



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:44 PM GMT

PDB ID : 3UT5  
Title : Tubulin-Colchicine-Ustiloxin: Stathmin-like domain complex  
Authors : Ranaivoson, F.M.; Gigant, B.; Knossow, M.  
Deposited on : 2011-11-25  
Resolution : 2.73 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

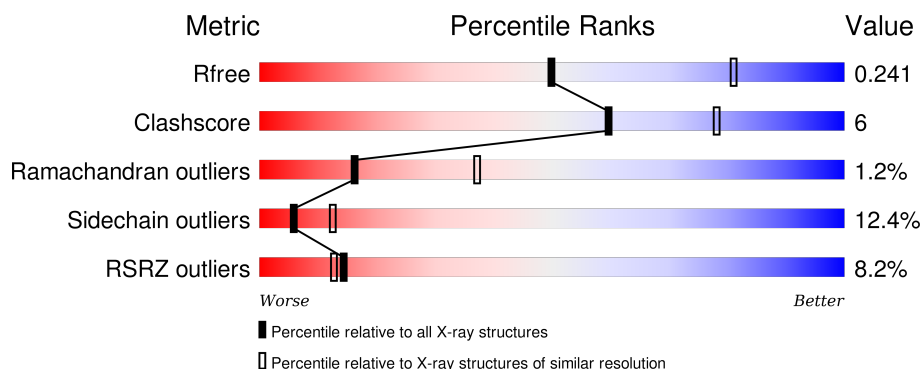
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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>8%</div> <div>77%</div> <div>16%</div> <div>• •</div> </div>
1	C	451	<div> <div>4%</div> <div>74%</div> <div>20%</div> <div>• •</div> </div>
2	B	445	<div> <div>12%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
2	D	445	<div> <div>6%</div> <div>76%</div> <div>16%</div> <div>• •</div> </div>
3	E	142	<div> <div>14%</div> <div>73%</div> <div>18%</div> <div>• 7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	4	

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
4	0E5	F	3	X	-	-	-
7	SO4	D	503	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15107 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
			3404	2158	575	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	3	0
			3417	2141	584	665	27			
2	D	432	Total	C	N	O	S	0	5	0
			3433	2153	584	670	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
			1077	666	195	212	4			

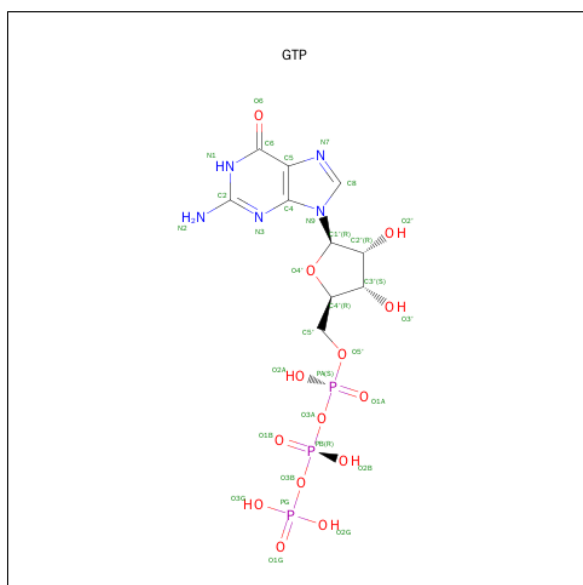
There are 3 discrepancies between the modelled and reference sequences:

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 a protein called Vinca tetrapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	0	0	0
			35	23	4	8			

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

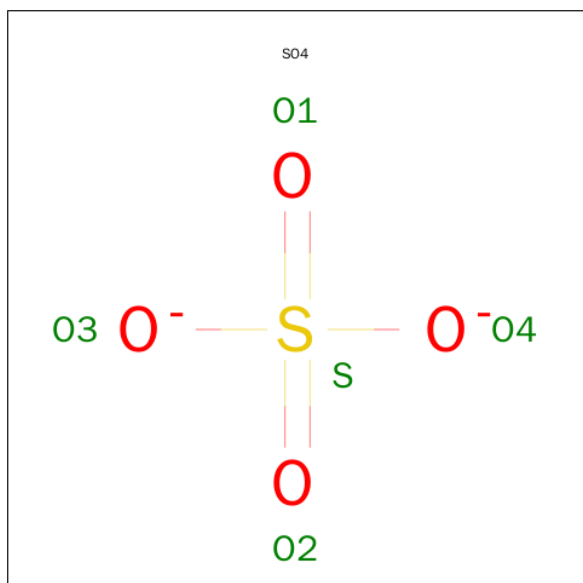


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

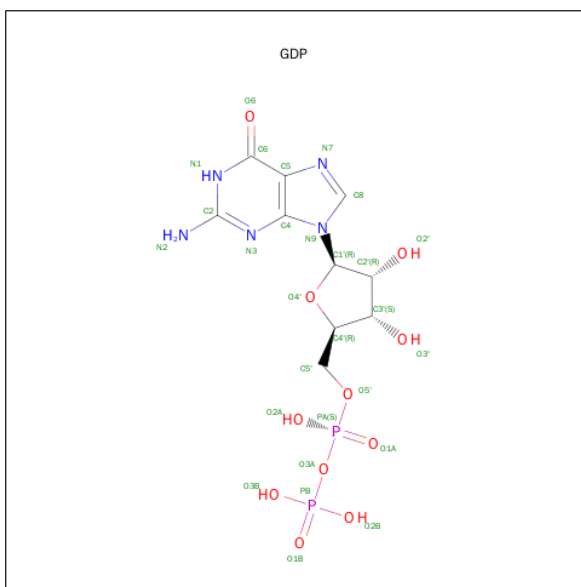
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



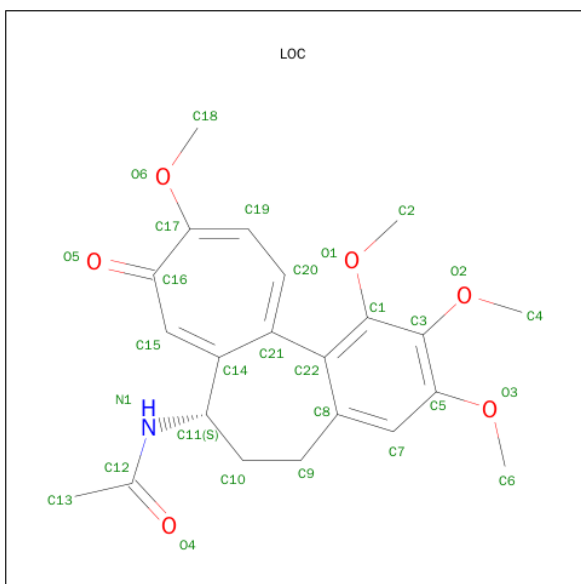
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 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
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 N-[(7S)-1,2,3,10-TETRAMETHOXY-9-OXO-6,7-DIHYDRO-5H-BENZO[D]H EPTALEN-7-YL]ETHANAMIDE (three-letter code: LOC) (formula:  $C_{22}H_{25}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			29	22	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 10 is water.

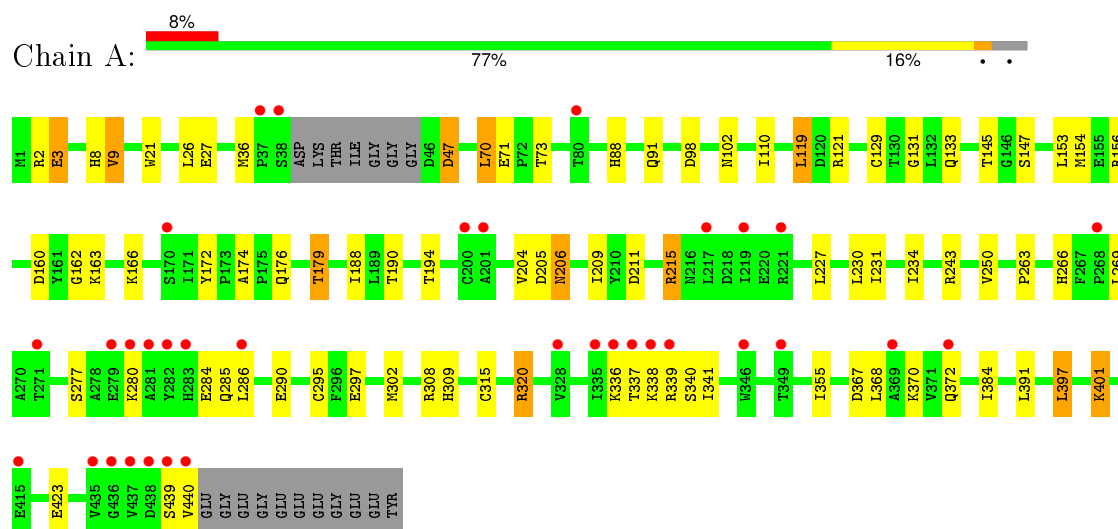
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	27	Total	O	0	0
			27	27		
10	B	28	Total	O	0	0
			28	28		
10	C	43	Total	O	0	0
			43	43		
10	D	36	Total	O	0	0
			36	36		
10	E	3	Total	O	0	0
			3	3		



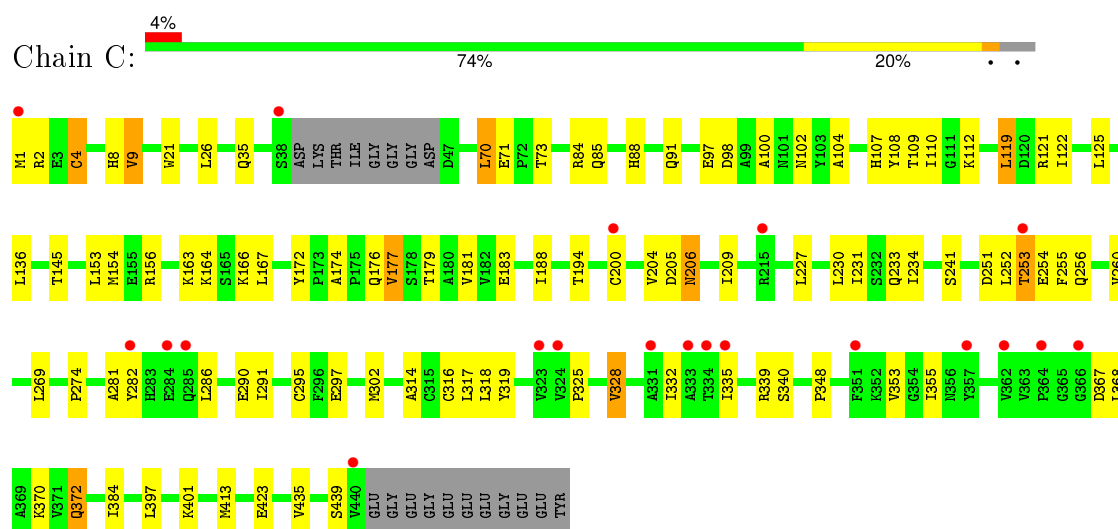
### 3 Residue-property plots [i](#)

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.

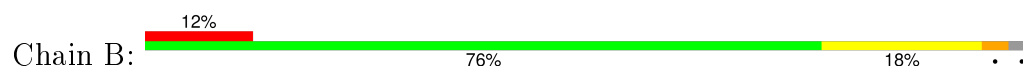
#### • Molecule 1: Tubulin alpha chain

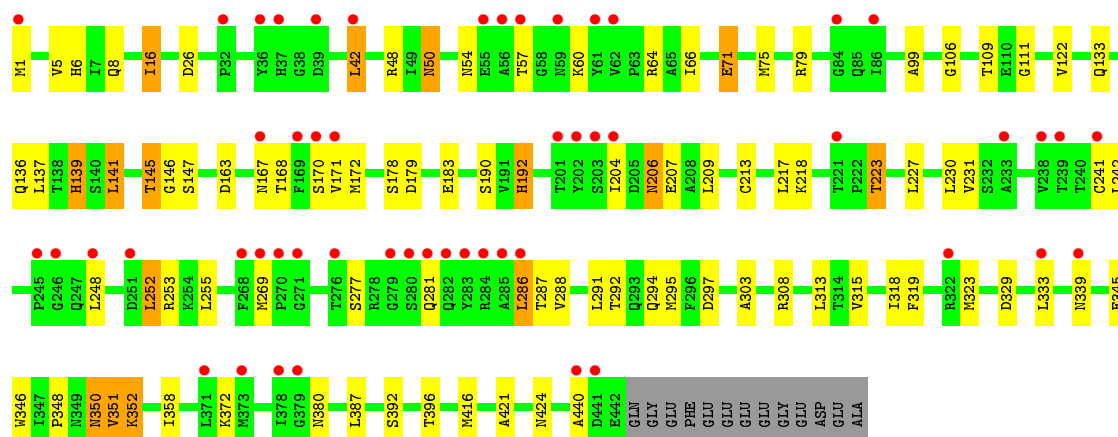


#### • Molecule 1: Tubulin alpha chain

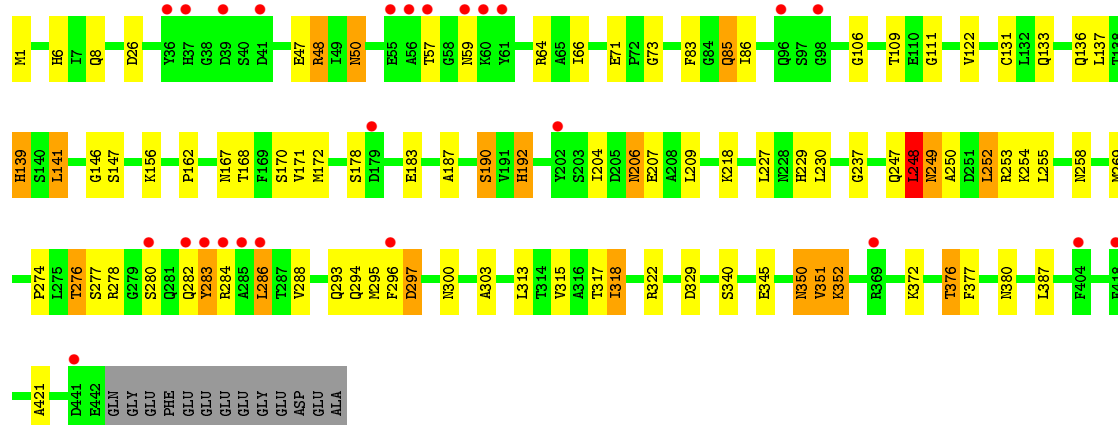
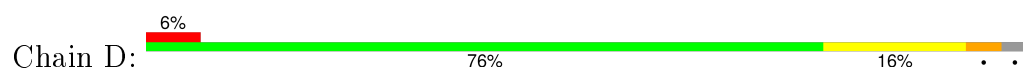


#### • Molecule 2: Tubulin beta chain

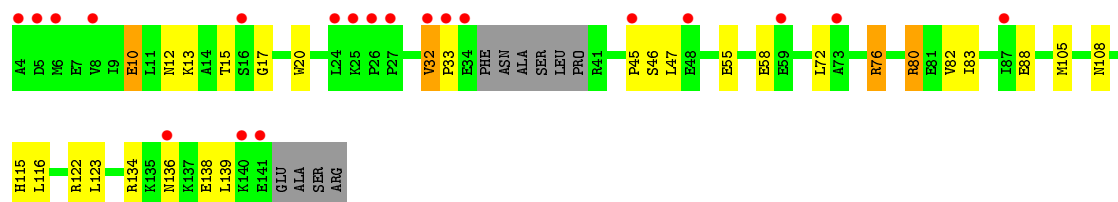




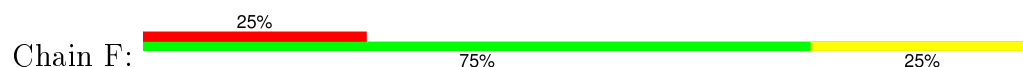
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Vinca tetrapeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.81Å 128.87Å 254.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.26 – 2.73 38.26 – 2.73	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.26-2.73) 97.6 (38.26-2.73)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.72Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.184 , 0.222 0.201 , 0.241	Depositor DCC
$R_{free}$ test set	2872 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 56364 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15107	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, LOC, MG, 0E5, GTP, SO4, 0EA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/3479	0.68	0/4723
1	C	0.45	0/3491	0.70	0/4741
2	B	0.42	0/3503	0.69	0/4744
2	D	0.43	0/3516	0.68	0/4762
3	E	0.46	0/1092	0.68	0/1455
4	F	1.32	0/10	0.38	0/9
All	All	0.44	0/15091	0.69	0/20434

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	0E5	C3

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	0	3312	31	0
1	C	3404	0	3311	39	0
2	B	3417	0	3283	47	0
2	D	3433	0	3301	53	0
3	E	1077	0	1068	7	0
4	F	35	0	28	1	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	D	10	0	0	0	0
8	B	28	0	12	3	0
8	D	28	0	12	2	0
9	B	29	0	25	4	0
9	D	29	0	25	3	0
10	A	27	0	0	0	0
10	B	28	0	0	1	0
10	C	43	0	0	0	0
10	D	36	0	0	1	0
10	E	3	0	0	0	0
All	All	15107	0	14401	168	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 6.

All (168) 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:206:ASN:HD21	8:B:501:GDP:HN22	1.24	0.86
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.59	0.85
1:C:206:ASN:HD21	5:C:600:GTP:HN22	1.24	0.83
1:A:206:ASN:HD21	5:A:501:GTP:HN22	1.26	0.82
2:D:206:ASN:HD21	8:D:501:GDP:HN22	1.25	0.82
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.51	0.76
2:D:237:GLY:CA	2:D:376:THR:HG21	2.17	0.74
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.37	0.72
2:D:318:ILE:HG23	2:D:376:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ASN:HD22	2:B:350:ASN:H	1.40	0.68
2:D:317:THR:HG22	2:D:377[B]:PHE:HD1	1.58	0.68
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.28	0.68
2:D:350:ASN:HD22	2:D:350:ASN:H	1.40	0.68
2:B:318:ILE:HD11	9:B:502:LOC:H4	1.76	0.68
2:D:172:MET:HG3	2:D:387:LEU:HD21	1.75	0.68
2:D:50:ASN:O	2:D:64:ARG:NH2	2.27	0.68
2:B:50:ASN:O	2:B:64:ARG:NH2	2.21	0.68
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.76	0.68
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.77	0.66
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.78	0.66
1:C:84:ARG:O	1:C:85:GLN:HB2	1.96	0.66
2:B:141:LEU:HD21	2:B:170:SER:HB3	1.78	0.65
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.79	0.64
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.79	0.64
2:B:71[B]:GLU:HG2	1:C:2:ARG:HH22	1.61	0.63
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.80	0.63
2:D:133:GLN:HE21	2:D:252:LEU:H	1.45	0.62
2:D:209:LEU:HB3	2:D:227:LEU:HG	1.83	0.60
2:D:352:LYS:HB2	9:D:502:LOC:H18B	1.84	0.59
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.83	0.59
2:D:66:ILE:HD13	2:D:122:VAL:HG12	1.84	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.03	0.59
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.86	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.87	0.57
1:C:70:LEU:HG	1:C:110:ILE:HG22	1.87	0.57
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.86	0.57
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.24	0.56
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.71	0.56
1:A:3:GLU:HG3	1:A:129:CYS:SG	2.46	0.56
1:A:70:LEU:HG	1:A:110:ILE:HG22	1.88	0.56
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.88	0.55
2:D:229:HIS:NE2	2:D:276:THR:HG22	2.21	0.55
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.53	0.55
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.88	0.55
3:E:10:GLU:HA	3:E:20:TRP:HB2	1.89	0.55
2:B:133:GLN:HE21	2:B:252:LEU:H	1.55	0.55
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.71	0.55
2:B:136:GLN:HA	2:B:167:ASN:O	2.08	0.54
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.89	0.54
1:A:397:LEU:HD23	2:B:348:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:HE22	1:A:372:GLN:H	1.57	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.08	0.53
2:B:315:VAL:HB	2:B:351:VAL:HB	1.92	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.58	0.52
2:D:133:GLN:NE2	2:D:252:LEU:H	2.08	0.52
2:B:392:SER:O	2:B:396:THR:HG23	2.09	0.52
1:C:97:GLU:HB2	2:D:1:MET:HG2	1.91	0.52
2:B:424:ASN:HB2	10:B:619:HOH:O	2.08	0.52
1:A:308:ARG:HH21	1:A:309:HIS:HD2	1.57	0.52
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.92	0.51
2:D:248:LEU:HD13	2:D:249:ASN:H	1.75	0.51
2:D:278:ARG:C	2:D:280:SER:H	2.14	0.51
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.24	0.51
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.57	0.51
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.43	0.51
1:C:241:SER:HB2	1:C:251:ASP:HA	1.93	0.50
1:A:211:ASP:O	1:A:215:ARG:HD2	2.11	0.50
2:B:99:ALA:HB2	2:B:145:THR:HG22	1.93	0.50
2:B:286:LEU:HD21	2:B:291:LEU:HD13	1.94	0.50
2:D:315:VAL:HB	2:D:351:VAL:HB	1.92	0.50
1:A:263:PRO:O	1:A:266:HIS:HD2	1.94	0.50
2:B:171:VAL:HA	2:B:204:ILE:O	2.11	0.50
2:B:42:LEU:HD12	2:B:358:ILE:HD11	1.94	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
1:C:325:PRO:HA	1:C:328:VAL:CG2	2.42	0.49
1:C:100:ALA:HA	2:D:254:LYS:HG2	1.93	0.49
3:E:115:HIS:HD2	3:E:116:LEU:HD22	1.77	0.49
2:D:350:ASN:ND2	2:D:350:ASN:H	2.09	0.49
2:B:223:THR:HA	4:F:3:OE5:H5	1.95	0.49
1:A:154:MET:HG3	1:A:194:THR:HG23	1.96	0.48
2:D:106:GLY:O	2:D:111:GLY:HA3	2.14	0.48
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.95	0.48
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.95	0.47
2:D:147[A]:SER:HB2	2:D:190:SER:HG	1.78	0.47
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.96	0.47
2:B:318:ILE:HD11	9:B:502:LOC:C4	2.45	0.47
1:A:174:ALA:HB1	1:A:176:GLN:HE21	1.80	0.47
1:C:174:ALA:HB1	1:C:176:GLN:HE21	1.79	0.47
1:A:2:ARG:HB3	1:A:133[A]:GLN:NE2	2.30	0.47
1:C:154:MET:HG3	1:C:194:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD23	2:B:172:MET:SD	2.56	0.46
2:B:183:GLU:OE2	8:B:501:GDP:H3'	2.16	0.46
1:A:355:ILE:O	3:E:17:GLY:HA2	2.15	0.46
2:D:183:GLU:OE2	8:D:501:GDP:H3'	2.16	0.46
1:C:179:THR:HG22	1:C:183:GLU:OE2	2.15	0.46
2:B:163:ASP:O	2:B:253[B]:ARG:NH2	2.48	0.45
2:D:85:GLN:CD	2:D:85:GLN:H	2.19	0.45
1:A:9:VAL:HG23	1:A:145:THR:HG22	1.98	0.45
1:C:181:VAL:HG22	2:D:258:ASN:HD22	1.80	0.45
2:B:16:ILE:HG12	2:B:231:VAL:HG11	1.98	0.45
2:D:141:LEU:HD23	2:D:172:MET:SD	2.56	0.45
2:B:346:TRP:HB3	2:B:440:ALA:HB2	1.99	0.45
2:D:253:ARG:NH2	10:D:633:HOH:O	2.49	0.45
2:D:139:HIS:HD2	2:D:146:GLY:O	2.00	0.45
2:B:99:ALA:CB	2:B:145:THR:HG22	2.46	0.45
2:D:350:ASN:HD22	2:D:350:ASN:N	2.10	0.45
2:B:350:ASN:H	2:B:350:ASN:ND2	2.09	0.44
1:C:286:LEU:HD21	1:C:291:ILE:HG23	1.99	0.44
1:C:9:VAL:HG23	1:C:145:THR:HG22	1.99	0.44
2:B:352:LYS:HE3	9:B:502:LOC:O5	2.18	0.44
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.35	0.44
1:A:230:LEU:O	1:A:234:ILE:HD12	2.17	0.44
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.44
2:D:294:GLN:HA	2:D:297:ASP:HB2	2.00	0.44
1:C:84:ARG:O	1:C:85:GLN:CB	2.66	0.44
2:D:162:PRO:HB2	3:E:116:LEU:HD12	2.00	0.43
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.58	0.43
1:A:2:ARG:HB3	1:A:133[A]:GLN:HE21	1.83	0.43
2:D:133:GLN:HE21	2:D:252:LEU:HB2	1.83	0.43
3:E:76:ARG:HG3	3:E:80:ARG:HH21	1.83	0.43
2:B:139:HIS:HD2	2:B:146:GLY:O	2.01	0.43
1:C:251:ASP:OD2	1:C:253:THR:OG1	2.37	0.43
1:A:401:LYS:HD3	2:B:346:TRP:CG	2.53	0.43
2:D:1:MET:HE3	2:D:133:GLN:HG3	2.00	0.43
2:B:1:MET:HE3	2:B:133:GLN:HG3	2.01	0.43
1:C:119:LEU:HD21	1:C:156:ARG:HB3	2.01	0.42
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.00	0.42
2:D:1:MET:N	2:D:131:CYS:SG	2.91	0.42
1:C:255:PHE:CE1	1:C:318:LEU:HD21	2.54	0.42
1:C:255:PHE:CD2	1:C:316:CYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.01	0.42
2:D:352:LYS:HE3	9:D:502:LOC:O5	2.20	0.42
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.84	0.42
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.55	0.42
2:B:241[A]:CYS:SG	9:B:502:LOC:O3	2.77	0.42
2:D:141:LEU:HB3	2:D:187:ALA:HA	2.02	0.42
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.37	0.42
2:B:206:ASN:HA	2:B:206:ASN:HD22	1.72	0.41
1:A:206:ASN:HD22	1:A:206:ASN:HA	1.67	0.41
2:B:133:GLN:NE2	2:B:252:LEU:H	2.18	0.41
1:A:286:LEU:HD23	1:A:290:GLU:HG2	2.03	0.41
1:A:71:GLU:OE2	1:A:73:THR:HB	2.20	0.41
1:A:27:GLU:OE2	1:A:320:ARG:NH2	2.53	0.41
2:B:192:HIS:CD2	2:B:421:ALA:HA	2.55	0.41
2:D:229:HIS:HB2	2:D:278:ARG:HB3	2.02	0.41
2:D:297:ASP:HB3	2:D:300:ASN:HD22	1.85	0.41
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.84	0.41
2:B:213:CYS:HA	2:B:217:LEU:HD12	2.03	0.41
1:C:286:LEU:HD11	1:C:291:ILE:CG2	2.51	0.41
1:C:317:LEU:HB2	1:C:353:VAL:HG22	2.03	0.41
2:D:250:ALA:HB1	9:D:502:LOC:H6B	2.02	0.41
1:A:440:VAL:CG2	3:E:33:PRO:HD2	2.51	0.41
2:D:274:PRO:HB3	2:D:286:LEU:HG	2.03	0.41
2:B:133:GLN:HE22	2:B:242:LEU:HD22	1.86	0.41
1:C:177:VAL:HG22	1:C:177:VAL:O	2.22	0.41
1:A:119:LEU:HD21	1:A:156:ARG:HB3	2.03	0.41
1:C:274:PRO:HG3	1:C:286:LEU:HG	2.03	0.40
1:C:107:HIS:HD2	1:C:108[A]:TYR:CE2	2.39	0.40
2:D:48:ARG:HE	2:D:248:LEU:HD11	1.87	0.40
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.40
1:C:372:GLN:HG3	1:C:372:GLN:H	1.73	0.40
2:B:206:ASN:HD21	8:B:501:GDP:N2	2.05	0.40
2:D:139:HIS:HE1	2:D:170:SER:OG	2.05	0.40
2:B:350:ASN:HD22	2:B:350:ASN:N	2.10	0.40
1:C:71:GLU:OE2	1:C:73:THR:HB	2.21	0.40
1:C:122:ILE:HA	1:C:125:LEU:HD12	2.04	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%)	404 (94%)	21 (5%)	5 (1%)	16	37
1	C	432/451 (96%)	406 (94%)	23 (5%)	3 (1%)	26	54
2	B	433/445 (97%)	411 (95%)	18 (4%)	4 (1%)	21	47
2	D	435/445 (98%)	411 (94%)	17 (4%)	7 (2%)	12	28
3	E	129/142 (91%)	118 (92%)	7 (5%)	4 (3%)	5	11
All	All	1859/1934 (96%)	1750 (94%)	86 (5%)	23 (1%)	16	37

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	178[A]	SER
2	D	178[B]	SER
2	D	248	LEU
2	B	178	SER
2	B	248	LEU
1	C	281	ALA
2	D	249	ASN
1	A	179	THR
1	A	340	SER
2	B	109	THR
2	D	109	THR
2	D	283	TYR
1	A	162	GLY
1	C	109	THR
3	E	45	PRO
2	B	286	LEU
1	C	314	ALA
3	E	10	GLU
3	E	32	VAL
3	E	46	SER
1	A	47	ASP

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Mol	Chain	Res	Type
2	D	73	GLY
1	A	131	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%)	326 (89%)	42 (11%)	7	15
1	C	369/379 (97%)	322 (87%)	47 (13%)	5	12
2	B	378/385 (98%)	331 (88%)	47 (12%)	6	12
2	D	380/385 (99%)	336 (88%)	44 (12%)	7	15
3	E	113/125 (90%)	93 (82%)	20 (18%)	2	5
4	F	1/1 (100%)	1 (100%)	0	100	100
All	All	1609/1654 (97%)	1409 (88%)	200 (12%)	6	12

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	9	VAL
1	A	26	LEU
1	A	36	MET
1	A	47	ASP
1	A	70	LEU
1	A	102	ASN
1	A	119	LEU
1	A	121	ARG
1	A	153	LEU
1	A	160	ASP
1	A	163	LYS
1	A	166	LYS
1	A	179	THR
1	A	188	ILE
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	215	ARG
1	A	227	LEU
1	A	250	VAL
1	A	269	LEU
1	A	277	SER
1	A	280	LYS
1	A	284	GLU
1	A	295	CYS
1	A	297	GLU
1	A	302	MET
1	A	315	CYS
1	A	320	ARG
1	A	336	LYS
1	A	337	THR
1	A	338	LYS
1	A	339	ARG
1	A	341	ILE
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	384	ILE
1	A	391	LEU
1	A	397	LEU
1	A	401	LYS
1	A	423	GLU
1	A	439	SER
2	B	5	VAL
2	B	16	ILE
2	B	26	ASP
2	B	42	LEU
2	B	48	ARG
2	B	50	ASN
2	B	54	ASN
2	B	57	THR
2	B	60	LYS
2	B	71[A]	GLU
2	B	71[B]	GLU
2	B	75	MET
2	B	79	ARG
2	B	139	HIS
2	B	141	LEU
2	B	145	THR

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Mol	Chain	Res	Type
2	B	147	SER
2	B	179	ASP
2	B	190	SER
2	B	192	HIS
2	B	206	ASN
2	B	207	GLU
2	B	218	LYS
2	B	223	THR
2	B	230	LEU
2	B	252	LEU
2	B	255	LEU
2	B	277	SER
2	B	281	GLN
2	B	287	THR
2	B	288	VAL
2	B	294	GLN
2	B	295	MET
2	B	297	ASP
2	B	308	ARG
2	B	313	LEU
2	B	323	MET
2	B	329	ASP
2	B	333	LEU
2	B	339	ASN
2	B	345	GLU
2	B	350	ASN
2	B	351	VAL
2	B	352	LYS
2	B	372	LYS
2	B	380	ASN
2	B	416	MET
1	C	1	MET
1	C	4[A]	CYS
1	C	4[B]	CYS
1	C	9	VAL
1	C	26	LEU
1	C	35	GLN
1	C	70	LEU
1	C	102	ASN
1	C	112	LYS
1	C	119	LEU
1	C	121	ARG

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Mol	Chain	Res	Type
1	C	153	LEU
1	C	163	LYS
1	C	164	LYS
1	C	166	LYS
1	C	177	VAL
1	C	188	ILE
1	C	206	ASN
1	C	227	LEU
1	C	233	GLN
1	C	252	LEU
1	C	253	THR
1	C	254	GLU
1	C	256	GLN
1	C	260	VAL
1	C	269	LEU
1	C	282	TYR
1	C	290	GLU
1	C	295	CYS
1	C	297	GLU
1	C	302	MET
1	C	328	VAL
1	C	332	ILE
1	C	335	ILE
1	C	339	ARG
1	C	340	SER
1	C	348	PRO
1	C	367	ASP
1	C	368	LEU
1	C	370	LYS
1	C	372	GLN
1	C	384	ILE
1	C	397	LEU
1	C	401	LYS
1	C	423	GLU
1	C	435	VAL
1	C	439	SER
2	D	26	ASP
2	D	47	GLU
2	D	48	ARG
2	D	50	ASN
2	D	57	THR
2	D	59	ASN

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Mol	Chain	Res	Type
2	D	71	GLU
2	D	85	GLN
2	D	139	HIS
2	D	141	LEU
2	D	156	LYS
2	D	190	SER
2	D	192	HIS
2	D	206	ASN
2	D	207	GLU
2	D	218	LYS
2	D	230	LEU
2	D	247	GLN
2	D	248	LEU
2	D	252	LEU
2	D	255	LEU
2	D	276	THR
2	D	277	SER
2	D	282	GLN
2	D	283	TYR
2	D	284	ARG
2	D	286	LEU
2	D	288	VAL
2	D	293	GLN
2	D	295	MET
2	D	296	PHE
2	D	297	ASP
2	D	313	LEU
2	D	318	ILE
2	D	322	ARG
2	D	329	ASP
2	D	340	SER
2	D	345	GLU
2	D	350	ASN
2	D	351	VAL
2	D	352	LYS
2	D	372	LYS
2	D	376	THR
2	D	380	ASN
3	E	12	ASN
3	E	13	LYS
3	E	15	THR
3	E	47	LEU

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Mol	Chain	Res	Type
3	E	55	GLU
3	E	58	GLU
3	E	72	LEU
3	E	76	ARG
3	E	80	ARG
3	E	82	VAL
3	E	83	ILE
3	E	88	GLU
3	E	105	MET
3	E	108	ASN
3	E	122	ARG
3	E	123	LEU
3	E	134	ARG
3	E	136	ASN
3	E	138	GLU
3	E	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	91	GLN
1	A	102	ASN
1	A	139	HIS
1	A	176	GLN
1	A	197	HIS
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	309	HIS
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	85	GLN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	206	ASN

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Mol	Chain	Res	Type
2	B	229	HIS
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	15	GLN
1	C	91	GLN
1	C	101	ASN
1	C	102	ASN
1	C	107	HIS
1	C	139	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	300	ASN
1	C	301	GLN
1	C	329	ASN
1	C	380	ASN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	85	GLN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	197	ASN
2	D	206	ASN
2	D	247	GLN
2	D	258	ASN
2	D	300	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	433	GLN
2	D	436	GLN
3	E	91	ASN
3	E	108	ASN
3	E	111	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 ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	0EA	F	1	4	14,15,16	2.68	8 (57%)	15,20,22	2.29	2 (13%)
4	0E5	F	3	4	6,7,9	1.16	0	7,8,13	3.97	5 (71%)

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	0EA	F	1	4	-	0/9/12/14	0/1/1/1
4	0E5	F	3	4	1/1/2/3	0/6/8/13	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	0EA	O5-C7	-4.84	1.26	1.36
4	F	1	0EA	C10-C11	2.15	1.55	1.51
4	F	1	0EA	C9-C10	2.40	1.43	1.39
4	F	1	0EA	O8-C11	2.63	1.48	1.42
4	F	1	0EA	C12-C11	2.92	1.59	1.54
4	F	1	0EA	C6-C10	3.45	1.44	1.39
4	F	1	0EA	O1-C5	3.85	1.44	1.36
4	F	1	0EA	C6-C5	4.08	1.44	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	0EA	C6-C5-C7	-5.91	114.46	119.82
4	F	3	0E5	O6-C20-C19	-3.75	115.54	125.44
4	F	3	0E5	C2-C3-C19	-2.69	103.90	111.13
4	F	3	0E5	C4-C3-C2	-2.11	106.50	111.87
4	F	3	0E5	C20-C19-N1	2.53	115.11	109.83
4	F	1	0EA	C8-C7-C5	4.77	125.77	119.72
4	F	3	0E5	C3-C19-C20	8.80	126.91	112.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	0E5	C3

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	0E5	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	1.44	3 (12%)	34,54,54	1.94	8 (23%)
7	SO4	A	503	-	4,4,4	0.27	0	6,6,6	0.13	0
7	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	GDP	B	501	-	23,30,30	1.48	5 (21%)	30,47,47	2.09	9 (30%)
9	LOC	B	502	-	29,31,31	2.16	6 (20%)	27,44,44	3.00	10 (37%)
7	SO4	B	503	-	4,4,4	0.12	0	6,6,6	0.09	0
5	GTP	C	600	6	25,34,34	1.47	5 (20%)	34,54,54	1.87	8 (23%)
8	GDP	D	501	-	23,30,30	1.29	4 (17%)	30,47,47	2.24	7 (23%)
9	LOC	D	502	-	29,31,31	2.27	6 (20%)	27,44,44	2.98	11 (40%)
7	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.09	0
7	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.12	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
7	SO4	A	503	-	-	0/0/0/0	0/0/0/0
7	SO4	A	504	-	-	0/0/0/0	0/0/0/0
8	GDP	B	501	-	-	0/12/32/32	0/3/3/3
9	LOC	B	502	-	-	0/10/25/25	0/3/3/3
7	SO4	B	503	-	-	0/0/0/0	0/0/0/0
5	GTP	C	600	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	-	-	0/12/32/32	0/3/3/3
9	LOC	D	502	-	-	0/10/25/25	0/3/3/3
7	SO4	D	503	-	-	0/0/0/0	0/0/0/0
7	SO4	D	504	-	-	0/0/0/0	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	502	LOC	C14-C11	-7.28	1.38	1.52
9	D	502	LOC	C9-C8	-6.01	1.39	1.51
9	B	502	LOC	C9-C8	-5.98	1.39	1.51
9	B	502	LOC	C21-C22	-5.77	1.41	1.49
9	B	502	LOC	C14-C11	-4.88	1.42	1.52
9	D	502	LOC	C21-C22	-4.30	1.43	1.49
9	D	502	LOC	O6-C18	-3.15	1.33	1.42
5	C	600	GTP	C8-N7	-2.84	1.29	1.34
9	B	502	LOC	O2-C3	-2.75	1.33	1.38
9	D	502	LOC	O2-C3	-2.57	1.33	1.38
8	D	501	GDP	C6-N1	2.01	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	LOC	C5-C3	2.01	1.45	1.40
5	C	600	GTP	C2-N2	2.06	1.38	1.34
8	B	501	GDP	C5-C4	2.08	1.45	1.40
8	D	501	GDP	C5-C4	2.14	1.45	1.40
5	A	501	GTP	C2-N1	2.23	1.39	1.35
5	C	600	GTP	C2-N1	2.27	1.39	1.35
8	B	501	GDP	C6-N1	2.28	1.37	1.33
8	B	501	GDP	C2-N1	2.30	1.39	1.35
5	C	600	GTP	C6-N1	2.31	1.37	1.33
8	B	501	GDP	PB-O3B	2.35	1.63	1.54
8	D	501	GDP	PB-O2B	2.45	1.63	1.54
8	D	501	GDP	C2-N1	2.45	1.39	1.35
5	A	501	GTP	C6-N1	2.58	1.37	1.33
9	B	502	LOC	C22-C8	2.95	1.45	1.40
8	B	501	GDP	C6-C5	3.11	1.47	1.41
9	D	502	LOC	C22-C8	3.37	1.46	1.40
5	C	600	GTP	O4'-C1'	3.40	1.45	1.41
5	A	501	GTP	O4'-C1'	3.87	1.46	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C6-N1	-6.30	114.97	123.59
9	D	502	LOC	C21-C22-C8	-5.70	114.47	120.63
9	B	502	LOC	C9-C8-C7	-5.24	107.70	119.10
5	C	600	GTP	PA-O3A-PB	-5.15	118.25	132.73
5	A	501	GTP	PA-O3A-PB	-5.12	118.34	132.73
8	B	501	GDP	C5-C6-N1	-5.08	116.65	123.59
5	A	501	GTP	N3-C2-N1	-4.38	120.77	127.44
8	B	501	GDP	C4-C5-N7	-4.32	105.51	109.48
5	C	600	GTP	N3-C2-N1	-4.20	121.04	127.44
9	D	502	LOC	C9-C8-C7	-4.07	110.24	119.10
8	D	501	GDP	N3-C2-N1	-4.06	121.26	127.44
9	B	502	LOC	C4-O2-C3	-3.95	104.44	114.82
8	B	501	GDP	PA-O3A-PB	-3.72	120.19	132.67
5	C	600	GTP	C6-C5-C4	-3.69	116.49	120.90
8	B	501	GDP	N3-C2-N1	-3.64	121.89	127.44
9	B	502	LOC	C21-C22-C8	-3.55	116.79	120.63
8	D	501	GDP	PA-O3A-PB	-3.52	120.88	132.67
5	A	501	GTP	C5-C6-N1	-3.45	118.88	123.59
5	A	501	GTP	C1'-N9-C4	-3.18	122.14	126.94
5	A	501	GTP	C6-C5-C4	-3.06	117.24	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	600	GTP	PB-O3B-PG	-3.06	122.41	132.67
5	C	600	GTP	C1'-N9-C4	-3.04	122.35	126.94
5	A	501	GTP	PB-O3B-PG	-3.01	122.57	132.67
8	D	501	GDP	C6-C5-C4	-2.94	117.38	120.90
8	D	501	GDP	C1'-N9-C4	-2.92	122.53	126.94
9	D	502	LOC	C6-O3-C5	-2.84	113.23	117.54
8	B	501	GDP	C6-C5-C4	-2.81	117.54	120.90
5	C	600	GTP	C5-C6-N1	-2.79	119.78	123.59
8	B	501	GDP	C1'-N9-C4	-2.70	122.87	126.94
9	D	502	LOC	C4-O2-C3	-2.68	107.77	114.82
5	A	501	GTP	C4-C5-N7	-2.65	107.04	109.48
8	D	501	GDP	C4-C5-N7	-2.46	107.21	109.48
5	C	600	GTP	C4-C5-N7	-2.24	107.42	109.48
9	B	502	LOC	O3-C5-C7	-2.06	120.70	124.21
9	B	502	LOC	O1-C1-C22	2.05	122.74	119.07
9	B	502	LOC	C7-C8-C22	2.09	122.52	119.79
8	B	501	GDP	O2A-PA-O3A	2.13	114.74	105.09
8	B	501	GDP	O2B-PB-O3A	2.13	114.75	105.09
9	D	502	LOC	C7-C8-C22	2.22	122.70	119.79
9	D	502	LOC	C5-C3-C1	2.24	122.31	119.62
9	D	502	LOC	O1-C1-C22	2.27	123.12	119.07
9	B	502	LOC	C21-C22-C1	2.47	124.66	121.05
9	B	502	LOC	O3-C5-C3	2.61	119.97	115.26
5	C	600	GTP	C6-N1-C2	3.24	120.44	115.94
5	A	501	GTP	C6-N1-C2	3.62	120.97	115.94
9	B	502	LOC	C10-C11-N1	3.88	117.05	109.96
9	D	502	LOC	C9-C10-C11	3.99	117.54	112.15
8	B	501	GDP	C6-N1-C2	5.01	122.89	115.94
9	D	502	LOC	C21-C22-C1	5.15	128.59	121.05
9	D	502	LOC	C10-C11-N1	5.85	120.65	109.96
8	D	501	GDP	C6-N1-C2	6.47	124.92	115.94
9	D	502	LOC	C9-C8-C22	8.19	127.05	119.24
9	B	502	LOC	C9-C8-C22	11.05	129.77	119.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	3	0
9	B	502	LOC	4	0
5	C	600	GTP	1	0
8	D	501	GDP	2	0
9	D	502	LOC	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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%)	0.42	34 (7%)	15 14	60, 97, 153, 198	0
1	C	432/451 (95%)	0.28	20 (4%)	36 36	42, 81, 133, 180	0
2	B	432/445 (97%)	0.58	53 (12%)	5 5	59, 90, 155, 215	2 (0%)
2	D	432/445 (97%)	0.28	25 (5%)	26 26	44, 77, 122, 162	2 (0%)
3	E	132/142 (92%)	1.02	20 (15%)	3 2	62, 107, 176, 214	0
4	F	2/4 (50%)	1.37	1 (50%)	0 0	117, 117, 117, 129	0
All	All	1863/1938 (96%)	0.44	153 (8%)	14 13	42, 89, 145, 215	4 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	34	GLU	8.6
3	E	141	GLU	8.0
2	B	283	TYR	7.7
3	E	140	LYS	7.5
3	E	32	VAL	7.4
2	D	283	TYR	6.9
1	A	337	THR	6.6
3	E	6	MET	6.1
3	E	4	ALA	5.7
3	E	33	PRO	5.4
2	B	279	GLY	5.1
3	E	5	ASP	5.0
2	D	56	ALA	5.0
2	D	284	ARG	4.8
1	C	335	ILE	4.6
2	D	39	ASP	4.6
1	A	338	LYS	4.4
1	C	366	GLY	4.3
1	C	323	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	36	TYR	4.3
1	A	280	LYS	4.2
2	B	276	THR	4.2
2	D	282	GLN	4.1
1	C	364	PRO	4.1
2	B	246	GLY	3.9
1	A	38	SER	3.8
1	A	437	VAL	3.8
1	C	1	MET	3.7
2	B	440	ALA	3.7
3	E	16	SER	3.7
1	A	221	ARG	3.7
1	A	37	PRO	3.6
1	A	282	TYR	3.6
1	A	346	TRP	3.6
1	A	440	VAL	3.5
2	B	441	ASP	3.5
2	B	61	TYR	3.5
2	B	55	GLU	3.5
2	B	281	GLN	3.5
2	D	57	THR	3.4
1	A	279	GLU	3.4
2	B	282	GLN	3.4
2	B	86	ILE	3.4
2	B	284	ARG	3.4
3	E	27	PRO	3.4
1	A	281	ALA	3.4
2	B	59	ASN	3.4
2	B	37	HIS	3.3
1	A	170	SER	3.3
2	D	60	LYS	3.3
2	D	285	ALA	3.3
2	D	37	HIS	3.3
1	C	334	THR	3.3
1	A	219	ILE	3.2
1	C	38	SER	3.2
2	B	379	GLY	3.2
1	C	357	TYR	3.1
2	B	241[A]	CYS	3.1
1	A	335	ILE	3.0
2	D	418	PHE	3.0
1	A	80	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	270	PRO	3.0
3	E	87	ILE	2.9
3	E	24	LEU	2.9
1	A	349	THR	2.9
2	B	56	ALA	2.9
2	D	296	PHE	2.8
2	B	285	ALA	2.8
1	C	282	TYR	2.8
2	B	203	SER	2.7
2	B	238	VAL	2.7
4	F	4	GLY	2.7
1	A	286	LEU	2.7
3	E	26	PRO	2.7
2	B	42	LEU	2.7
2	B	286	LEU	2.7
2	D	179[A]	ASP	2.7
2	B	245	PRO	2.6
2	B	269	MET	2.6
2	B	373	MET	2.6
1	A	439	SER	2.6
1	A	435	VAL	2.6
2	B	202	TYR	2.6
2	B	62	VAL	2.6
1	A	201	ALA	2.6
2	B	36	TYR	2.6
3	E	8	VAL	2.5
2	D	59	ASN	2.5
3	E	136	ASN	2.5
1	C	253	THR	2.5
1	A	339	ARG	2.5
3	E	73	ALA	2.5
2	B	322	ARG	2.5
2	B	201	THR	2.4
3	E	48	GLU	2.4
2	B	271	GLY	2.4
2	B	1	MET	2.4
2	B	371	LEU	2.4
1	A	283	HIS	2.4
1	A	268	PRO	2.4
3	E	59	GLU	2.3
1	C	331	ALA	2.3
2	B	280	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	200	CYS	2.3
2	B	268	PHE	2.3
2	D	55	GLU	2.3
2	B	339	ASN	2.3
2	B	32	PRO	2.3
3	E	25	LYS	2.3
1	A	336	LYS	2.3
2	B	39	ASP	2.3
1	C	362	VAL	2.3
2	D	280	SER	2.2
2	D	41	ASP	2.2
1	A	328	VAL	2.2
2	B	204	ILE	2.2
2	D	61	TYR	2.2
2	B	333	LEU	2.2
2	B	170	SER	2.2
2	B	378	ILE	2.2
2	B	248	LEU	2.2
2	B	233	ALA	2.2
1	A	438	ASP	2.2
2	B	239	THR	2.2
1	A	372	GLN	2.2
2	D	96	GLN	2.2
1	C	285	GLN	2.2
2	B	169	PHE	2.1
1	C	215	ARG	2.1
2	D	441	ASP	2.1
1	C	324	VAL	2.1
2	B	57	THR	2.1
1	C	333	ALA	2.1
1	A	436	GLY	2.1
2	D	369	ARG	2.1
1	A	271	THR	2.1
2	B	167	ASN	2.1
2	D	286	LEU	2.1
2	B	221	THR	2.1
2	D	202	TYR	2.1
1	A	415	GLU	2.1
1	A	200	CYS	2.1
1	A	369	ALA	2.1
2	B	171	VAL	2.0
2	D	404	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	84	GLY	2.0
1	A	217	LEU	2.0
1	C	351	PHE	2.0
2	B	251	ASP	2.0
3	E	45	PRO	2.0
2	D	98	GLY	2.0
1	C	284	GLU	2.0
1	C	440	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
4	0E5	F	3	8/10	0.93	0.27	-	110,113,121,122	0
4	0EA	F	1	15/16	0.93	0.26	-	113,115,118,119	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	SO4	D	503	5/5	0.95	0.30	2.37	142,143,148,149	0
5	GTP	A	501	32/32	0.98	0.20	0.17	63,70,76,76	0
7	SO4	D	504	5/5	0.88	0.19	0.08	141,143,147,149	0
8	GDP	B	501	28/28	0.98	0.18	-0.32	69,71,76,76	0
7	SO4	A	504	5/5	0.90	0.20	-0.36	140,143,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GTP	C	600	32/32	0.98	0.17	-0.39	57,59,66,68	0
8	GDP	D	501	28/28	0.98	0.17	-0.47	62,66,70,73	0
9	LOC	D	502	29/29	0.97	0.18	-0.48	51,63,67,67	0
6	MG	A	502	1/1	0.95	0.16	-0.67	74,74,74,74	0
9	LOC	B	502	29/29	0.94	0.18	-1.08	75,79,83,85	0
6	MG	C	601	1/1	0.96	0.13	-1.10	56,56,56,56	0
7	SO4	B	503	5/5	0.92	0.09	-1.43	157,160,165,165	0
7	SO4	A	503	5/5	0.91	0.16	-	127,130,133,134	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.