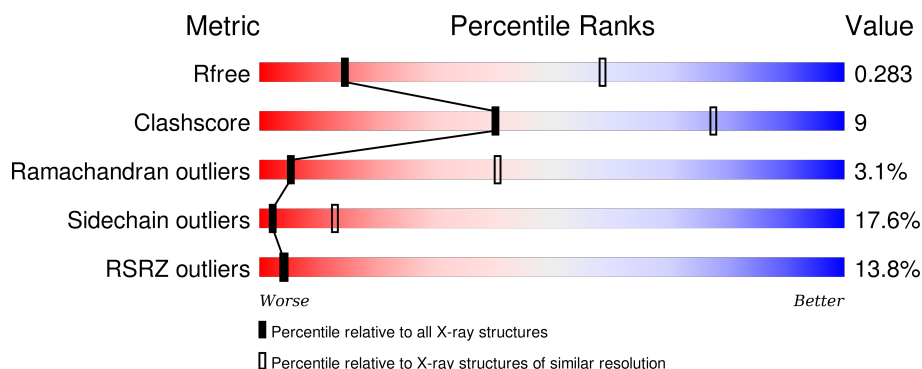
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>18%</div> <div>63%</div> <div>28%</div> <div>• •</div> </div>
1	C	451	<div> <div>11%</div> <div>65%</div> <div>26%</div> <div>5%</div> <div>•</div> </div>
2	B	445	<div> <div>14%</div> <div>64%</div> <div>28%</div> <div>5%</div> <div>•</div> </div>
2	D	445	<div> <div>9%</div> <div>64%</div> <div>29%</div> <div>• •</div> </div>
3	E	142	<div> <div>18%</div> <div>68%</div> <div>21%</div> <div>• • 7%</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	SO4	A	504	-	-	-	X
6	SO4	D	502	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14918 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	433	Total	C	N	O	S	0	1	0
			3399	2153	577	647	22			
1	C	432	Total	C	N	O	S	0	4	0
			3408	2161	576	648	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	2	0
			3400	2130	582	662	26			
2	D	432	Total	C	N	O	S	0	1	0
			3394	2127	580	661	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

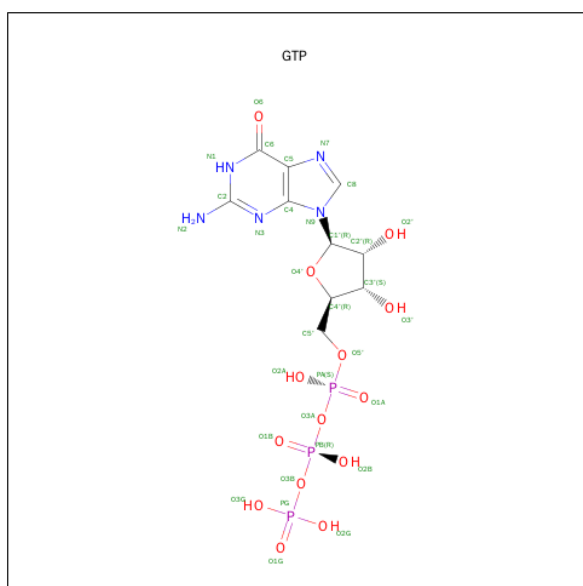
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	132	Total	C	N	O	S	0	1	0
			1080	669	195	212	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043
E	14	ALA	CYS	ENGINEERED MUTATION	UNP P63043
E	20	TRP	PHE	ENGINEERED MUTATION	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

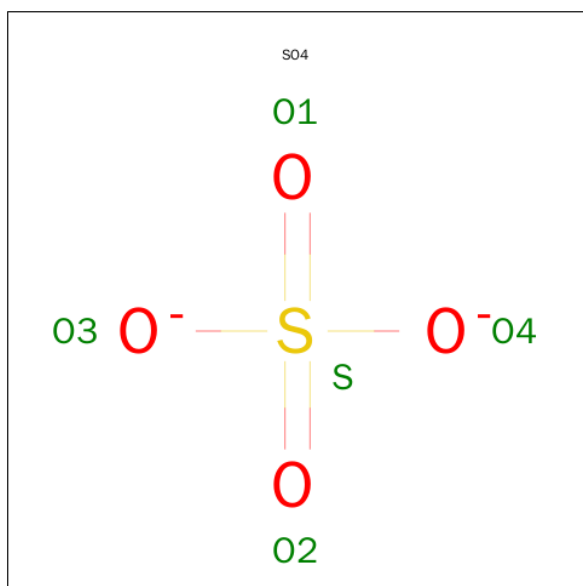
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

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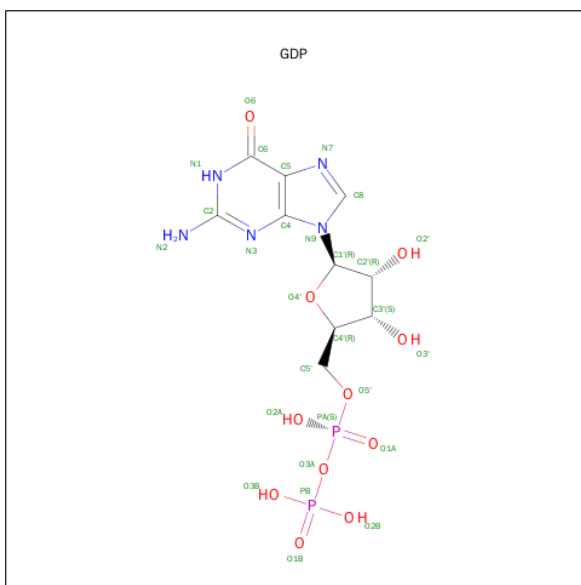
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



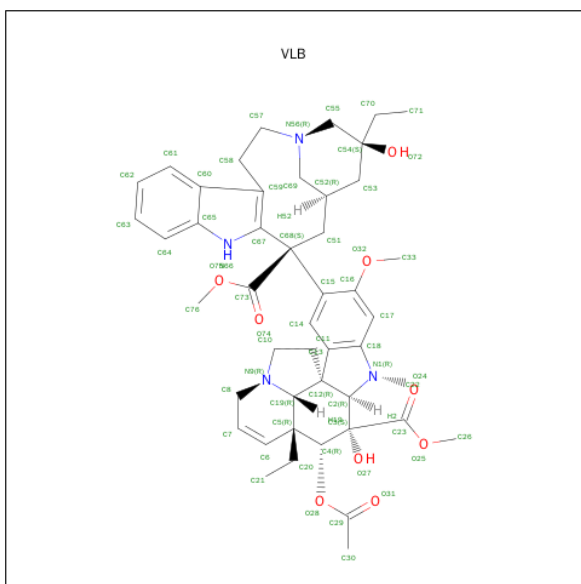
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

- Molecule 8 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula:  $C_{46}H_{58}N_4O_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			59	46	4	9		

- Molecule 9 is water.

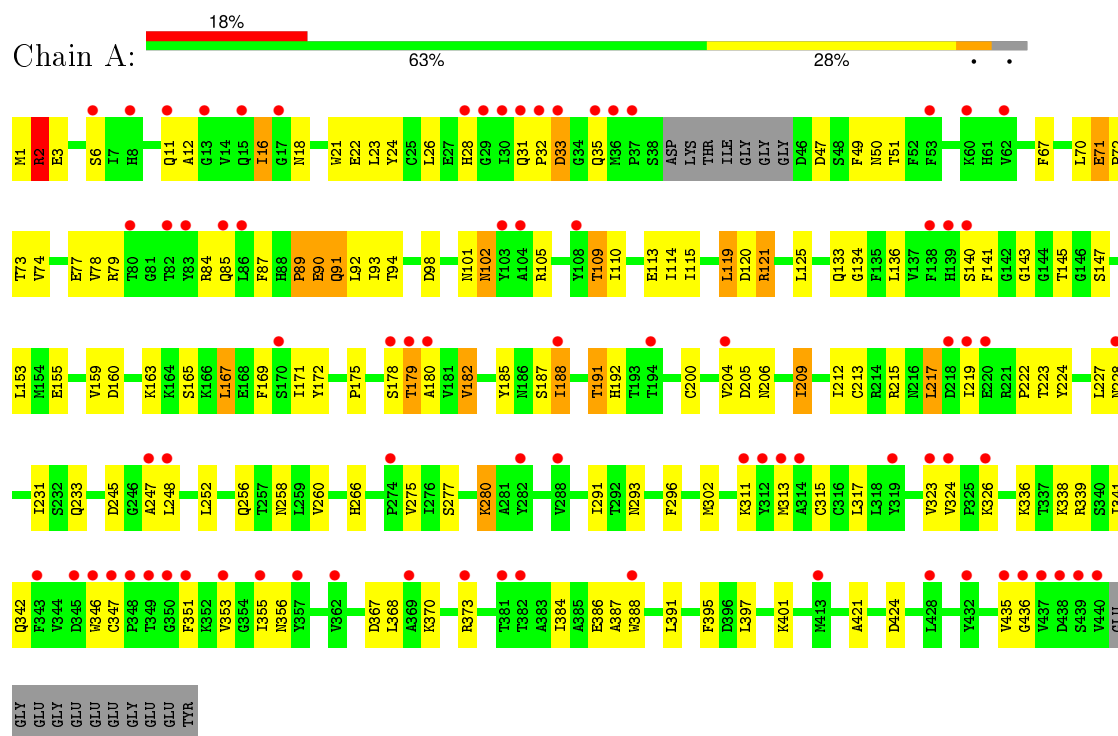
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total 5	O 5	0	0
9	B	3	Total 3	O 3	0	0
9	C	13	Total 13	O 13	0	0
9	D	9	Total 9	O 9	0	0
9	E	1	Total 1	O 1	0	0



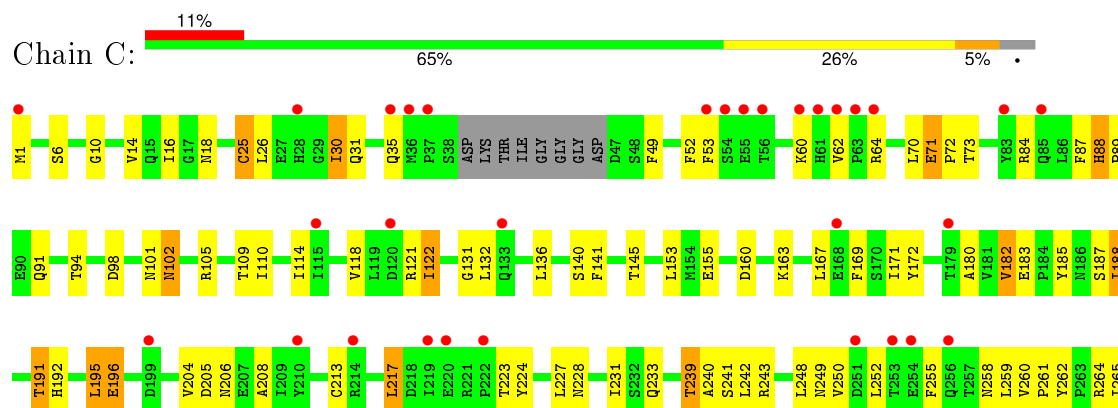
### 3 Residue-property plots [i](#)

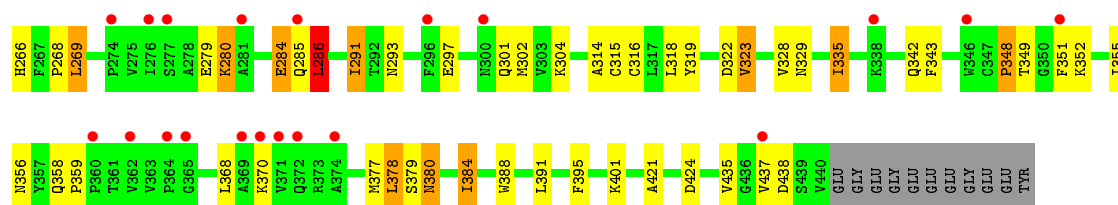
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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

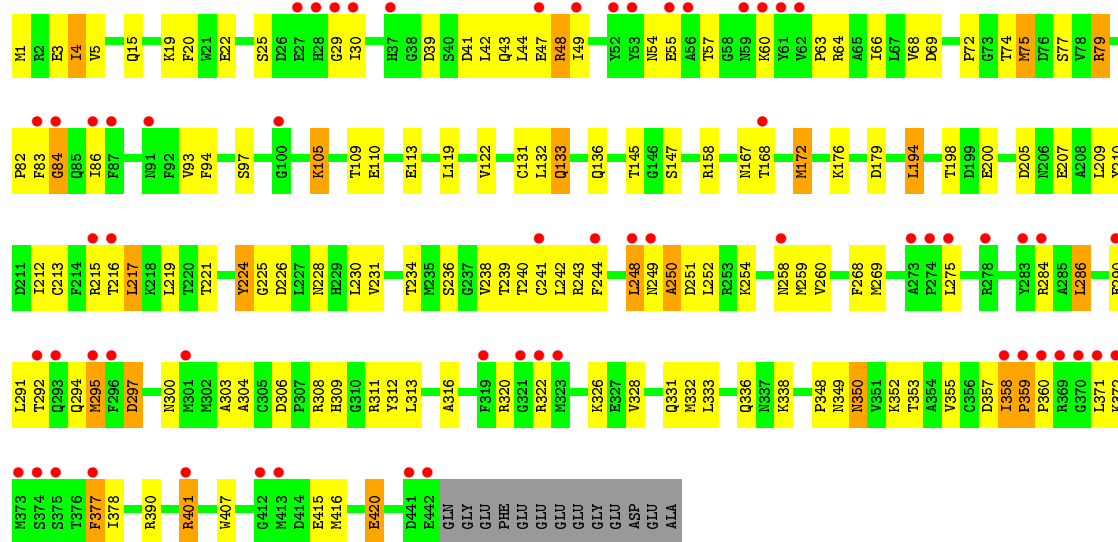


#### • Molecule 1: Tubulin alpha chain

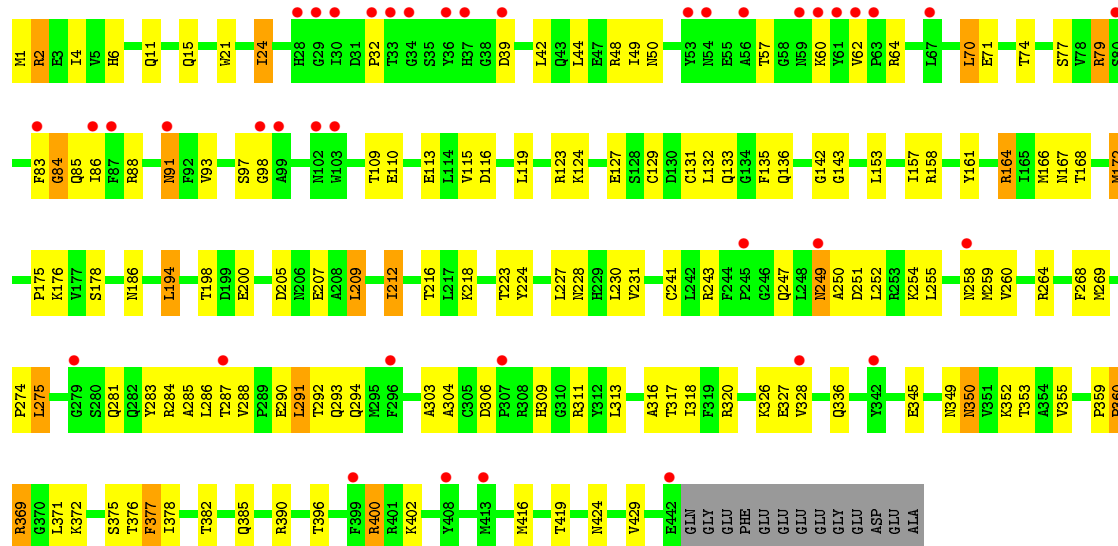




• Molecule 2: Tubulin beta chain

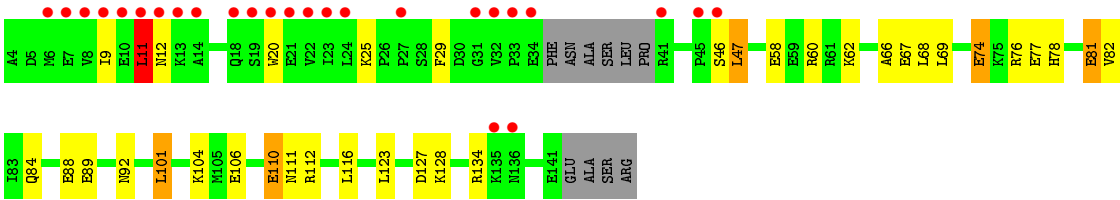


• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.69Å 129.68Å 252.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 3.47 43.06 – 3.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.06-3.47) 99.2 (43.06-3.47)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.213 , 0.253 0.235 , 0.283	Depositor DCC
$R_{free}$ test set	1424 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	119.2	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 140.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	2 of 28150 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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, GTP, MG, VLB, SO4

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	0.40	0/3479	0.72	1/4723 (0.0%)
1	C	0.40	0/3495	0.73	1/4745 (0.0%)
2	B	0.40	0/3485	0.73	0/4720
2	D	0.41	0/3471	0.73	0/4701
3	E	0.40	0/1095	0.68	0/1459
All	All	0.40	0/15025	0.73	2/20348 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	PRO	N-CA-C	5.41	126.17	112.10
1	C	348	PRO	C-N-CA	5.20	134.70	121.70

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	3399	0	3312	54	0
1	C	3408	0	3322	61	0
2	B	3400	0	3266	68	0
2	D	3394	0	3268	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1080	0	1077	10	0
4	A	32	0	12	4	0
4	C	32	0	12	3	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	10	0	0	0	0
6	B	5	0	0	0	0
6	D	10	0	0	0	0
7	B	28	0	12	0	0
7	D	28	0	12	2	0
8	C	59	0	58	13	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
9	C	13	0	0	0	0
9	D	9	0	0	0	0
9	E	1	0	0	0	0
All	All	14918	0	14351	255	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 (255) 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)
8:C:503:VLB:H303	8:C:503:VLB:H213	1.50	0.93
2:B:212:ILE:HA	2:B:217:LEU:HG	1.55	0.86
2:B:221:THR:HA	8:C:503:VLB:H761	1.61	0.83
8:C:503:VLB:H582	8:C:503:VLB:H511	1.64	0.78
2:B:5:VAL:HG12	2:B:64:ARG:HG2	1.67	0.77
2:D:62:VAL:HG21	2:D:88:ARG:HG3	1.68	0.76
2:D:2:ARG:HB2	2:D:131:CYS:HB3	1.67	0.76
2:D:172:MET:HE1	2:D:390:ARG:HH22	1.53	0.74
2:D:317:THR:HG22	2:D:377:PHE:HD1	1.52	0.74
1:C:259:LEU:HD21	1:C:378:LEU:HB3	1.71	0.73
1:A:180:ALA:HA	2:B:258:ASN:HD21	1.53	0.73
2:B:359:PRO:HB2	2:B:360:PRO:CD	2.18	0.73
2:B:172:MET:HE1	2:B:390:ARG:HH22	1.53	0.73
2:D:212:ILE:HD11	2:D:230:LEU:HD22	1.72	0.71
1:C:206:ASN:HD21	4:C:501:GTP:HN22	1.38	0.70
1:A:206:ASN:HD21	4:A:501:GTP:HN22	1.38	0.69
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD21	1:A:252:LEU:HB2	1.75	0.68
2:D:21:TRP:HA	2:D:24:ILE:HG22	1.75	0.68
1:C:213:CYS:HA	1:C:217:LEU:HB2	1.77	0.66
2:D:320:ARG:HB3	2:D:359:PRO:HA	1.76	0.66
2:B:407:TRP:HZ2	1:C:260:VAL:HG13	1.62	0.65
2:B:297:ASP:HA	2:B:308:ARG:HH12	1.62	0.64
2:B:248:LEU:HG	2:B:249:ASN:H	1.63	0.64
2:D:11:GLN:HE21	2:D:15:GLN:HE22	1.47	0.63
2:B:228:ASN:HA	2:B:231:VAL:HG12	1.81	0.63
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.79	0.63
2:B:1:MET:N	2:B:131:CYS:SG	2.72	0.63
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.81	0.62
8:C:503:VLB:H332	8:C:503:VLB:H512	1.80	0.62
1:C:101:ASN:HD22	1:C:180:ALA:HB2	1.64	0.62
1:A:70:LEU:HD23	1:A:110:ILE:HG23	1.81	0.61
1:C:25:CYS:HB2	1:C:30:ILE:HB	1.83	0.61
2:B:216:THR:H	2:B:217:LEU:HD22	1.66	0.60
2:D:320:ARG:HE	2:D:360:PRO:HG3	1.65	0.60
1:C:191:THR:HG21	1:C:388:TRP:CH2	2.36	0.60
2:D:133:GLN:HG2	2:D:252:LEU:HB2	1.83	0.59
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.82	0.59
1:A:87:PHE:HB3	1:A:91:GLN:HG3	1.83	0.59
1:A:101:ASN:HD22	1:A:180:ALA:HB2	1.66	0.59
3:E:11:LEU:H	3:E:20:TRP:HA	1.68	0.59
2:B:210:TYR:HE2	8:C:503:VLB:H333	1.67	0.59
1:C:241:SER:HA	1:C:249:ASN:HD21	1.66	0.59
2:D:209:LEU:HB3	2:D:230:LEU:HD11	1.86	0.58
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.84	0.58
1:C:239:THR:O	1:C:241:SER:N	2.36	0.58
1:A:2:ARG:HB2	1:A:133[A]:GLN:HE21	1.67	0.57
1:C:262:TYR:HB2	1:C:265:ILE:HD12	1.86	0.57
1:A:247:ALA:HB1	3:E:12:ASN:HB2	1.85	0.57
2:B:401:ARG:HH11	2:B:401:ARG:HB3	1.69	0.57
8:C:503:VLB:H691	8:C:503:VLB:C59	2.35	0.56
2:B:172:MET:CE	2:B:390:ARG:HH22	2.18	0.56
1:C:208:ALA:HB2	1:C:304:LYS:HG2	1.88	0.56
2:D:172:MET:CE	2:D:390:ARG:HH22	2.18	0.56
1:A:191:THR:HG21	1:A:388:TRP:CH2	2.41	0.56
2:D:142:GLY:HA3	7:D:501:GDP:H4'	1.88	0.56
2:D:133:GLN:HE21	2:D:252:LEU:H	1.53	0.56
1:A:33:ASP:HA	1:A:85:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.88	0.55
2:B:306:ASP:HB3	2:B:309:HIS:HB2	1.88	0.55
2:D:21:TRP:HA	2:D:24:ILE:CG2	2.37	0.55
1:A:28:HIS:CD2	1:A:49:PHE:HB2	2.42	0.55
2:B:79:ARG:HA	2:B:84:GLY:HA3	1.89	0.55
1:A:16:ILE:HD11	1:A:231:ILE:HG13	1.89	0.54
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.90	0.54
1:A:213:CYS:SG	1:A:222:PRO:HG3	2.48	0.53
1:A:217:LEU:HA	1:A:277:SER:HB3	1.89	0.53
1:C:87:PHE:HB2	1:C:91:GLN:NE2	2.23	0.53
2:D:318:ILE:HB	2:D:376:THR:HG23	1.91	0.53
2:D:249:ASN:HB2	2:D:255:LEU:HA	1.91	0.52
2:B:407:TRP:CZ2	1:C:260:VAL:HG13	2.43	0.52
2:B:86:ILE:HD12	2:B:86:ILE:H	1.74	0.52
1:A:67:PHE:HB2	1:A:92:LEU:HD22	1.91	0.52
2:B:241:CYS:SG	2:B:248:LEU:HD11	2.49	0.52
2:D:116:ASP:HA	2:D:119:LEU:HG	1.92	0.52
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.90	0.52
2:D:24:ILE:HD11	2:D:243:ARG:HD3	1.91	0.51
1:C:206:ASN:ND2	4:C:501:GTP:HN22	2.07	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG2	1.92	0.51
1:A:206:ASN:ND2	4:A:501:GTP:HN22	2.08	0.51
2:B:5:VAL:HG22	2:B:132:LEU:HD11	1.93	0.51
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.93	0.51
2:D:241:CYS:HB2	2:D:250:ALA:HA	1.93	0.51
1:C:204:VAL:HG11	1:C:231:ILE:HD12	1.92	0.51
1:C:318:LEU:HD13	1:C:378:LEU:HD23	1.94	0.50
1:A:397:LEU:HD23	2:B:348:PRO:HG3	1.93	0.50
2:D:161:TYR:HB3	2:D:164:ARG:HG3	1.92	0.50
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.93	0.50
2:D:251:ASP:HB3	2:D:254:LYS:HB2	1.93	0.50
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.94	0.50
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.93	0.50
1:C:31:GLN:HB2	1:C:35:GLN:HB2	1.93	0.50
1:A:175:PRO:HA	1:A:179:THR:HG21	1.93	0.50
2:B:234:THR:O	2:B:238:VAL:HG23	2.11	0.50
1:A:140:SER:HA	1:A:171:ILE:HB	1.94	0.50
2:D:396:THR:O	2:D:400:ARG:HB2	2.11	0.50
1:C:242:LEU:HD11	1:C:252:LEU:HB3	1.94	0.50
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.94	0.49
2:D:153:LEU:O	2:D:157:ILE:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.94	0.49
2:B:63:PRO:HD3	2:B:86:ILE:HG22	1.95	0.49
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.94	0.49
2:B:286:LEU:HD11	2:B:291:LEU:HD13	1.95	0.49
2:D:175:PRO:HA	2:D:178:SER:HB3	1.95	0.49
1:C:259:LEU:HD11	1:C:316:CYS:HB2	1.95	0.49
2:B:41:ASP:HA	2:B:44:LEU:HD12	1.95	0.49
1:A:105:ARG:HA	1:A:109:THR:HG23	1.95	0.48
1:C:269:LEU:HD12	1:C:384:ILE:HD12	1.96	0.48
2:B:236:SER:HA	2:B:239:THR:OG1	2.13	0.48
2:D:2:ARG:HB2	2:D:131:CYS:CB	2.41	0.48
2:D:79:ARG:HA	2:D:84:GLY:HA3	1.94	0.48
3:E:66:ALA:HA	3:E:69:LEU:HD12	1.94	0.48
1:C:70:LEU:HD22	1:C:145:THR:HG22	1.96	0.48
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.94	0.48
8:C:503:VLB:C58	8:C:503:VLB:H511	2.40	0.48
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.96	0.47
1:C:136:LEU:HD22	1:C:169:PHE:HE1	1.79	0.47
2:D:291:LEU:HG	2:D:375:SER:HB2	1.95	0.47
1:C:196:GLU:CD	1:C:196:GLU:H	2.18	0.47
1:C:356:ASN:HD21	1:C:358:GLN:HB2	1.80	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.97	0.47
1:C:328:VAL:HG21	1:C:355:ILE:HD11	1.96	0.47
2:B:4:ILE:HD11	2:B:252:LEU:HD13	1.96	0.47
2:B:133:GLN:HE21	2:B:252:LEU:H	1.63	0.47
2:B:225:GLY:HA2	2:B:228:ASN:HB2	1.97	0.46
2:B:77:SER:H	2:B:79:ARG:HH21	1.64	0.46
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.96	0.46
1:C:206:ASN:HD21	4:C:501:GTP:N2	2.10	0.46
1:A:2:ARG:HG3	1:A:51:THR:HG22	1.97	0.46
2:B:22:GLU:HB3	2:B:83:PHE:HB2	1.98	0.46
1:A:219:ILE:HD12	1:A:222:PRO:HB3	1.96	0.46
1:A:317:LEU:HB2	1:A:353:VAL:HG13	1.98	0.46
7:D:501:GDP:H8	7:D:501:GDP:H5''	1.80	0.45
2:D:264:ARG:NH2	2:D:424:ASN:O	2.43	0.45
1:A:21:TRP:HA	1:A:24:TYR:HB2	1.97	0.45
1:A:145:THR:O	4:A:501:GTP:O2B	2.35	0.45
2:B:44:LEU:O	2:B:49:ILE:HG13	2.17	0.45
2:D:77:SER:H	2:D:79:ARG:HH21	1.65	0.45
2:B:48:ARG:HH22	2:B:250:ALA:HB1	1.82	0.45
1:C:314:ALA:HB3	1:C:380:ASN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASN:HD21	8:C:503:VLB:H66	1.62	0.45
1:A:167:LEU:HD12	1:A:200:CYS:HB3	1.98	0.45
1:A:90:GLU:C	1:A:121:ARG:HH12	2.20	0.45
2:B:243:ARG:HD2	2:B:243:ARG:N	2.32	0.45
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.99	0.45
2:D:157:ILE:HG13	2:D:166:MET:HE3	1.97	0.45
2:D:216:THR:HG21	2:D:275:LEU:HD13	1.99	0.45
1:C:88:HIS:HB2	1:C:89:PRO:HD2	1.98	0.45
2:D:227:LEU:O	2:D:230:LEU:HG	2.17	0.44
2:D:143:GLY:O	2:D:186:ASN:ND2	2.50	0.44
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.99	0.44
1:A:209:ILE:HD11	1:A:227:LEU:HG	2.00	0.44
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.99	0.44
2:D:205:ASP:CB	2:D:303:ALA:HA	2.48	0.44
2:B:350:ASN:HD22	2:B:350:ASN:H	1.65	0.44
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.99	0.44
1:C:286:LEU:HD21	1:C:291:ILE:HG23	1.99	0.44
2:D:274:PRO:HD2	2:D:371:LEU:HD23	1.99	0.44
2:D:176:LYS:HD2	2:D:207:GLU:HG3	1.98	0.44
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.98	0.44
2:D:350:ASN:H	2:D:350:ASN:HD22	1.66	0.44
2:B:238:VAL:HG22	2:B:378:ILE:HD11	1.99	0.44
3:E:106:GLU:O	3:E:110:GLU:HG3	2.18	0.44
2:B:68:VAL:HG22	2:B:93:VAL:HG13	2.00	0.44
2:B:350:ASN:HD22	2:B:350:ASN:N	2.16	0.44
1:C:239:THR:HB	1:C:243:ARG:HD3	2.01	0.43
1:A:31:GLN:O	1:A:33:ASP:N	2.51	0.43
2:D:228:ASN:HA	2:D:231:VAL:HB	2.00	0.43
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.36	0.43
2:B:205:ASP:CB	2:B:303:ALA:HA	2.48	0.43
1:C:10:GLY:O	1:C:14:VAL:HG22	2.18	0.43
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.99	0.43
1:C:241:SER:HA	1:C:249:ASN:ND2	2.32	0.43
2:B:105:LYS:HG3	2:B:110:GLU:HG2	2.00	0.43
3:E:74:GLU:HA	3:E:77:GLU:HG2	2.00	0.43
1:A:136:LEU:HD22	1:A:169:PHE:HE1	1.84	0.43
8:C:503:VLB:H692	8:C:503:VLB:H713	2.01	0.43
2:B:248:LEU:CG	2:B:249:ASN:H	2.30	0.43
1:C:195:LEU:HD12	1:C:264:ARG:HG2	2.00	0.43
2:D:115:VAL:HG22	2:D:119:LEU:HD23	2.01	0.43
2:B:48:ARG:NH2	2:B:250:ALA:HB1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:SER:HB3	2:B:30:ILE:HG13	2.00	0.43
1:C:180:ALA:O	1:C:183:GLU:HG3	2.19	0.43
1:C:180:ALA:HA	2:D:258:ASN:HD21	1.84	0.43
1:C:319:TYR:HB3	1:C:323:VAL:HG21	2.01	0.43
1:C:88:HIS:HB2	1:C:89:PRO:CD	2.49	0.43
1:C:118:VAL:O	1:C:122:ILE:HB	2.18	0.43
1:C:378:LEU:HD13	1:C:378:LEU:HA	1.85	0.43
1:C:228:ASN:HA	1:C:231:ILE:HG12	2.01	0.43
1:C:358:GLN:HA	1:C:359:PRO:HD3	1.95	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.19	0.43
2:D:350:ASN:HD22	2:D:350:ASN:N	2.17	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
3:E:78:HIS:O	3:E:81:GLU:HG3	2.19	0.42
1:C:155:GLU:HB3	3:E:101:LEU:HD11	2.01	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.42
1:C:255:PHE:HA	1:C:258:ASN:HD22	1.83	0.42
2:D:286:LEU:HD22	2:D:290:GLU:HB3	2.00	0.42
2:D:259:MET:HB3	2:D:268:PHE:CE2	2.53	0.42
1:A:12:ALA:O	1:A:16:ILE:HB	2.20	0.42
1:A:102:ASN:HD22	1:A:105:ARG:H	1.67	0.42
2:D:200:GLU:HB2	2:D:268:PHE:HE1	1.84	0.42
2:B:176:LYS:O	8:C:503:VLB:H222	2.20	0.42
2:D:62:VAL:HG23	2:D:86:ILE:O	2.19	0.42
1:C:102:ASN:HD22	1:C:105:ARG:H	1.67	0.42
1:A:206:ASN:HD21	4:A:501:GTP:N2	2.10	0.42
1:A:91:GLN:HA	1:A:121:ARG:NH1	2.35	0.42
2:D:172:MET:SD	2:D:205:ASP:HA	2.60	0.42
1:A:28:HIS:HD2	1:A:49:PHE:HB2	1.84	0.42
2:B:292:THR:HG21	2:B:331:GLN:HB3	2.01	0.42
2:B:240:THR:HG21	2:B:320:ARG:HD2	2.01	0.42
8:C:503:VLB:H582	8:C:503:VLB:C51	2.44	0.42
2:D:2:ARG:NH2	2:D:132:LEU:H	2.18	0.42
1:A:228:ASN:HA	1:A:231:ILE:HG12	2.01	0.42
1:A:143:GLY:O	1:A:147:SER:OG	2.32	0.42
2:D:132:LEU:HD23	2:D:164:ARG:HD3	2.01	0.42
1:A:182:VAL:O	1:A:185:TYR:HB2	2.20	0.42
2:B:19:LYS:HA	2:B:22:GLU:HG2	2.00	0.41
2:B:200:GLU:HB2	2:B:268:PHE:HE2	1.84	0.41
1:C:182:VAL:O	1:C:185:TYR:HB2	2.20	0.41
2:B:401:ARG:HH21	1:C:435:VAL:HG12	1.84	0.41
1:C:70:LEU:HD23	1:C:110:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:THR:HA	2:B:244:PHE:HD1	1.85	0.41
2:D:70:LEU:HB3	2:D:98:GLY:HA2	2.02	0.41
3:E:58:GLU:HG2	3:E:62:LYS:HD2	2.03	0.41
8:C:503:VLB:N1	8:C:503:VLB:H212	2.36	0.41
1:A:79:ARG:HG3	1:A:92:LEU:HD12	2.02	0.41
2:B:69:ASP:HB3	2:B:94:PHE:CD1	2.55	0.41
1:C:266:HIS:O	1:C:268:PRO:HD3	2.20	0.41
2:B:72:PRO:HA	2:B:75:MET:HG2	2.02	0.41
2:D:306:ASP:HB3	2:D:309:HIS:CG	2.55	0.41
1:A:313:MET:HE3	1:A:313:MET:HB3	1.91	0.41
2:D:136:GLN:HA	2:D:167:ASN:O	2.21	0.41
2:D:129:CYS:HB3	2:D:131:CYS:O	2.21	0.41
2:B:416:MET:O	2:B:420:GLU:HG3	2.21	0.41
8:C:503:VLB:C14	8:C:503:VLB:H52	2.51	0.41
1:C:188:ILE:HD13	1:C:395:PHE:HB2	2.02	0.41
2:B:136:GLN:HA	2:B:167:ASN:O	2.21	0.41
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.03	0.41
1:C:335:ILE:HD11	1:C:351:PHE:CZ	2.56	0.41
2:D:88:ARG:HB2	2:D:91:ASN:OD1	2.21	0.41
2:B:259:MET:HB3	2:B:268:PHE:CE1	2.56	0.41
1:A:346:TRP:HB3	3:E:29:PHE:HD2	1.85	0.41
2:B:194:LEU:HD23	2:B:198:THR:HG21	2.02	0.41
1:C:224:TYR:HA	1:C:227:LEU:HB2	2.03	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.41
2:D:311:ARG:H	2:D:382:THR:HG1	1.69	0.41
1:A:188:ILE:HD13	1:A:395:PHE:HB2	2.02	0.40
1:C:259:LEU:O	1:C:261:PRO:HD3	2.21	0.40
2:D:194:LEU:HD23	2:D:198:THR:HG21	2.02	0.40
2:B:69:ASP:HA	2:B:145:THR:HG21	2.03	0.40
1:A:115:ILE:O	1:A:119:LEU:HD13	2.22	0.40
2:B:172:MET:SD	2:B:205:ASP:HA	2.61	0.40
1:A:224:TYR:HA	1:A:227:LEU:HB2	2.03	0.40
1:C:285:GLN:O	1:C:286:LEU:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/451 (95%)	374 (87%)	43 (10%)	13 (3%)	5	41
1	C	432/451 (96%)	382 (88%)	35 (8%)	15 (4%)	4	38
2	B	432/445 (97%)	380 (88%)	38 (9%)	14 (3%)	5	40
2	D	431/445 (97%)	385 (89%)	33 (8%)	13 (3%)	5	41
3	E	129/142 (91%)	114 (88%)	13 (10%)	2 (2%)	12	54
All	All	1854/1934 (96%)	1635 (88%)	162 (9%)	57 (3%)	5	41

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	89	PRO
1	A	179	THR
1	A	245	ASP
2	B	215	ARG
2	B	359	PRO
1	C	240	ALA
1	C	379	SER
1	C	437	VAL
2	D	369	ARG
3	E	11	LEU
1	A	2	ARG
1	A	3	GLU
1	A	178	SER
2	B	82	PRO
2	B	109	THR
2	B	224	TYR
2	B	372	LYS
1	C	109	THR
1	C	239	THR
1	C	284	GLU

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Mol	Chain	Res	Type
1	C	286	LEU
1	C	322	ASP
1	C	348	PRO
2	D	84	GLY
2	D	97	SER
2	D	109	THR
1	A	280	LYS
2	B	84	GLY
2	B	295	MET
2	D	281	GLN
2	D	285	ALA
2	B	57	THR
2	B	286	LEU
2	B	304	ALA
2	B	358	ILE
1	C	280	LYS
2	D	50	ASN
2	D	249	ASN
2	D	283	TYR
2	D	294	GLN
2	D	304	ALA
2	D	360	PRO
3	E	46	SER
1	A	338	LYS
1	A	387	ALA
2	B	250	ALA
1	C	342	GLN
1	C	349	THR
2	D	57	THR
1	A	260	VAL
1	C	438	ASP
1	A	72	PRO
1	C	72	PRO
1	C	131	GLY
2	B	29	GLY
1	A	212	ILE

### 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%)	295 (80%)	73 (20%)	1	9
1	C	370/379 (98%)	311 (84%)	59 (16%)	3	18
2	B	375/385 (97%)	313 (84%)	62 (16%)	3	16
2	D	374/385 (97%)	313 (84%)	61 (16%)	3	17
3	E	114/125 (91%)	89 (78%)	25 (22%)	1	6
All	All	1601/1653 (97%)	1321 (82%)	280 (18%)	2	13

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	6	SER
1	A	16	ILE
1	A	18	ASN
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	33	ASP
1	A	35	GLN
1	A	47	ASP
1	A	50	ASN
1	A	71	GLU
1	A	73	THR
1	A	77	GLU
1	A	78	VAL
1	A	84	ARG
1	A	90	GLU
1	A	91	GLN
1	A	94	THR
1	A	102	ASN
1	A	109	THR
1	A	113	GLU
1	A	114	ILE
1	A	119	LEU
1	A	120	ASP
1	A	121	ARG
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	141	PHE
1	A	153	LEU
1	A	155	GLU
1	A	160	ASP
1	A	163	LYS
1	A	167	LEU
1	A	182	VAL
1	A	188	ILE
1	A	191	THR
1	A	209	ILE
1	A	215	ARG
1	A	217	LEU
1	A	223	THR
1	A	233	GLN
1	A	248	LEU
1	A	256	GLN
1	A	258	ASN
1	A	266	HIS
1	A	275	VAL
1	A	280	LYS
1	A	291	ILE
1	A	293	ASN
1	A	296	PHE
1	A	302	MET
1	A	315	CYS
1	A	323	VAL
1	A	324	VAL
1	A	326	LYS
1	A	336	LYS
1	A	339	ARG
1	A	341	ILE
1	A	342	GLN
1	A	347	CYS
1	A	351	PHE
1	A	355	ILE
1	A	356	ASN
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	373	ARG
1	A	384	ILE
1	A	386	GLU

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Mol	Chain	Res	Type
1	A	401	LYS
1	A	424	ASP
1	A	435	VAL
2	B	3	GLU
2	B	4	ILE
2	B	15	GLN
2	B	20	PHE
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	47	GLU
2	B	48	ARG
2	B	54	ASN
2	B	55	GLU
2	B	60	LYS
2	B	74	THR
2	B	75	MET
2	B	79	ARG
2	B	97	SER
2	B	105	LYS
2	B	113	GLU
2	B	119	LEU
2	B	133	GLN
2	B	147	SER
2	B	158	ARG
2	B	168	THR
2	B	172	MET
2	B	179	ASP
2	B	194	LEU
2	B	209	LEU
2	B	213	CYS
2	B	217	LEU
2	B	219	LEU
2	B	224	TYR
2	B	226	ASP
2	B	230	LEU
2	B	242	LEU
2	B	248	LEU
2	B	260	VAL
2	B	284	ARG
2	B	290	GLU
2	B	294	GLN

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Mol	Chain	Res	Type
2	B	295	MET
2	B	297	ASP
2	B	311	ARG
2	B	313	LEU
2	B	322	ARG
2	B	326	LYS
2	B	328	VAL
2	B	332	MET
2	B	333	LEU
2	B	336	GLN
2	B	338	LYS
2	B	349	ASN
2	B	350	ASN
2	B	352	LYS
2	B	353	THR
2	B	355	VAL
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	377	PHE
2	B	401	ARG
2	B	415	GLU
2	B	420	GLU
1	C	1	MET
1	C	6	SER
1	C	16	ILE
1	C	18	ASN
1	C	25	CYS
1	C	26	LEU
1	C	30	ILE
1	C	49	PHE
1	C	52	PHE
1	C	53	PHE
1	C	60	LYS
1	C	62	VAL
1	C	64	ARG
1	C	71	GLU
1	C	73	THR
1	C	84	ARG
1	C	88	HIS
1	C	94	THR
1	C	102	ASN

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Mol	Chain	Res	Type
1	C	114	ILE
1	C	121	ARG
1	C	122	ILE
1	C	132	LEU
1	C	141	PHE
1	C	153	LEU
1	C	160	ASP
1	C	163	LYS
1	C	167	LEU
1	C	182	VAL
1	C	188	ILE
1	C	191	THR
1	C	195	LEU
1	C	196	GLU
1	C	217	LEU
1	C	223	THR
1	C	233	GLN
1	C	248	LEU
1	C	269	LEU
1	C	279	GLU
1	C	280	LYS
1	C	284	GLU
1	C	286	LEU
1	C	291	ILE
1	C	293	ASN
1	C	297	GLU
1	C	301	GLN
1	C	302	MET
1	C	315	CYS
1	C	323	VAL
1	C	335	ILE
1	C	343	PHE
1	C	368	LEU
1	C	370	LYS
1	C	377	MET
1	C	378	LEU
1	C	380	ASN
1	C	384	ILE
1	C	401	LYS
1	C	424	ASP
2	D	1	MET
2	D	2	ARG

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Mol	Chain	Res	Type
2	D	4	ILE
2	D	24	ILE
2	D	39	ASP
2	D	42	LEU
2	D	44	LEU
2	D	48	ARG
2	D	49	ILE
2	D	60	LYS
2	D	64	ARG
2	D	70	LEU
2	D	71	GLU
2	D	74	THR
2	D	79	ARG
2	D	85	GLN
2	D	91	ASN
2	D	93	VAL
2	D	110	GLU
2	D	113	GLU
2	D	123	ARG
2	D	124	LYS
2	D	127	GLU
2	D	135	PHE
2	D	158	ARG
2	D	164	ARG
2	D	168	THR
2	D	172	MET
2	D	194	LEU
2	D	209	LEU
2	D	212	ILE
2	D	218	LYS
2	D	223	THR
2	D	224	TYR
2	D	247	GLN
2	D	260	VAL
2	D	275	LEU
2	D	284	ARG
2	D	287	THR
2	D	288	VAL
2	D	291	LEU
2	D	292	THR
2	D	293	GLN
2	D	313	LEU

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Mol	Chain	Res	Type
2	D	326	LYS
2	D	327	GLU
2	D	328	VAL
2	D	336	GLN
2	D	345	GLU
2	D	349	ASN
2	D	350	ASN
2	D	352	LYS
2	D	353	THR
2	D	355	VAL
2	D	369	ARG
2	D	372	LYS
2	D	377	PHE
2	D	400	ARG
2	D	402	LYS
2	D	416	MET
2	D	419	THR
3	E	9	ILE
3	E	11	LEU
3	E	25	LYS
3	E	47	LEU
3	E	60	ARG
3	E	67	GLU
3	E	68	LEU
3	E	74	GLU
3	E	76	ARG
3	E	81	GLU
3	E	82	VAL
3	E	84	GLN
3	E	88	GLU
3	E	89	GLU
3	E	92	ASN
3	E	101	LEU
3	E	104	LYS
3	E	110	GLU
3	E	111	ASN
3	E	112	ARG
3	E	116	LEU
3	E	123	LEU
3	E	127	ASP
3	E	128	LYS
3	E	134	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	35	GLN
1	A	101	ASN
1	A	102	ASN
1	A	206	ASN
1	A	285	GLN
1	A	356	ASN
1	A	358	GLN
1	A	380	ASN
2	B	14	ASN
2	B	50	ASN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	249	ASN
2	B	258	ASN
2	B	331	GLN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	436	GLN
1	C	8	HIS
1	C	11	GLN
1	C	101	ASN
1	C	102	ASN
1	C	139	HIS
1	C	206	ASN
1	C	249	ASN
1	C	293	ASN
1	C	356	ASN
2	D	14	ASN
2	D	15	GLN
2	D	85	GLN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	186	ASN
2	D	258	ASN
2	D	334	ASN
2	D	350	ASN
2	D	380	ASN

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Mol	Chain	Res	Type
2	D	385	GLN
2	D	436	GLN
3	E	90	ASN
3	E	91	ASN
3	E	115	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z  > 2$
4	GTP	A	501	5	25,34,34	1.51	5 (20%)	34,54,54	2.20	10 (29%)
6	SO4	A	503	-	4,4,4	0.21	0	6,6,6	0.06	0
6	SO4	A	504	-	4,4,4	0.08	0	6,6,6	0.09	0
7	GDP	B	501	-	23,30,30	1.50	3 (13%)	30,47,47	1.90	7 (23%)
6	SO4	B	502	-	4,4,4	0.10	0	6,6,6	0.10	0
4	GTP	C	501	5	25,34,34	1.53	3 (12%)	34,54,54	2.12	10 (29%)
8	VLB	C	503	-	62,67,67	1.63	10 (16%)	77,108,108	2.43	22 (28%)
7	GDP	D	501	-	23,30,30	1.84	5 (21%)	30,47,47	2.14	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	D	502	-	4,4,4	0.10	0	6,6,6	0.08	0
6	SO4	D	503	-	4,4,4	0.07	0	6,6,6	0.08	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
4	GTP	A	501	5	-	0/18/38/38	0/3/3/3
6	SO4	A	503	-	-	0/0/0/0	0/0/0/0
6	SO4	A	504	-	-	0/0/0/0	0/0/0/0
7	GDP	B	501	-	-	0/12/32/32	0/3/3/3
6	SO4	B	502	-	-	0/0/0/0	0/0/0/0
4	GTP	C	501	5	-	0/18/38/38	0/3/3/3
8	VLB	C	503	-	-	0/38/131/131	0/7/9/9
7	GDP	D	501	-	-	0/12/32/32	0/3/3/3
6	SO4	D	502	-	-	0/0/0/0	0/0/0/0
6	SO4	D	503	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	503	VLB	C8-C7	-4.93	1.39	1.49
8	C	503	VLB	C5-C6	-4.44	1.42	1.51
7	D	501	GDP	C8-N7	-2.83	1.29	1.34
8	C	503	VLB	C18-N1	-2.65	1.34	1.39
8	C	503	VLB	C30-C29	-2.31	1.41	1.49
4	A	501	GTP	C8-N7	-2.17	1.30	1.34
4	C	501	GTP	C8-N7	-2.04	1.30	1.34
4	A	501	GTP	C2-N2	2.03	1.38	1.34
4	C	501	GTP	C2-N2	2.03	1.38	1.34
7	B	501	GDP	PB-O2B	2.05	1.62	1.54
4	A	501	GTP	C2-N1	2.09	1.39	1.35
8	C	503	VLB	C63-C64	2.16	1.41	1.36
4	A	501	GTP	C6-N1	2.18	1.37	1.33
7	D	501	GDP	PB-O3B	2.19	1.62	1.54
8	C	503	VLB	O25-C23	2.19	1.37	1.33
7	D	501	GDP	C2-N2	2.55	1.39	1.34
7	B	501	GDP	C6-N1	2.63	1.38	1.33
8	C	503	VLB	O75-C73	2.66	1.38	1.33
7	D	501	GDP	PB-O2B	2.72	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	503	VLB	C16-C15	2.95	1.44	1.39
8	C	503	VLB	C68-C67	3.19	1.57	1.53
4	A	501	GTP	O4'-C1'	3.92	1.46	1.41
4	C	501	GTP	O4'-C1'	4.11	1.46	1.41
7	B	501	GDP	O4'-C1'	4.13	1.46	1.41
8	C	503	VLB	C6-C7	4.16	1.41	1.32
7	D	501	GDP	O4'-C1'	5.21	1.47	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	503	VLB	C33-O32-C16	-6.14	108.23	117.54
8	C	503	VLB	O32-C16-C17	-5.86	114.21	124.21
4	A	501	GTP	PA-O3A-PB	-5.40	117.58	132.73
4	C	501	GTP	PA-O3A-PB	-5.34	117.74	132.73
4	A	501	GTP	PB-O3B-PG	-5.00	115.89	132.67
7	D	501	GDP	N3-C2-N1	-4.97	119.88	127.44
4	C	501	GTP	PB-O3B-PG	-4.79	116.60	132.67
7	B	501	GDP	PA-O3A-PB	-4.79	116.61	132.67
7	D	501	GDP	PA-O3A-PB	-4.49	117.62	132.67
4	A	501	GTP	N3-C2-N1	-4.35	120.81	127.44
4	C	501	GTP	N3-C2-N1	-4.27	120.94	127.44
8	C	503	VLB	C22-N1-C2	-4.26	108.60	119.52
7	B	501	GDP	N3-C2-N1	-4.20	121.05	127.44
7	B	501	GDP	C5-C6-N1	-4.17	117.88	123.59
4	A	501	GTP	C5-C6-N1	-4.09	118.00	123.59
7	D	501	GDP	C5-C6-N1	-3.85	118.33	123.59
8	C	503	VLB	C22-N1-C18	-3.69	107.82	120.95
7	D	501	GDP	C2'-C1'-N9	-3.68	108.66	114.29
8	C	503	VLB	C17-C18-C13	-3.60	117.67	122.03
4	A	501	GTP	C4-C5-N7	-3.37	106.38	109.48
4	C	501	GTP	C4-C5-N7	-3.31	106.43	109.48
4	C	501	GTP	C6-C5-C4	-3.14	117.15	120.90
4	C	501	GTP	C5-C6-N1	-3.13	119.31	123.59
7	B	501	GDP	C4-C5-N7	-3.09	106.64	109.48
4	C	501	GTP	C1'-N9-C4	-2.86	122.63	126.94
8	C	503	VLB	C13-C12-C19	-2.73	105.62	115.13
4	A	501	GTP	C1'-N9-C4	-2.61	123.00	126.94
4	A	501	GTP	C6-C5-C4	-2.58	117.81	120.90
8	C	503	VLB	O74-C73-C68	-2.53	117.77	124.02
7	D	501	GDP	C4-C5-N7	-2.43	107.25	109.48
8	C	503	VLB	O28-C29-O31	-2.38	118.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	501	GDP	C6-C5-C4	-2.35	118.09	120.90
8	C	503	VLB	C76-O75-C73	-2.31	111.95	116.00
4	C	501	GTP	C4'-O4'-C1'	-2.20	107.30	109.72
7	B	501	GDP	C6-C5-C4	-2.17	118.30	120.90
8	C	503	VLB	O75-C73-O74	-2.13	120.14	123.90
8	C	503	VLB	C8-N9-C10	-2.08	110.59	116.36
4	A	501	GTP	O2G-PG-O3B	2.00	114.18	105.09
8	C	503	VLB	O28-C4-C3	2.05	109.43	106.44
8	C	503	VLB	C14-C13-C18	2.06	122.06	120.25
8	C	503	VLB	C52-C69-N56	2.12	113.54	110.71
7	D	501	GDP	N2-C2-N3	2.18	121.98	117.80
7	D	501	GDP	O3A-PA-O5'	2.41	109.33	102.94
7	B	501	GDP	O3A-PA-O5'	2.43	109.37	102.94
8	C	503	VLB	C2-C12-C19	2.54	118.66	114.10
8	C	503	VLB	C17-C18-N1	2.75	130.25	127.44
4	C	501	GTP	O3A-PA-O5'	2.84	110.47	102.94
4	A	501	GTP	O3A-PA-O5'	3.01	110.91	102.94
8	C	503	VLB	O25-C23-C3	3.39	118.24	112.65
4	C	501	GTP	C6-N1-C2	3.45	120.72	115.94
8	C	503	VLB	C69-N56-C55	3.65	116.05	110.89
7	B	501	GDP	C6-N1-C2	3.84	121.27	115.94
4	A	501	GTP	C6-N1-C2	4.02	121.52	115.94
8	C	503	VLB	C53-C54-C55	4.43	115.10	109.22
7	D	501	GDP	C6-N1-C2	4.85	122.67	115.94
8	C	503	VLB	O28-C29-C30	6.57	123.50	111.10
8	C	503	VLB	O32-C16-C15	7.29	124.78	116.16
8	C	503	VLB	O75-C73-C68	8.71	122.08	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GTP	4	0
4	C	501	GTP	3	0
8	C	503	VLB	13	0
7	D	501	GDP	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	433/451 (96%)	0.94	79 (18%) 2 2	125, 187, 248, 265	0
1	C	432/451 (95%)	0.70	51 (11%) 6 6	105, 169, 233, 267	0
2	B	432/445 (97%)	0.74	61 (14%) 4 4	107, 165, 243, 269	2 (0%)
2	D	432/445 (97%)	0.54	40 (9%) 11 10	73, 142, 234, 251	2 (0%)
3	E	132/142 (92%)	1.04	26 (19%) 1 2	139, 209, 254, 266	0
All	All	1861/1934 (96%)	0.75	257 (13%) 4 4	73, 170, 244, 269	4 (0%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	HIS	11.3
1	A	313	MET	8.2
3	E	22	VAL	7.6
2	B	274	PRO	7.4
3	E	23	ILE	7.2
2	B	61	TYR	7.0
1	A	438	ASP	7.0
1	C	62	VAL	6.5
2	B	28	HIS	5.9
1	C	60	LYS	5.7
2	D	53	TYR	5.6
3	E	34	GLU	5.5
1	A	349	THR	5.5
2	D	62	VAL	5.4
3	E	18	GLN	5.4
1	A	347	CYS	5.4
1	A	348	PRO	5.4
2	B	359	PRO	5.3
3	E	8	VAL	5.2
1	A	369	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	5.2
1	C	55	GLU	5.2
1	A	32	PRO	5.1
2	B	55	GLU	4.9
2	B	295	MET	4.9
1	C	253	THR	4.9
3	E	6	MET	4.9
1	A	346	TRP	4.8
2	B	375	SER	4.8
2	D	28	HIS	4.8
3	E	33	PRO	4.8
1	A	312	TYR	4.8
2	D	61	TYR	4.8
1	A	439	SER	4.7
2	D	80	SER	4.6
2	D	99	ALA	4.6
2	B	86	ILE	4.3
2	D	413	MET	4.3
3	E	13	LYS	4.2
2	B	249	ASN	4.2
3	E	24	LEU	4.1
2	B	216	THR	4.1
2	D	32	PRO	4.1
2	B	49	ILE	4.1
2	D	63	PRO	4.1
2	B	84	GLY	4.0
2	D	36	TYR	4.0
2	D	34	GLY	3.9
2	B	374	SER	3.9
3	E	7	GLU	3.9
1	A	170	SER	3.9
3	E	19	SER	3.9
3	E	32	VAL	3.8
2	B	371	LEU	3.8
2	B	273	ALA	3.8
1	C	346	TRP	3.8
2	D	87	PHE	3.8
2	D	59	ASN	3.8
1	A	345	ASP	3.8
1	A	220	GLU	3.8
1	A	311	LYS	3.7
1	C	296	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	293	GLN	3.7
1	A	413	MET	3.7
1	A	28	HIS	3.7
2	B	284	ARG	3.6
1	C	120[A]	ASP	3.6
1	A	381	THR	3.6
1	A	139	HIS	3.6
1	A	37	PRO	3.5
2	D	37	HIS	3.5
2	B	373	MET	3.5
2	B	372	LYS	3.5
2	D	91	ASN	3.5
1	A	319	TYR	3.5
2	B	358	ILE	3.5
1	A	62	VAL	3.4
1	A	35	GLN	3.4
2	D	83	PHE	3.4
2	B	27	GLU	3.4
1	A	435	VAL	3.4
1	A	274	PRO	3.4
1	A	282	TYR	3.4
1	A	440	VAL	3.4
2	B	62	VAL	3.3
1	A	83	TYR	3.3
2	D	408	TYR	3.3
2	D	30	ILE	3.3
2	B	83	PHE	3.3
1	A	247	ALA	3.3
1	C	364	PRO	3.3
2	B	59	ASN	3.2
2	B	442	GLU	3.2
3	E	135	LYS	3.2
1	C	36	MET	3.2
1	A	103	TYR	3.2
1	A	80	THR	3.2
3	E	41	ARG	3.2
2	B	369	ARG	3.2
1	A	343	PHE	3.1
1	C	276	ILE	3.1
1	C	277	SER	3.1
2	D	296	PHE	3.1
2	B	283	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	37	PRO	3.1
1	A	248	LEU	3.1
2	B	275	LEU	3.1
1	A	86	LEU	3.1
1	C	115	ILE	3.0
2	B	56	ALA	3.0
1	A	323	VAL	3.0
1	A	428	LEU	3.0
1	A	13	GLY	3.0
3	E	20	TRP	3.0
1	C	370	LYS	3.0
1	C	437	VAL	3.0
3	E	11	LEU	3.0
2	D	29	GLY	2.9
2	D	56	ALA	2.9
2	D	33	THR	2.9
1	C	54	SER	2.9
3	E	10	GLU	2.9
1	A	178	SER	2.9
2	B	319	PHE	2.9
2	B	53	TYR	2.9
1	C	365	GLY	2.9
1	A	355	ILE	2.8
1	A	179	THR	2.8
1	C	199	ASP	2.8
2	B	241	CYS	2.8
2	B	244	PHE	2.8
2	D	60	LYS	2.8
2	B	401	ARG	2.8
2	B	100	GLY	2.8
3	E	12	ASN	2.8
3	E	21	GLU	2.7
1	A	350	GLY	2.7
2	B	301	MET	2.7
2	B	412	GLY	2.7
2	D	86	ILE	2.7
2	B	37	HIS	2.7
1	A	357	TYR	2.7
1	C	274	PRO	2.7
1	C	222	PRO	2.7
1	C	256	GLN	2.7
2	D	98	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	220	GLU	2.7
2	B	248	LEU	2.7
2	D	258	ASN	2.7
1	C	219	ILE	2.7
1	A	29	GLY	2.7
1	A	432	TYR	2.6
1	C	351	PHE	2.6
3	E	27	PRO	2.6
2	B	377	PHE	2.6
1	C	168	GLU	2.6
1	C	64	ARG	2.6
3	E	14	ALA	2.6
1	C	63	PRO	2.6
1	C	179	THR	2.6
2	B	370	GLY	2.5
2	B	30	ILE	2.5
2	B	323	MET	2.5
2	D	67	LEU	2.5
1	A	204	VAL	2.5
1	A	108	TYR	2.5
1	C	254	GLU	2.5
2	B	321	GLY	2.5
2	B	296	PHE	2.5
1	A	31	GLN	2.5
1	A	53	PHE	2.5
2	B	29	GLY	2.5
2	B	87	PHE	2.5
2	B	322	ARG	2.5
3	E	136	ASN	2.5
1	C	338	LYS	2.5
1	C	362	VAL	2.4
1	C	374	ALA	2.4
1	A	85	GLN	2.4
1	A	288	VAL	2.4
1	A	326	LYS	2.4
1	A	17	GLY	2.4
1	A	388	TRP	2.4
2	B	47	GLU	2.4
1	A	82	THR	2.4
1	C	133	GLN	2.4
1	A	104	ALA	2.4
2	B	215	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	140	SER	2.4
1	A	324	VAL	2.4
1	C	372	GLN	2.3
3	E	45	PRO	2.3
1	A	351	PHE	2.3
2	D	39	ASP	2.3
2	D	103	TRP	2.3
1	A	228	ASN	2.3
2	D	54	ASN	2.3
1	A	15	GLN	2.3
1	A	30	ILE	2.3
2	B	60	LYS	2.3
1	A	314	ALA	2.3
2	B	441	ASP	2.3
2	B	168	THR	2.3
1	C	285	GLN	2.3
3	E	31	GLY	2.3
1	A	382	THR	2.3
3	E	46	SER	2.3
1	A	218	ASP	2.3
2	D	399	PHE	2.3
2	B	413	MET	2.2
2	B	91	ASN	2.2
2	B	258	ASN	2.2
1	C	35	GLN	2.2
1	C	281	ALA	2.2
1	A	60	LYS	2.2
1	C	53	PHE	2.2
2	D	249	ASN	2.2
1	C	85	GLN	2.2
2	B	278	ARG	2.2
1	C	56	THR	2.2
2	D	442	GLU	2.2
1	A	436	GLY	2.2
2	D	279	GLY	2.2
2	B	290	GLU	2.2
1	C	369	ALA	2.2
1	A	33	ASP	2.2
2	D	102	ASN	2.2
1	A	188	ILE	2.2
2	D	328	VAL	2.2
1	A	373	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	245	PRO	2.1
1	C	251	ASP	2.1
2	B	52	TYR	2.1
1	A	36	MET	2.1
1	C	371	VAL	2.1
1	C	300	ASN	2.1
2	D	287	THR	2.1
1	A	219	ILE	2.1
1	A	353	VAL	2.1
1	A	194	THR	2.1
2	B	292	THR	2.1
1	A	11	GLN	2.1
1	A	362	VAL	2.1
1	C	1	MET	2.1
1	C	214	ARG	2.1
1	A	138	PHE	2.1
2	B	360	PRO	2.1
2	D	307	PRO	2.1
1	A	8	HIS	2.1
1	C	360	PRO	2.1
2	D	342	TYR	2.0
1	C	28	HIS	2.0
1	A	180	ALA	2.0
3	E	9	ILE	2.0
1	C	210	TYR	2.0
1	C	83	TYR	2.0
1	A	6	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	D	502	5/5	0.80	0.48	2.28	219,223,224,224	0
6	SO4	A	504	5/5	0.66	0.48	1.81	246,250,251,251	0
6	SO4	D	503	5/5	0.85	0.23	-0.28	159,164,165,165	0
4	GTP	A	501	32/32	0.97	0.31	-0.33	140,148,158,159	0
4	GTP	C	501	32/32	0.95	0.28	-0.34	134,138,144,149	0
8	VLB	C	503	59/59	0.90	0.26	-0.35	154,159,166,170	0
7	GDP	D	501	28/28	0.97	0.16	-0.99	113,117,125,130	0
7	GDP	B	501	28/28	0.98	0.21	-1.04	126,131,138,140	0
6	SO4	A	503	5/5	0.67	0.45	-	232,237,238,238	0
6	SO4	B	502	5/5	0.84	0.19	-	243,248,249,249	0
5	MG	C	502	1/1	0.98	0.22	-	121,121,121,121	0
5	MG	A	502	1/1	0.98	0.30	-	116,116,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.