



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:58 PM BST

PDB ID : 5J2T  
Title : Tubulin-vinblastine complex  
Authors : Waight, A.B.; Bargsten, K.; Doronina, S.; Steinmetz, M.O.; Sussman, D.;  
Prota, A.E.  
Deposited on : 2016-03-30  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

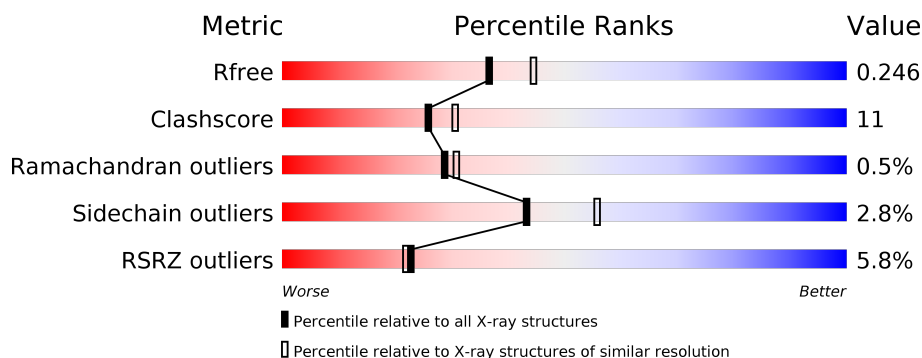
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. 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>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>80%</div> <div>17%</div> <div>•</div> </div>
2	B	445	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
2	D	445	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• 5%</div> </div> </div>
3	E	143	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>• 16%</div> </div> </div>
4	F	384	<div> <div>21%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>• 14%</div> </div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17989 atoms, of which 71 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	9	0
			3469	2202	584	659	24			
1	C	440	Total	C	N	O	S	0	9	0
			3476	2204	585	663	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	0	4	0
			3347	2105	568	646	28			
2	B	428	Total	C	N	O	S	0	2	0
			3370	2118	576	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

There are 2 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

- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	6	0
			2740	1771	458	497	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

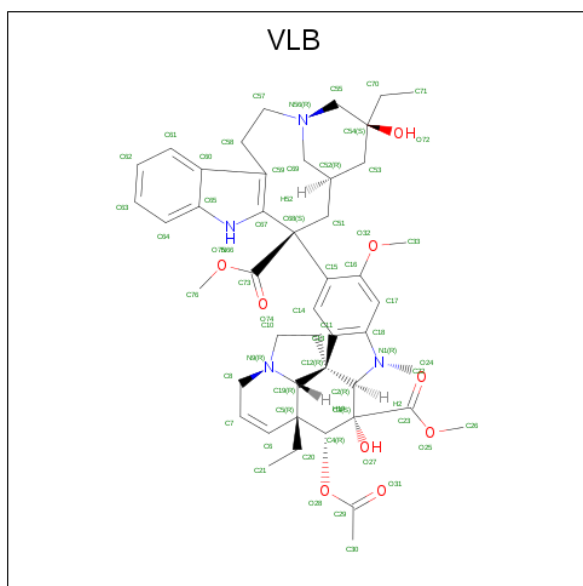
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

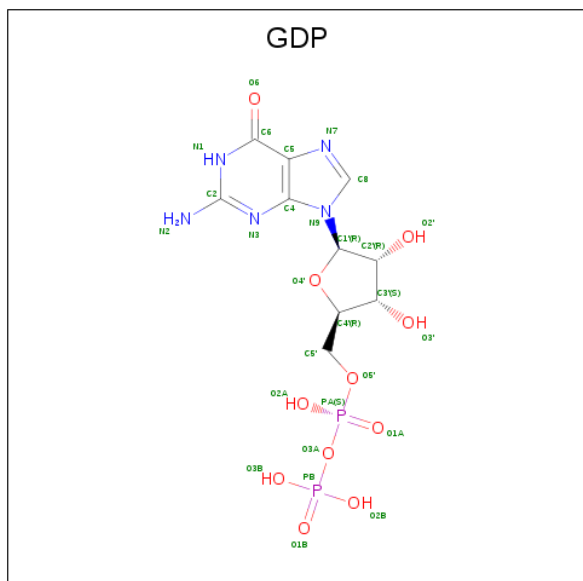
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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



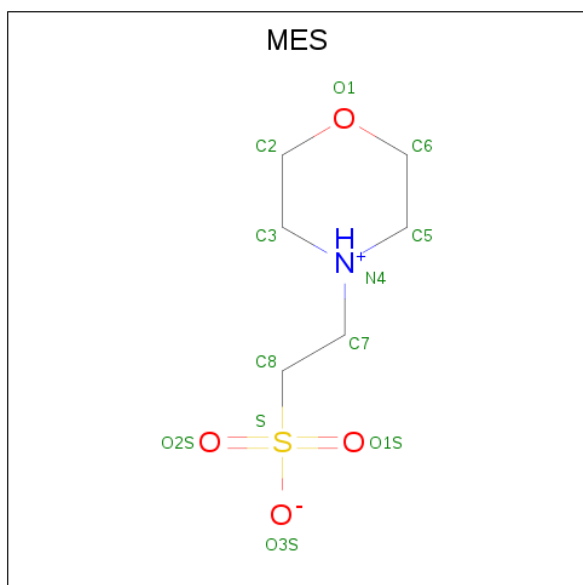
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			117	46	58	4	9		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

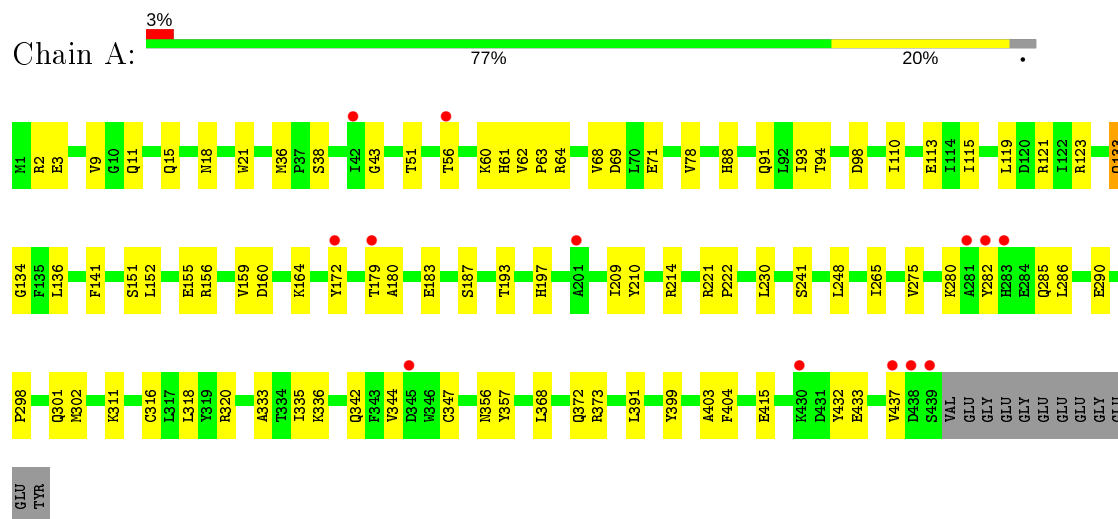
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	59	Total	O	0	0
			59	59		
11	C	124	Total	O	0	0
			124	124		
11	D	26	Total	O	0	0
			26	26		
11	E	10	Total	O	0	0
			10	10		
11	F	31	Total	O	0	0
			31	31		
11	B	80	Total	O	0	0
			80	80		

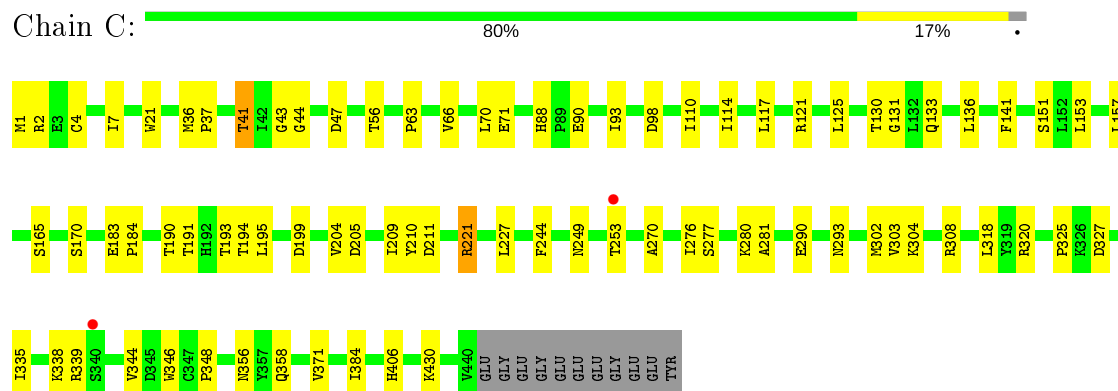
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

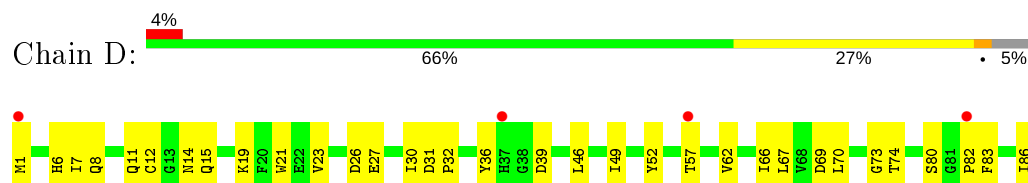
- Molecule 1: Tubulin alpha-1B chain

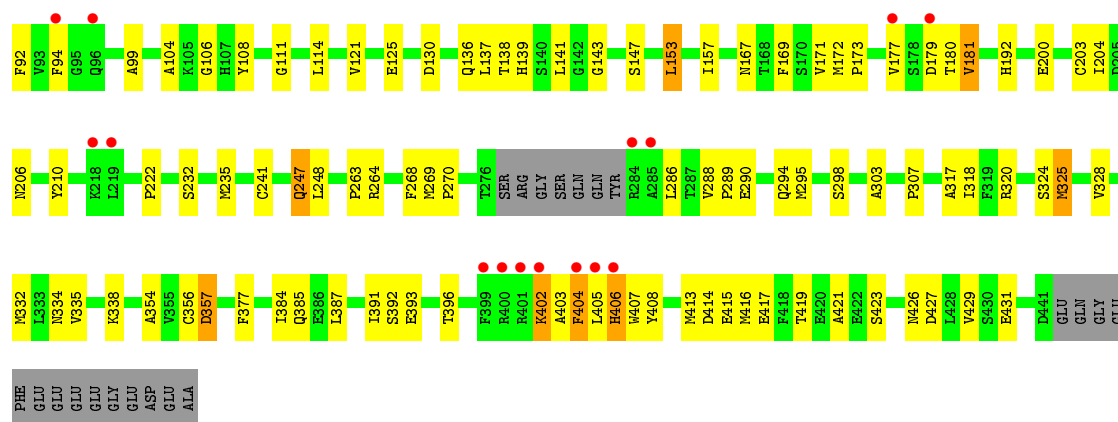


- Molecule 1: Tubulin alpha-1B chain

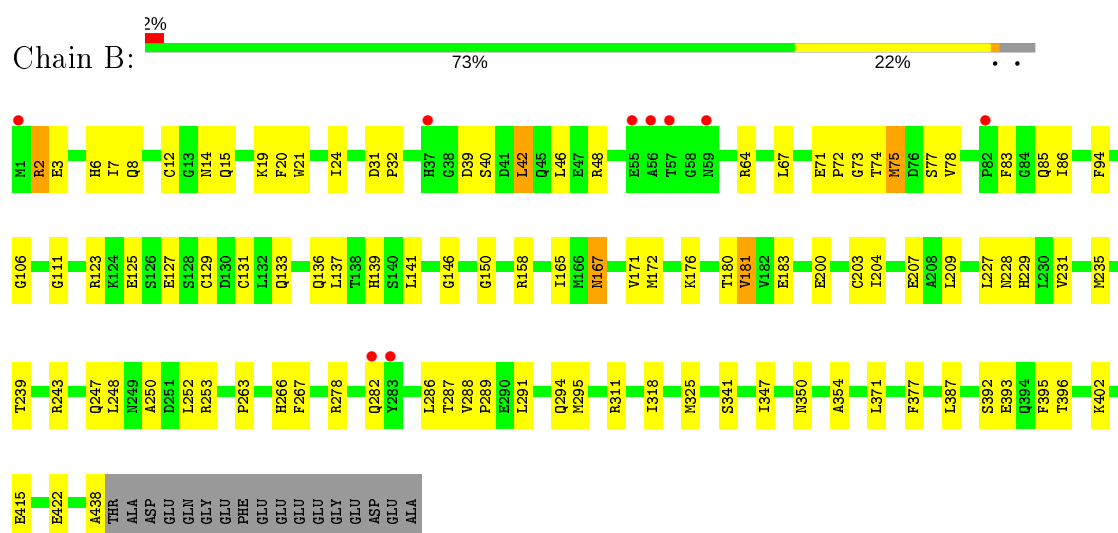


- Molecule 2: Tubulin beta-2B chain

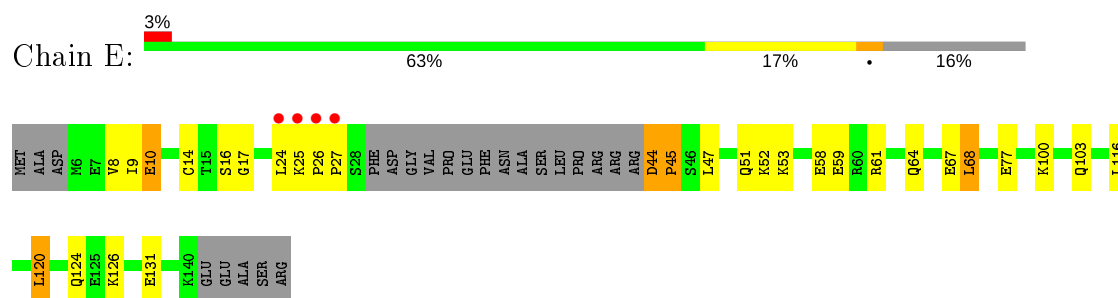




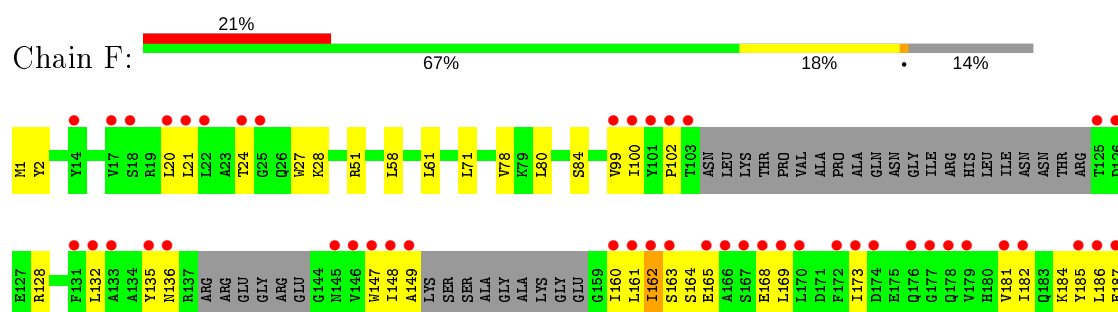
• Molecule 2: Tubulin beta-2B chain



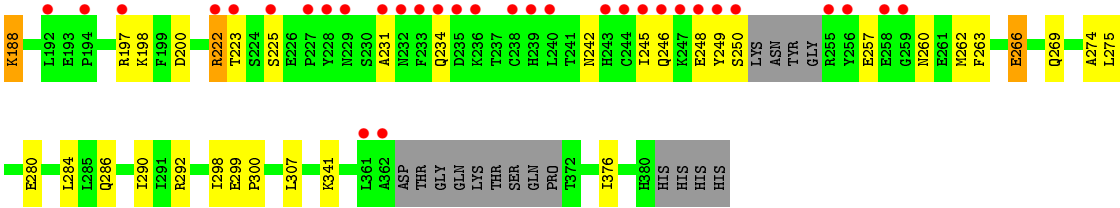
• Molecule 3: Stathmin-4



• Molecule 4: TUBULIN-TYROSINE LIGASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.25Å 157.74Å 182.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.20 48.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.17-2.20) 97.8 (48.17-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.193 , 0.244 0.197 , 0.246	Depositor DCC
$R_{free}$ test set	7499 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, 0.333 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, CA, VLB, GTP, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/3575	0.53	0/4854
1	C	0.48	0/3581	0.58	0/4863
2	B	0.46	0/3451	0.56	0/4675
2	D	0.36	0/3432	0.50	0/4649
3	E	0.41	0/999	0.45	0/1325
4	F	0.32	0/2819	0.48	0/3812
All	All	0.42	0/17857	0.53	0/24178

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	3469	0	3406	62	1
1	C	3476	0	3409	71	1
2	B	3370	0	3250	71	0
2	D	3347	0	3242	96	0
3	E	991	0	1012	21	0
4	F	2740	0	2734	51	0
5	A	32	0	12	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
8	C	59	58	58	5	0
9	B	28	0	12	1	0
9	D	28	0	12	4	0
10	B	12	13	13	1	0
11	A	59	0	0	5	0
11	B	80	0	0	3	0
11	C	124	0	0	5	0
11	D	26	0	0	5	0
11	E	10	0	0	0	0
11	F	31	0	0	1	0
All	All	17918	71	17172	366	1

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 11.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.34	1.06
2:B:2:ARG:HD3	2:B:133:GLN:HG2	1.46	0.94
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.50	0.90
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.54	0.90
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.54	0.88
1:A:333:ALA:N	11:A:602:HOH:O	2.08	0.83
4:F:262:MET:HG3	4:F:266:GLU:HG2	1.59	0.83
4:F:280:GLU:HA	4:F:284[B]:LEU:HD12	1.62	0.81
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.60	0.81
2:B:2:ARG:HA	2:B:131:CYS:O	1.81	0.80
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.17	0.80
3:E:68:LEU:HD11	2:B:158:ARG:NH2	2.01	0.75
2:D:426:ASN:OD1	11:D:601:HOH:O	2.04	0.74
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.53	0.73
1:A:285:GLN:HG2	1:A:372[B]:GLN:CD	2.10	0.72
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.24	0.72
2:B:83:PHE:HD2	2:B:86:ILE:HD13	1.53	0.72
3:E:25:LYS:HD2	3:E:26:PRO:HD2	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:MET:HE3	4:F:28:LYS:HB3	1.73	0.71
2:D:173:PRO:HD2	2:D:391:ILE:HD11	1.73	0.71
5:A:501:GTP:O2G	11:A:601:HOH:O	2.08	0.71
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.71	0.71
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.26	0.70
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.72	0.70
2:B:253:ARG:NH1	10:B:503:MES:O3S	2.22	0.70
2:D:66:ILE:HD11	2:D:125:GLU:HG3	1.74	0.70
8:C:503:VLB:C23	8:C:503:VLB:H223	2.22	0.69
2:D:294:GLN:NE2	11:D:603:HOH:O	2.23	0.69
1:A:151:SER:HB2	1:A:193:THR:HG22	1.75	0.69
2:B:282:GLN:HG3	2:B:371:LEU:HD23	1.73	0.69
1:A:88:HIS:O	1:A:91:GLN:HG2	1.94	0.68
11:A:659:HOH:O	2:B:131:CYS:SG	2.50	0.67
1:C:88:HIS:NE2	1:C:90:GLU:HG3	2.08	0.67
2:D:334:ASN:HD21	2:D:338:LYS:HE2	1.59	0.67
1:A:210:TYR:CD2	1:A:214:ARG:HD2	2.29	0.67
1:C:209:ILE:HD11	1:C:302[B]:MET:HE1	1.77	0.67
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.77	0.67
1:C:293[B]:ASN:ND2	11:C:602:HOH:O	2.28	0.66
4:F:262:MET:CG	4:F:266:GLU:HG2	2.24	0.66
4:F:99:VAL:O	4:F:100:ILE:HD12	1.96	0.66
2:D:66:ILE:HD12	2:D:121:VAL:CG1	2.24	0.65
4:F:149:ALA:HA	4:F:182:ILE:HG12	1.79	0.65
2:B:48:ARG:NH2	2:B:250:ALA:O	2.28	0.65
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.64
2:D:62:VAL:HG11	2:D:88:ARG:HG3	1.80	0.64
2:B:83:PHE:O	2:B:86:ILE:HG12	1.97	0.64
2:D:402:LYS:HD2	2:D:402:LYS:N	2.12	0.63
3:E:100:LYS:O	3:E:103:GLN:HG3	1.98	0.63
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.14	0.63
2:D:66:ILE:HD12	2:D:121:VAL:HG12	1.79	0.63
1:C:253:THR:HG22	11:C:696:HOH:O	1.97	0.63
4:F:225:SER:HB2	4:F:260:ASN:HD21	1.64	0.63
1:A:110:ILE:O	1:A:113:GLU:HG2	1.99	0.62
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.62
1:C:209:ILE:HD11	1:C:302[B]:MET:CE	2.29	0.62
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.18	0.62
2:B:123:ARG:O	2:B:127:GLU:HG2	2.00	0.62
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.81	0.61
2:D:83:PHE:O	2:D:86:ILE:HG22	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:THR:O	2:B:78:VAL:HG23	2.00	0.61
1:A:180:ALA:O	1:A:183:GLU:HG3	1.99	0.61
1:C:2:ARG:HD3	1:C:133:GLN:CG	2.31	0.61
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.19	0.61
2:D:247:GLN:NE2	11:D:604:HOH:O	2.34	0.60
4:F:200:ASP:OD1	4:F:222:ARG:NE	2.30	0.60
1:C:209:ILE:HD11	1:C:302[B]:MET:SD	2.42	0.60
2:D:104:ALA:HB2	2:D:413:MET:CE	2.33	0.59
3:E:47:LEU:O	3:E:51:GLN:HG2	2.01	0.59
1:A:285:GLN:HG2	1:A:372[B]:GLN:CG	2.32	0.59
2:D:19:LYS:O	2:D:23:VAL:HG23	2.03	0.59
2:D:357:ASP:OD1	2:D:357:ASP:N	2.32	0.59
3:E:120:LEU:O	3:E:124:GLN:HG2	2.03	0.59
2:B:287:THR:HB	2:B:289:PRO:HD2	1.85	0.58
1:C:204:VAL:HG13	1:C:302[B]:MET:HE3	1.85	0.58
2:D:334:ASN:ND2	2:D:338:LYS:HE2	2.18	0.58
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.03	0.58
2:D:286:LEU:HB2	2:D:290:GLU:OE2	2.03	0.58
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.37	0.58
2:D:317:ALA:O	2:D:318:ILE:HD13	2.04	0.58
4:F:102:PRO:HG3	4:F:173:ILE:HG22	1.84	0.58
2:B:438:ALA:HB3	11:B:630:HOH:O	2.03	0.58
4:F:99:VAL:C	4:F:100:ILE:HD12	2.24	0.58
1:A:209:ILE:HD11	1:A:302:MET:SD	2.44	0.57
4:F:197:ARG:NH1	4:F:223:THR:HG21	2.19	0.57
2:B:282:GLN:HG3	2:B:371:LEU:CD2	2.34	0.57
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.86	0.57
5:A:501:GTP:O1B	11:A:601:HOH:O	2.17	0.57
4:F:286:GLN:O	4:F:290:ILE:HG13	2.03	0.57
1:A:285:GLN:HG2	1:A:372[B]:GLN:HG2	1.87	0.57
2:B:3:GLU:OE2	2:B:129:CYS:HB3	2.04	0.57
2:B:146:GLY:O	2:B:150:GLY:HA3	2.05	0.56
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.38	0.56
1:C:41:THR:OG1	1:C:41:THR:O	2.22	0.56
8:C:503:VLB:H711	2:B:227:LEU:HD22	1.87	0.56
3:E:25:LYS:HD2	3:E:26:PRO:CD	2.35	0.56
1:A:3:GLU:O	1:A:133:GLN:HG3	2.05	0.56
2:D:153:LEU:O	2:D:157:ILE:HG13	2.05	0.56
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.88	0.56
2:D:408:TYR:HB3	2:D:413:MET:CE	2.36	0.56
1:A:311:LYS:HZ2	1:A:342:GLN:HG2	1.71	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:242:ASN:O	4:F:245:ILE:HG22	2.06	0.56
1:C:2:ARG:HD3	1:C:133:GLN:HG2	1.88	0.55
1:A:115:ILE:HD13	1:A:152:LEU:HG	1.88	0.55
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.88	0.55
3:E:25:LYS:CD	3:E:26:PRO:HD2	2.37	0.55
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.37	0.55
3:E:53:LYS:HD3	3:E:53:LYS:N	2.21	0.55
2:B:176:LYS:NZ	11:B:604:HOH:O	2.40	0.55
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.07	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.07	0.54
1:C:293[A]:ASN:HA	1:C:335:ILE:HD11	1.89	0.54
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.22	0.54
1:A:179:THR:HG21	2:B:247:GLN:HG3	1.90	0.54
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.38	0.54
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.07	0.54
2:B:83:PHE:HB3	2:B:86:ILE:CD1	2.37	0.54
4:F:160:ILE:HG22	4:F:161:LEU:H	1.71	0.54
1:C:293[B]:ASN:HA	1:C:335:ILE:HD11	1.89	0.54
2:B:75:MET:CE	2:B:94:PHE:HB3	2.30	0.53
2:D:106:GLY:O	2:D:111:GLY:HA3	2.08	0.53
2:D:408:TYR:HB3	2:D:413:MET:HE2	1.89	0.53
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.90	0.53
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.90	0.53
1:C:1:MET:HG2	1:C:130:THR:OG1	2.08	0.53
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.91	0.53
2:D:180:THR:O	2:D:181:VAL:HG22	2.09	0.53
2:D:1:MET:HE3	2:D:130:ASP:HB2	1.91	0.53
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.91	0.53
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.07	0.53
2:B:83:PHE:CD2	2:B:86:ILE:HD13	2.38	0.53
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.91	0.53
1:C:371:VAL:HG22	11:C:664:HOH:O	2.09	0.53
2:D:169:PHE:CG	2:D:235:MET:HE1	2.44	0.53
2:D:171:VAL:HA	2:D:204:ILE:O	2.09	0.53
2:D:393:GLU:O	2:D:396:THR:HG22	2.09	0.53
2:D:403:ALA:O	2:D:405:LEU:N	2.42	0.52
3:E:25:LYS:HG3	3:E:26:PRO:O	2.09	0.52
2:B:67:LEU:HD12	2:B:67:LEU:N	2.24	0.52
1:C:88:HIS:CD2	1:C:90:GLU:HG3	2.44	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.52
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.49	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:148:ILE:O	4:F:182:ILE:HG12	2.09	0.52
1:A:403:ALA:O	1:A:404:PHE:HB2	2.10	0.52
8:C:503:VLB:C22	8:C:503:VLB:C23	2.85	0.52
4:F:280:GLU:CA	4:F:284[B]:LEU:HD12	2.35	0.52
2:B:171:VAL:HA	2:B:204:ILE:O	2.10	0.52
2:B:2:ARG:HG2	2:B:131:CYS:SG	2.49	0.52
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.92	0.52
2:D:286:LEU:H	2:D:286:LEU:HD23	1.75	0.52
2:B:83:PHE:HB3	2:B:86:ILE:HD11	1.90	0.52
2:B:71:GLU:HB2	2:B:72:PRO:HD2	1.90	0.51
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.43	0.51
2:B:75:MET:HE2	2:B:94:PHE:CB	2.32	0.51
2:D:268:PHE:O	2:D:270:PRO:HD3	2.11	0.51
2:D:298:SER:HB2	2:D:307:PRO:HD2	1.91	0.51
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.92	0.51
4:F:147:TRP:HA	4:F:185:TYR:H	1.75	0.51
2:D:210:TYR:CE2	2:D:222:PRO:HD2	2.45	0.51
2:D:104:ALA:HB2	2:D:413:MET:HE2	1.93	0.51
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.93	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.93	0.51
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.10	0.51
2:B:106:GLY:O	2:B:111:GLY:HA3	2.10	0.51
4:F:148:ILE:HG12	4:F:149:ALA:N	2.26	0.51
4:F:162:ILE:HD12	4:F:162:ILE:H	1.75	0.51
2:D:406:HIS:ND1	2:D:407:TRP:HD1	2.08	0.50
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.46	0.50
2:D:332:MET:O	2:D:335:VAL:HG12	2.11	0.50
2:D:70:LEU:HD23	2:D:114:LEU:HD23	1.92	0.50
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.93	0.50
2:D:192:HIS:ND1	2:D:421:ALA:HA	2.26	0.50
4:F:187:GLU:HB2	4:F:188:LYS:HE3	1.93	0.50
3:E:131:GLU:HA	3:E:131:GLU:OE2	2.11	0.50
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.42	0.50
1:A:60:LYS:HG3	1:A:62:VAL:HG12	1.94	0.50
1:C:70:LEU:HD13	1:C:110:ILE:HG22	1.93	0.50
1:A:69:ASP:O	1:A:94:THR:HA	2.13	0.49
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.94	0.49
2:D:1:MET:CE	2:D:130:ASP:HB2	2.42	0.49
2:D:210:TYR:HE2	2:D:222:PRO:HD2	1.77	0.49
2:D:403:ALA:HB1	2:D:404:PHE:CD2	2.48	0.49
2:D:423:SER:HA	2:D:426:ASN:HB2	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:HD12	2:D:172:MET:SD	2.52	0.49
2:D:320:ARG:HA	2:D:356:CYS:O	2.13	0.49
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48
2:D:324:SER:O	2:D:328:VAL:HG23	2.13	0.48
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	1.96	0.48
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.95	0.48
2:B:40:SER:HB3	2:B:42:LEU:HB2	1.94	0.48
1:C:293[A]:ASN:OD1	1:C:339:ARG:NH2	2.27	0.48
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.48
4:F:132:LEU:O	4:F:135:TYR:HB3	2.14	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.53	0.48
4:F:160:ILE:HG22	4:F:161:LEU:N	2.27	0.48
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.53	0.48
1:C:204:VAL:HG13	1:C:302[B]:MET:CE	2.43	0.48
1:C:221:ARG:CG	2:D:325:MET:HE3	2.44	0.48
2:B:180:THR:O	2:B:183:GLU:HG3	2.14	0.48
2:B:75:MET:HE2	2:B:94:PHE:CD2	2.48	0.48
2:D:30:ILE:HD11	2:D:49:ILE:CD1	2.44	0.48
4:F:162:ILE:HD12	4:F:162:ILE:N	2.29	0.48
2:D:203:CYS:SG	2:D:384[A]:ILE:HD11	2.54	0.48
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.46	0.48
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.49	0.48
2:D:414:ASP:N	2:D:414:ASP:OD1	2.41	0.48
2:B:392:SER:O	2:B:396:THR:HG22	2.13	0.47
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.36	0.47
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	1.95	0.47
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.54	0.47
1:C:210:TYR:OH	1:C:221:ARG:HD3	2.14	0.47
1:C:276:ILE:HD11	1:C:281:ALA:N	2.29	0.47
4:F:100:ILE:HG13	4:F:128:ARG:HA	1.96	0.47
8:C:503:VLB:O24	8:C:503:VLB:H223	2.14	0.47
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.49	0.47
2:D:11:GLN:HA	2:D:74:THR:HG21	1.96	0.47
4:F:262:MET:SD	4:F:266:GLU:HG2	2.55	0.47
4:F:376:ILE:HD12	4:F:376:ILE:N	2.30	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.50	0.47
1:C:327:ASP:OD1	11:C:601:HOH:O	2.20	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.47
2:B:229:HIS:CG	2:B:278:ARG:HG3	2.49	0.47
1:C:98:ASP:HB2	5:C:501:GTP:O3G	2.15	0.47
1:A:43:GLY:HA2	1:A:56:THR:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:HIS:CD2	2:D:263:PRO:HD3	2.50	0.47
2:B:19:LYS:NZ	2:B:228:ASN:HD22	2.13	0.47
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.47	0.47
2:D:7:ILE:O	2:D:137:LEU:HD12	2.15	0.47
2:D:11:GLN:HB3	9:D:501:GDP:O2A	2.14	0.47
1:A:298:PRO:HD2	11:A:634:HOH:O	2.15	0.47
1:A:123:ARG:NH2	1:A:160:ASP:HB3	2.30	0.46
2:B:32:PRO:O	2:B:85:GLN:HG3	2.14	0.46
1:C:325:PRO:HB3	8:C:503:VLB:C65	2.44	0.46
2:D:286:LEU:N	2:D:286:LEU:HD23	2.30	0.46
1:A:399:TYR:OH	1:A:415:GLU:HG2	2.15	0.46
2:D:153:LEU:HD13	2:D:157:ILE:HG13	1.97	0.46
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.46
4:F:20:LEU:O	4:F:24:THR:HG23	2.15	0.46
2:D:241[A]:CYS:SG	2:D:318:ILE:HD12	2.56	0.46
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.98	0.46
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.96	0.46
2:D:30:ILE:N	2:D:30:ILE:HD12	2.31	0.46
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.98	0.46
2:D:387:LEU:C	2:D:387:LEU:HD23	2.35	0.46
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.16	0.46
1:C:43:GLY:HA2	1:C:56:THR:O	2.16	0.46
1:A:134:GLY:HA2	1:A:164:LYS:HB3	1.97	0.46
4:F:163:SER:HB3	4:F:169:LEU:HD11	1.98	0.45
2:D:416:MET:O	2:D:419:THR:N	2.49	0.45
2:D:66:ILE:HD12	2:D:121:VAL:HG11	1.99	0.45
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.98	0.45
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.52	0.45
1:A:221:ARG:HG2	2:B:325:MET:HB3	1.99	0.45
2:B:318:ILE:HD12	2:B:318:ILE:N	2.32	0.45
2:B:75:MET:HE2	2:B:94:PHE:HD2	1.82	0.45
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.31	0.45
9:D:501:GDP:O1A	11:D:602:HOH:O	2.21	0.45
2:B:231:VAL:O	2:B:235:MET:HG3	2.17	0.45
2:B:263:PRO:O	2:B:266:HIS:ND1	2.38	0.45
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.98	0.45
2:D:248:LEU:HD23	2:D:354:ALA:CB	2.37	0.45
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.45
2:D:392:SER:OG	11:D:601:HOH:O	2.21	0.45
2:B:286:LEU:HD21	2:B:294:GLN:NE2	2.32	0.44
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.51	0.44
3:E:44:ASP:HA	3:E:45:PRO:HD3	1.67	0.44
3:E:8:VAL:C	3:E:9:ILE:HD12	2.38	0.44
1:A:155:GLU:HG2	1:A:197:HIS:NE2	2.32	0.44
1:A:285:GLN:CG	1:A:372[B]:GLN:HG2	2.47	0.44
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.53	0.44
4:F:248:GLU:O	4:F:250:SER:N	2.42	0.44
4:F:80:LEU:O	4:F:84:SER:HB3	2.18	0.44
1:C:153:LEU:O	1:C:157:LEU:HG	2.18	0.44
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.46	0.44
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.49	0.44
3:E:52:LYS:HD3	3:E:52:LYS:O	2.18	0.44
4:F:71:LEU:HD22	4:F:298:ILE:HD13	1.98	0.44
1:C:183:GLU:N	1:C:184:PRO:CD	2.81	0.44
1:C:348:PRO:HG3	11:B:653:HOH:O	2.18	0.44
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.99	0.44
1:C:191:THR:O	1:C:195:LEU:HB2	2.18	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.52	0.43
1:C:320:ARG:HA	1:C:356:ASN:O	2.18	0.43
2:D:177:VAL:HG11	2:D:206:ASN:HB3	2.00	0.43
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.79	0.43
2:D:23:VAL:O	2:D:27:GLU:HG3	2.19	0.43
1:A:433:GLU:O	1:A:437:VAL:HG13	2.18	0.43
2:B:8:GLN:HG3	2:B:14:ASN:OD1	2.18	0.43
1:C:205:ASP:CB	1:C:303:VAL:HA	2.48	0.43
1:C:276:ILE:HD11	1:C:280:LYS:C	2.39	0.43
1:A:123:ARG:HH22	1:A:160:ASP:HB3	1.84	0.43
1:C:327:ASP:HA	11:C:601:HOH:O	2.18	0.43
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.54	0.43
1:C:41:THR:HG21	1:C:47:ASP:OD2	2.19	0.43
1:A:320:ARG:HA	1:A:356:ASN:O	2.18	0.43
1:A:372[B]:GLN:HG3	1:A:373:ARG:CZ	2.48	0.43
2:B:402:LYS:HZ1	2:B:415:GLU:CD	2.22	0.43
1:A:241:SER:HB2	1:A:248:LEU:O	2.18	0.43
1:C:270:ALA:O	1:C:302[A]:MET:HG2	2.19	0.43
2:D:8:GLN:OE1	2:D:14:ASN:HA	2.19	0.43
4:F:2:TYR:O	4:F:27:TRP:HA	2.19	0.43
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.01	0.42
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.49	0.42
1:C:88:HIS:CD2	1:C:90:GLU:H	2.37	0.42
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.54	0.42
2:D:385:GLN:HB2	2:D:429:VAL:HG13	2.01	0.42
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.86	0.42
1:C:221:ARG:HG3	2:D:325:MET:HE3	2.00	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.18	0.42
4:F:274:ALA:HB3	4:F:275[A]:LEU:HD22	2.01	0.42
2:D:67:LEU:N	2:D:67:LEU:HD12	2.34	0.42
3:E:14:CYS:SG	3:E:16:SER:HB2	2.59	0.42
4:F:184:LYS:NZ	4:F:187:GLU:HG2	2.34	0.42
4:F:307:LEU:HA	4:F:307:LEU:HD12	1.88	0.42
2:D:179:ASP:O	2:D:181:VAL:HG13	2.19	0.42
1:A:286:LEU:HD22	1:A:286:LEU:H	1.85	0.42
1:C:276:ILE:HG12	1:C:277:SER:O	2.20	0.42
1:C:36:MET:HA	1:C:37:PRO:HD2	1.84	0.42
4:F:269:GLN:HB3	11:F:420:HOH:O	2.20	0.42
3:E:9:ILE:HG22	3:E:10:GLU:N	2.34	0.41
1:C:338:LYS:O	1:C:339:ARG:HG2	2.20	0.41
2:D:137:LEU:HD12	2:D:138:THR:N	2.34	0.41
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.55	0.41
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.02	0.41
4:F:58:LEU:HA	4:F:58:LEU:HD23	1.91	0.41
1:A:141:PHE:HB3	1:A:187:SER:OG	2.21	0.41
1:C:348:PRO:HG2	2:B:181:VAL:HG23	2.02	0.41
1:C:318:LEU:HD12	1:C:318:LEU:N	2.35	0.41
2:B:239:THR:O	2:B:243:ARG:HG3	2.20	0.41
2:B:2:ARG:HD3	2:B:133:GLN:CG	2.34	0.41
2:B:393:GLU:HA	2:B:396:THR:HG22	2.03	0.41
4:F:163:SER:OG	4:F:164:SER:N	2.54	0.41
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.41
2:D:427:ASP:O	2:D:431:GLU:HG3	2.21	0.41
2:D:52:TYR:OH	2:D:136:GLN:NE2	2.43	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.50	0.41
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.86	0.41
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.23	0.41
4:F:225:SER:HB2	4:F:260:ASN:ND2	2.34	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.41
2:B:311:ARG:NH2	2:B:341:SER:O	2.53	0.41
4:F:21:LEU:HD22	4:F:27:TRP:CD1	2.56	0.41
1:A:60:LYS:CG	1:A:62:VAL:HG12	2.50	0.41
2:B:286:LEU:N	2:B:286:LEU:HD12	2.36	0.41
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:GLU:HG3	2:D:416:MET:N	2.36	0.41
1:C:41:THR:HB	1:C:44:GLY:O	2.21	0.40
1:C:88:HIS:HD2	1:C:90:GLU:HB2	1.86	0.40
4:F:165:GLU:O	4:F:168:GLU:HG2	2.21	0.40
4:F:197:ARG:NH2	4:F:257:GLU:OE1	2.44	0.40
2:D:104:ALA:HB2	2:D:413:MET:HE1	2.02	0.40
4:F:51:ARG:HD3	4:F:51:ARG:HH11	1.76	0.40
1:A:11:GLN:O	1:A:15:GLN:HG3	2.21	0.40
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.03	0.40
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.56	0.40
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	2.03	0.40
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.56	0.40
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.51	0.40
1:C:93:ILE:HD11	1:C:121:ARG:CG	2.36	0.40
2:D:141:LEU:HA	2:D:147:SER:HB3	2.03	0.40
2:D:36:TYR:CE2	2:D:46:LEU:HD11	2.56	0.40
2:B:32:PRO:O	2:B:86:ILE:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:OE1	1:C:308:ARG:NH1[3_555]	2.16	0.04

## 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	446/451 (99%)	427 (96%)	18 (4%)	1 (0%)	47	55
1	C	447/451 (99%)	433 (97%)	13 (3%)	1 (0%)	47	55
2	B	428/445 (96%)	416 (97%)	11 (3%)	1 (0%)	47	55

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	424/445 (95%)	405 (96%)	16 (4%)	3 (1%)	22	22
3	E	116/143 (81%)	114 (98%)	1 (1%)	1 (1%)	17	16
4	F	325/384 (85%)	302 (93%)	19 (6%)	4 (1%)	13	10
All	All	2186/2319 (94%)	2097 (96%)	78 (4%)	11 (0%)	29	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	181	VAL
2	D	404	PHE
4	F	231	ALA
1	C	41	THR
4	F	249	TYR
1	A	282	TYR
4	F	234	GLN
2	B	73	GLY
4	F	136	ASN
3	E	27	PRO
2	D	73	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	379/379 (100%)	374 (99%)	5 (1%)	69	81
1	C	380/379 (100%)	375 (99%)	5 (1%)	69	81
2	B	369/383 (96%)	357 (97%)	12 (3%)	38	49
2	D	370/383 (97%)	357 (96%)	13 (4%)	36	46
3	E	108/127 (85%)	97 (90%)	11 (10%)	7	6
4	F	305/342 (89%)	298 (98%)	7 (2%)	50	63
All	All	1911/1993 (96%)	1858 (97%)	53 (3%)	43	56

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	71	GLU
1	A	133	GLN
1	A	280	LYS
1	A	335	ILE
1	C	71	GLU
1	C	221	ARG
1	C	290	GLU
1	C	384	ILE
1	C	430	LYS
2	D	15	GLN
2	D	26	ASP
2	D	39	ASP
2	D	57	THR
2	D	80	SER
2	D	90	ASP
2	D	139	HIS
2	D	153	LEU
2	D	247	GLN
2	D	325	MET
2	D	357	ASP
2	D	402	LYS
2	D	406	HIS
3	E	10	GLU
3	E	44	ASP
3	E	45	PRO
3	E	59	GLU
3	E	64	GLN
3	E	67	GLU
3	E	68	LEU
3	E	77	GLU
3	E	116	LEU
3	E	120	LEU
3	E	126	LYS
4	F	162	ILE
4	F	186	LEU
4	F	188	LYS
4	F	198	LYS
4	F	222	ARG
4	F	266	GLU
4	F	292	ARG
2	B	2	ARG
2	B	15	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	39	ASP
2	B	42	LEU
2	B	46	LEU
2	B	75	MET
2	B	77	SER
2	B	139	HIS
2	B	167	ASN
2	B	181	VAL
2	B	200	GLU
2	B	207	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	HIS
4	F	260	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
10	MES	B	503	-	12,12,12	2.68	1 (8%)	14,16,16	1.59	3 (21%)
8	VLB	C	503	-	63,67,67	2.31	15 (23%)	79,108,108	2.46	25 (31%)
9	GDP	D	501	-	24,30,30	1.17	2 (8%)	31,47,47	2.00	8 (25%)
5	GTP	A	501	-	26,34,34	1.03	1 (3%)	33,54,54	1.70	7 (21%)
9	GDP	B	501	6	24,30,30	1.05	3 (12%)	31,47,47	1.90	9 (29%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.97	9 (27%)

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
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
8	VLB	C	503	-	-	6/38/131/131	0/7/9/9
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3
5	GTP	A	501	-	-	8/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	503	VLB	C59-C67	9.82	1.53	1.39
10	B	503	MES	C8-S	-9.17	1.64	1.77
8	C	503	VLB	C16-C15	6.69	1.51	1.39
8	C	503	VLB	O75-C73	5.45	1.43	1.33
8	C	503	VLB	O25-C23	4.82	1.42	1.33
8	C	503	VLB	C18-C13	4.76	1.45	1.39
9	D	501	GDP	C6-C5	4.11	1.48	1.41
8	C	503	VLB	O28-C29	4.00	1.44	1.35
8	C	503	VLB	C68-C67	3.30	1.57	1.53
9	B	501	GDP	C6-C5	3.30	1.47	1.41
8	C	503	VLB	C57-N56	2.95	1.54	1.47
5	A	501	GTP	C6-N1	2.80	1.37	1.33
8	C	503	VLB	C68-C73	-2.70	1.51	1.53
8	C	503	VLB	C64-C65	-2.62	1.37	1.41
9	D	501	GDP	C5-C4	2.51	1.47	1.40
8	C	503	VLB	C51-C52	2.49	1.60	1.53
8	C	503	VLB	C61-C60	-2.41	1.37	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	503	VLB	C51-C68	2.18	1.58	1.56
9	B	501	GDP	O4'-C1'	2.16	1.44	1.41
5	C	501	GTP	C6-N1	2.13	1.36	1.33
8	C	503	VLB	C18-N1	-2.08	1.35	1.39
9	B	501	GDP	C5-C4	2.05	1.46	1.40
8	C	503	VLB	C57-C58	2.03	1.58	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	503	VLB	C52-C69-N56	10.67	127.99	111.28
5	C	501	GTP	N3-C2-N1	-5.81	119.48	127.22
8	C	503	VLB	O75-C73-C68	5.19	119.12	111.32
8	C	503	VLB	O32-C16-C15	5.15	121.85	116.58
8	C	503	VLB	C33-O32-C16	5.03	125.12	117.53
9	D	501	GDP	C2-N3-C4	4.87	120.92	115.36
5	A	501	GTP	N3-C2-N1	-4.71	120.95	127.22
8	C	503	VLB	C58-C57-N56	4.59	123.69	113.44
9	D	501	GDP	C6-N1-C2	4.36	122.86	115.93
9	B	501	GDP	C6-N1-C2	4.33	122.81	115.93
8	C	503	VLB	O25-C23-C3	4.32	119.48	112.22
9	B	501	GDP	C6-C5-C4	-4.25	116.75	120.80
9	D	501	GDP	C5-C6-N1	-4.23	117.64	123.43
5	C	501	GTP	C6-N1-C2	4.13	122.50	115.93
8	C	503	VLB	C20-C5-C6	-4.10	103.11	107.99
5	C	501	GTP	C5-C6-N1	-4.04	117.91	123.43
9	B	501	GDP	C5-C6-N1	-3.87	118.14	123.43
9	B	501	GDP	C2-N3-C4	3.83	119.73	115.36
8	C	503	VLB	C12-C19-C5	-3.74	115.42	118.20
8	C	503	VLB	C19-C5-C6	3.72	112.09	108.28
5	C	501	GTP	C2-N3-C4	3.66	119.53	115.36
9	D	501	GDP	C6-C5-C4	-3.57	117.39	120.80
8	C	503	VLB	O25-C23-O24	-3.57	117.68	123.93
8	C	503	VLB	C2-C12-C19	3.55	120.08	114.07
8	C	503	VLB	C54-C53-C52	3.53	120.37	110.02
8	C	503	VLB	O28-C29-C30	3.45	117.43	111.09
9	D	501	GDP	N3-C2-N1	-3.42	122.66	127.22
8	C	503	VLB	C53-C52-C69	-3.37	104.78	108.72
9	B	501	GDP	N3-C2-N1	-3.34	122.76	127.22
5	A	501	GTP	C2-N3-C4	3.34	119.17	115.36
5	A	501	GTP	C5-C6-N1	-3.29	118.93	123.43
8	C	503	VLB	O32-C16-C17	-3.28	118.47	124.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	503	VLB	O75-C73-O74	-3.26	118.22	123.93
8	C	503	VLB	C8-N9-C19	3.22	120.91	112.50
8	C	503	VLB	C5-C19-N9	3.07	118.19	111.72
9	D	501	GDP	PA-O3A-PB	-2.95	122.69	132.83
8	C	503	VLB	C61-C60-C65	2.95	122.08	118.17
10	B	503	MES	O3S-S-C8	2.93	110.51	105.77
8	C	503	VLB	C76-O75-C73	2.90	120.82	115.94
8	C	503	VLB	C22-N1-C2	2.85	126.17	119.21
5	A	501	GTP	O2G-PG-O3B	2.85	114.20	104.64
9	D	501	GDP	C4-C5-N7	-2.81	106.47	109.40
5	A	501	GTP	C6-N1-C2	2.75	120.30	115.93
9	B	501	GDP	O2B-PB-O3A	2.75	113.84	104.64
8	C	503	VLB	C17-C16-C15	-2.73	119.68	122.20
10	B	503	MES	O1S-S-C8	2.67	110.13	106.92
10	B	503	MES	C6-O1-C2	2.59	118.54	109.89
5	A	501	GTP	PA-O3A-PB	-2.57	124.00	132.83
5	C	501	GTP	PB-O3B-PG	-2.55	124.08	132.83
8	C	503	VLB	C61-C60-C59	-2.47	129.91	134.17
9	B	501	GDP	C4-C5-N7	-2.42	106.87	109.40
9	B	501	GDP	PA-O3A-PB	-2.41	124.57	132.83
8	C	503	VLB	C11-C12-C13	-2.40	107.98	112.35
5	C	501	GTP	C6-C5-C4	-2.33	118.57	120.80
5	A	501	GTP	PB-O3B-PG	-2.25	125.10	132.83
9	D	501	GDP	O4'-C1'-C2'	-2.18	103.74	106.93
5	C	501	GTP	PA-O3A-PB	-2.18	125.35	132.83
5	C	501	GTP	O4'-C1'-C2'	-2.09	103.87	106.93
9	B	501	GDP	C1'-N9-C4	-2.09	122.97	126.64
8	C	503	VLB	C64-C65-C60	-2.02	117.07	120.76
5	C	501	GTP	N2-C2-N3	2.00	121.05	117.79

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	503	VLB	C3-C23-O25-C26
9	D	501	GDP	C5'-O5'-PA-O1A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O2A
8	C	503	VLB	O24-C23-O25-C26
8	C	503	VLB	O24-C23-C3-C4
8	C	503	VLB	O25-C23-C3-C4
8	C	503	VLB	C53-C54-C70-C71
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	PB-O3A-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
8	C	503	VLB	C58-C57-N56-C69
10	B	503	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A

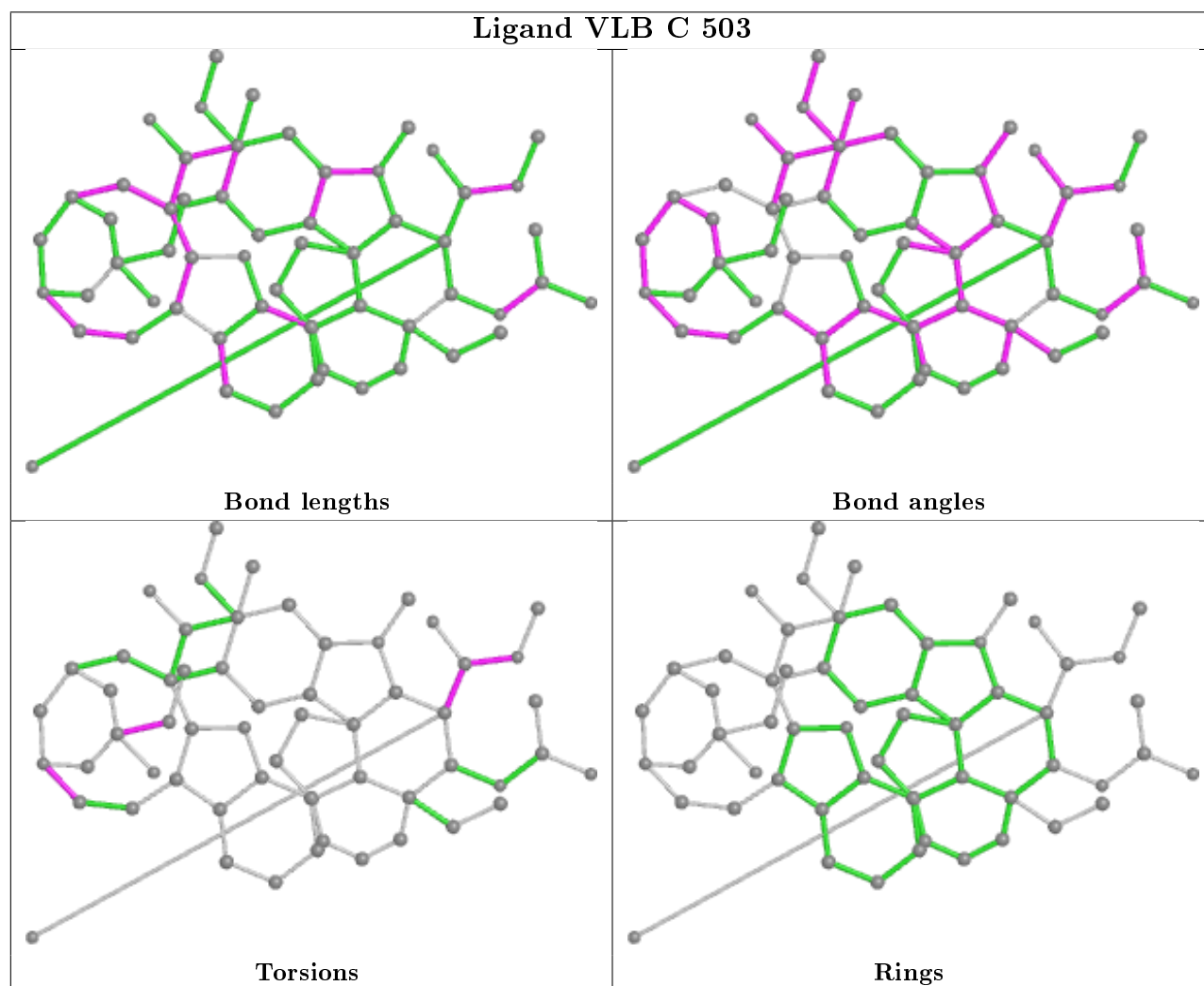
There are no ring outliers.

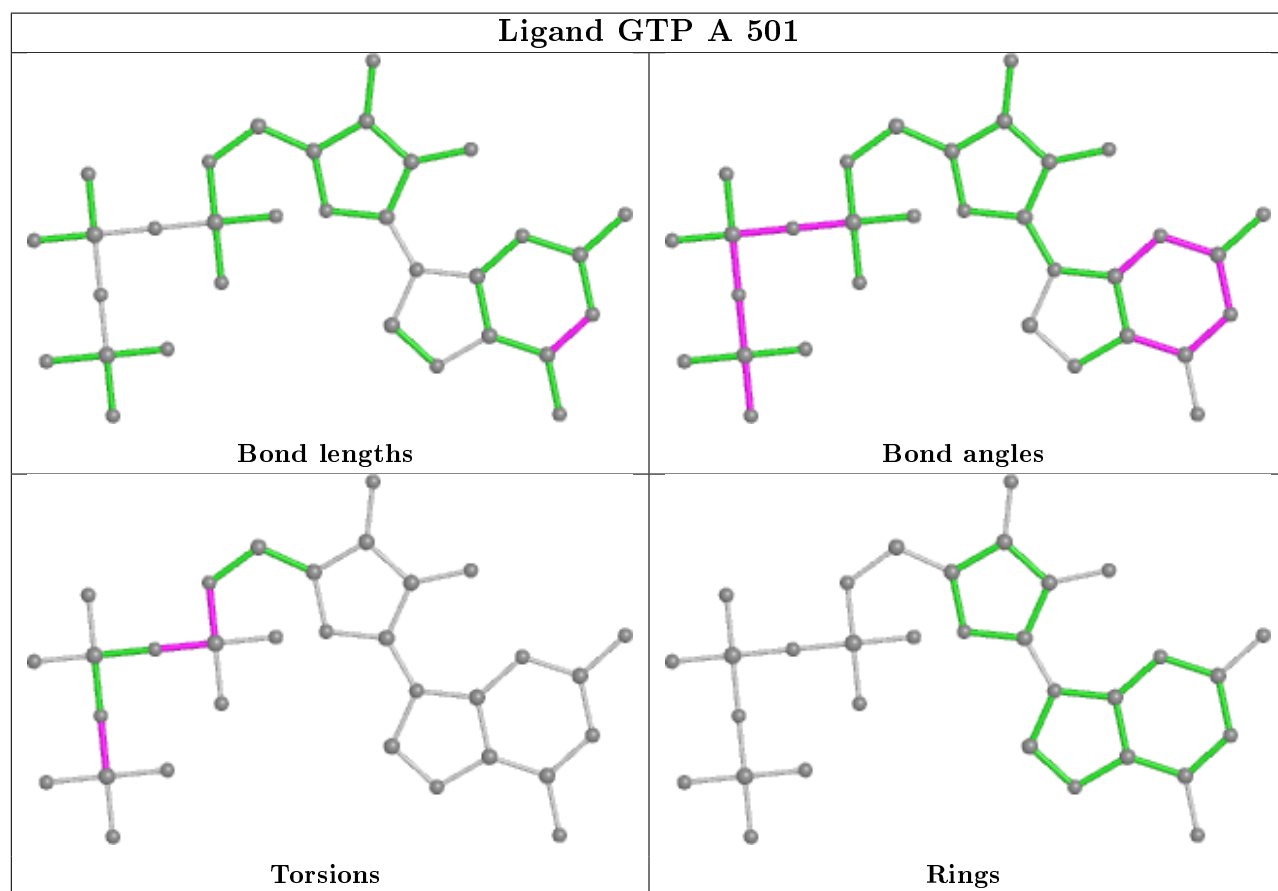
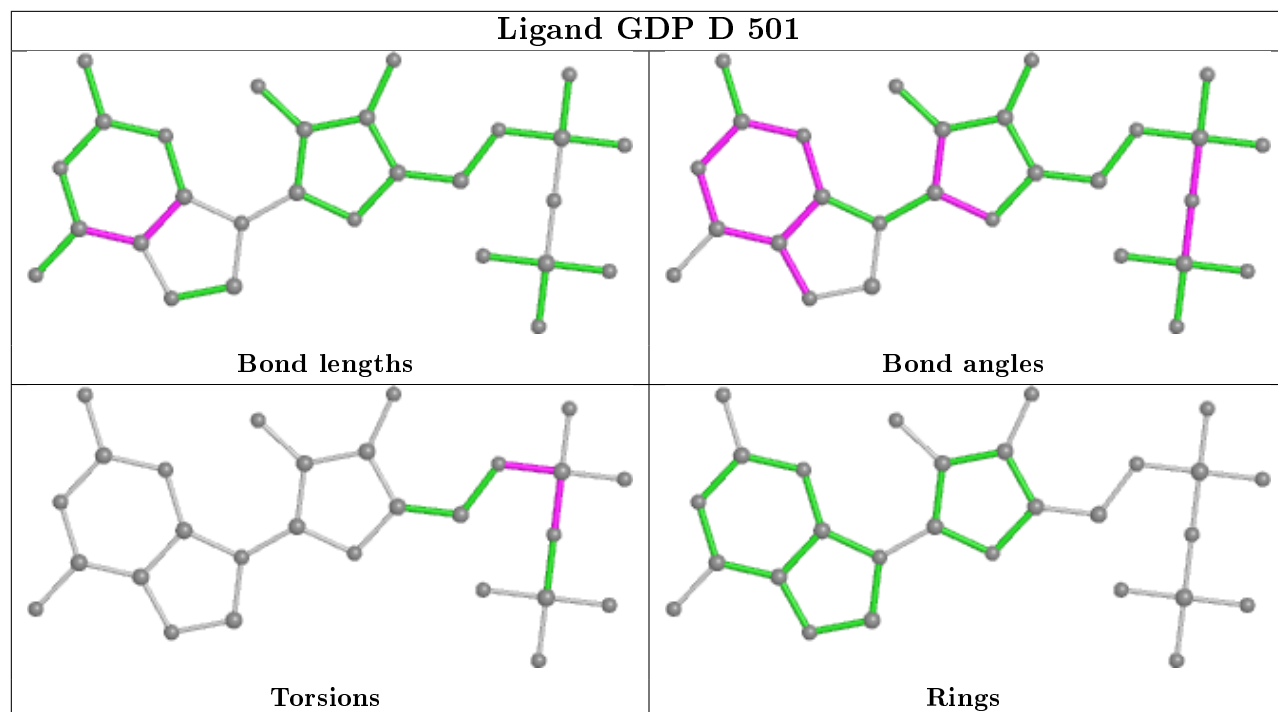
6 monomers are involved in 15 short contacts:

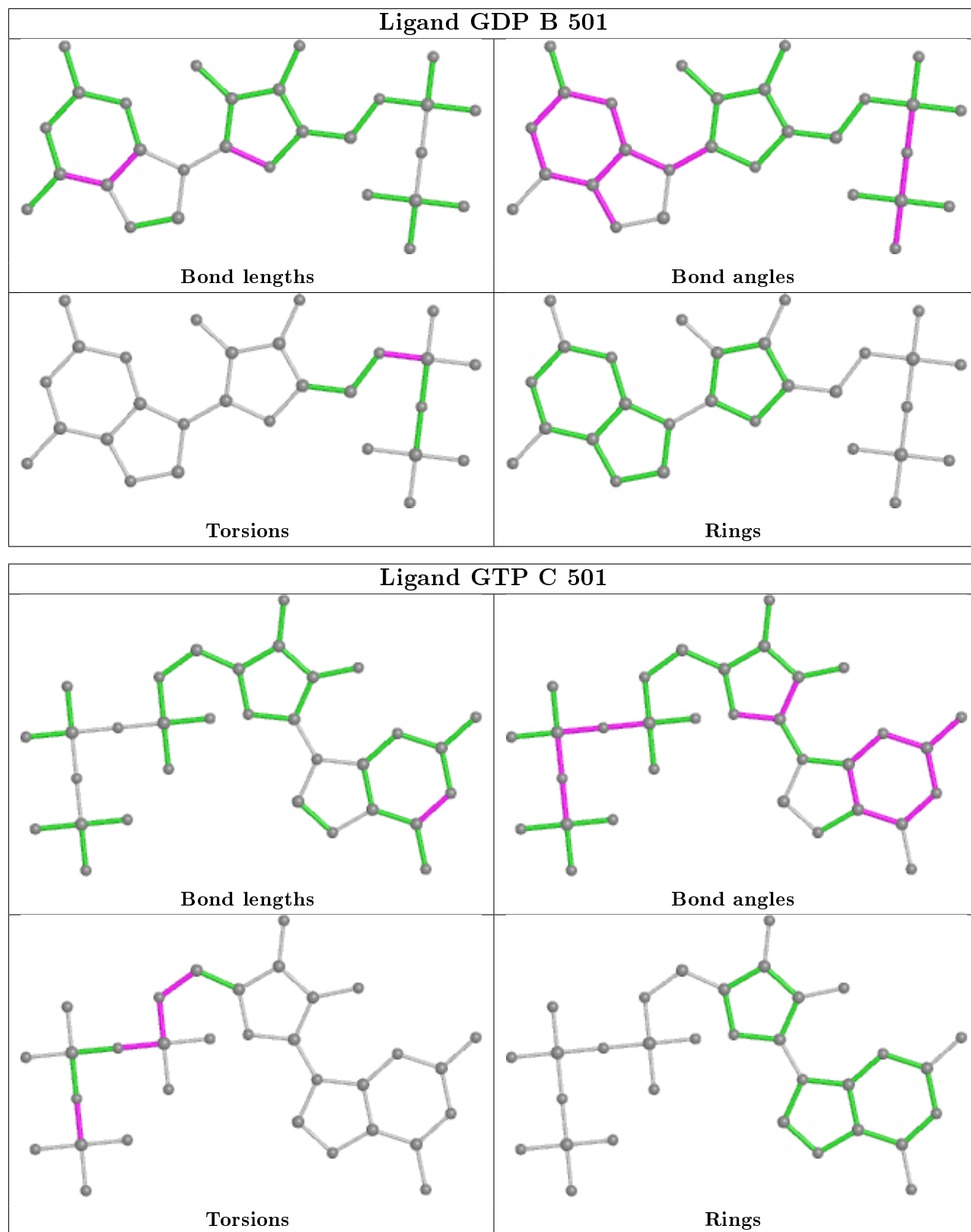
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	1	0
8	C	503	VLB	5	0
9	D	501	GDP	4	0
5	A	501	GTP	3	0
9	B	501	GDP	1	0
5	C	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

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	439/451 (97%)	0.03	13 (2%) 50 48	41, 63, 97, 155	0
1	C	440/451 (97%)	-0.15	2 (0%) 91 90	35, 50, 83, 105	0
2	B	428/445 (96%)	-0.02	9 (2%) 63 61	34, 52, 90, 141	2 (0%)
2	D	424/445 (95%)	0.17	19 (4%) 33 32	46, 75, 112, 162	6 (1%)
3	E	120/143 (83%)	0.02	4 (3%) 46 44	47, 78, 107, 121	0
4	F	331/384 (86%)	0.84	79 (23%) 0 0	47, 84, 152, 186	0
All	All	2182/2319 (94%)	0.13	126 (5%) 23 22	34, 64, 114, 186	8 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	8.1
2	D	1	MET	7.4
4	F	233	PHE	7.3
4	F	161	LEU	6.7
4	F	232	ASN	6.3
4	F	133	ALA	5.6
4	F	100	ILE	4.8
4	F	132	LEU	4.8
4	F	231	ALA	4.8
4	F	182	ILE	4.6
4	F	225	SER	4.6
4	F	234	GLN	4.6
4	F	255	ARG	4.5
4	F	173	ILE	4.5
4	F	250	SER	4.4
4	F	256	TYR	4.3
4	F	249	TYR	4.2
4	F	136	ASN	4.2
4	F	239	HIS	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	362	ALA	4.1
2	D	37	HIS	4.1
4	F	235	ASP	4.0
4	F	236	LYS	4.0
4	F	186	LEU	3.9
4	F	361	LEU	3.9
4	F	177	GLY	3.9
4	F	147	TRP	3.8
4	F	103	THR	3.8
2	D	284	ARG	3.8
2	D	400	ARG	3.8
1	A	438	ASP	3.7
4	F	160	ILE	3.7
2	D	57	THR	3.7
4	F	245	ILE	3.7
1	A	42	ILE	3.6
4	F	101	TYR	3.6
4	F	146	VAL	3.6
1	A	282	TYR	3.6
2	B	59	ASN	3.5
4	F	163	SER	3.5
4	F	17	VAL	3.5
4	F	131	PHE	3.4
4	F	172	PHE	3.4
3	E	27	PRO	3.4
2	D	179	ASP	3.4
4	F	20	LEU	3.4
4	F	148	ILE	3.3
2	D	405	LEU	3.3
4	F	99	VAL	3.3
4	F	21	LEU	3.3
4	F	169	LEU	3.2
4	F	162	ILE	3.2
4	F	102	PRO	3.2
4	F	170	LEU	3.2
2	D	219	LEU	3.1
3	E	25	LYS	3.1
4	F	228	TYR	3.1
1	C	253	THR	3.1
4	F	238	CYS	3.1
2	D	218	LYS	3.0
2	D	285	ALA	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	404	PHE	3.0
4	F	178	GLN	3.0
4	F	247	LYS	3.0
4	F	176	GLN	2.9
1	A	439	SER	2.9
2	B	56	ALA	2.9
4	F	246	GLN	2.8
1	A	281	ALA	2.8
4	F	135	TYR	2.8
4	F	185	TYR	2.8
1	A	283	HIS	2.8
1	A	345	ASP	2.7
4	F	197	ARG	2.8
2	B	282	GLN	2.7
4	F	149	ALA	2.7
4	F	223	THR	2.7
4	F	259	GLY	2.7
4	F	227	PRO	2.6
4	F	243	HIS	2.6
2	B	57	THR	2.6
4	F	22	LEU	2.6
2	D	82	PRO	2.6
2	D	94	PHE	2.6
4	F	229	ASN	2.6
4	F	258	GLU	2.6
2	D	406	HIS	2.5
4	F	179	VAL	2.5
1	A	201	ALA	2.5
4	F	174	ASP	2.5
1	A	179	THR	2.5
4	F	181	VAL	2.4
4	F	24	THR	2.4
4	F	192	LEU	2.4
4	F	248	GLU	2.4
2	D	96	GLN	2.4
2	D	401	ARG	2.4
4	F	240	LEU	2.4
2	B	82	PRO	2.4
4	F	222	ARG	2.4
4	F	165	GLU	2.4
4	F	18	SER	2.3
1	A	437	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	2.3
2	D	177	VAL	2.3
2	B	55	GLU	2.2
4	F	167	SER	2.2
4	F	187	GLU	2.2
2	D	402	LYS	2.2
4	F	125	THR	2.2
4	F	168	GLU	2.2
4	F	194	PRO	2.2
1	A	172	TYR	2.2
1	C	340	SER	2.2
4	F	25	GLY	2.2
1	A	430	LYS	2.1
4	F	145	ASN	2.1
4	F	166	ALA	2.1
4	F	14	TYR	2.1
1	A	56	THR	2.1
3	E	24	LEU	2.1
2	B	283	TYR	2.1
2	D	399	PHE	2.1
3	E	26	PRO	2.0
2	B	37	HIS	2.0
4	F	126	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

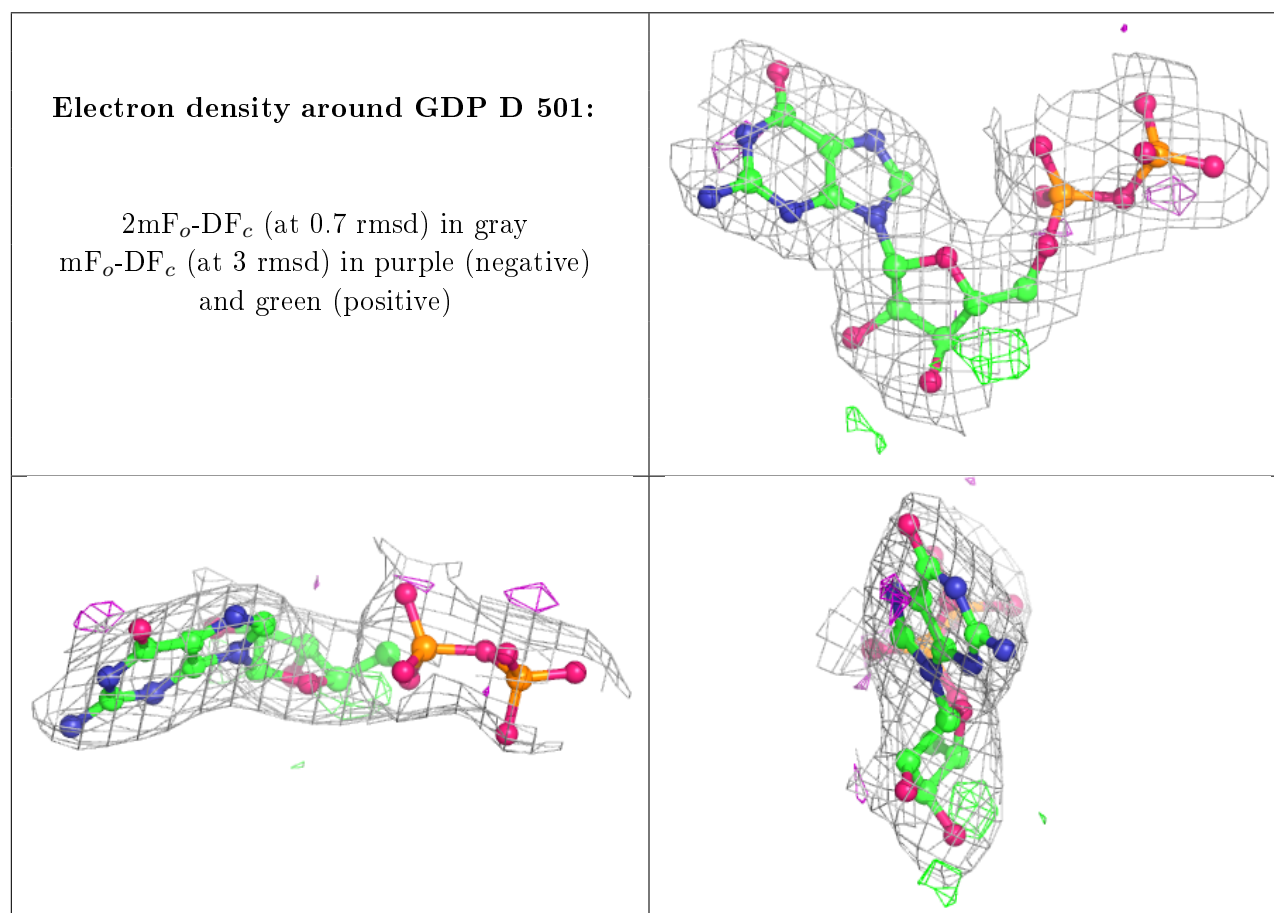
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

*Continued on next page...*

*Continued from previous page...*

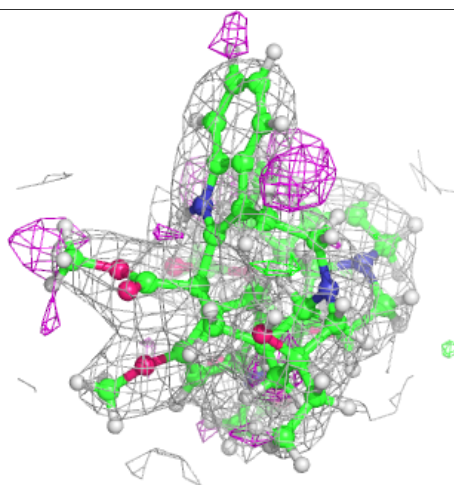
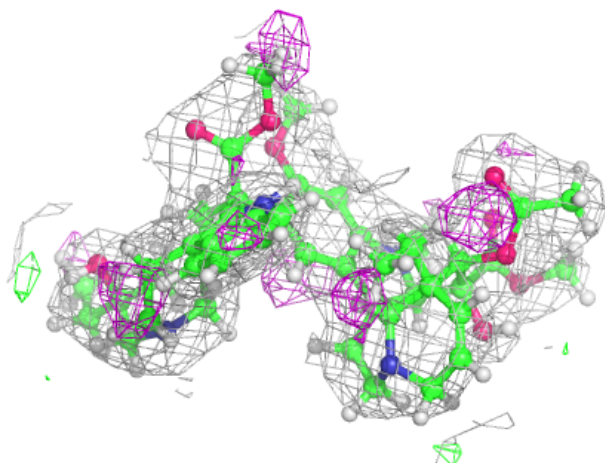
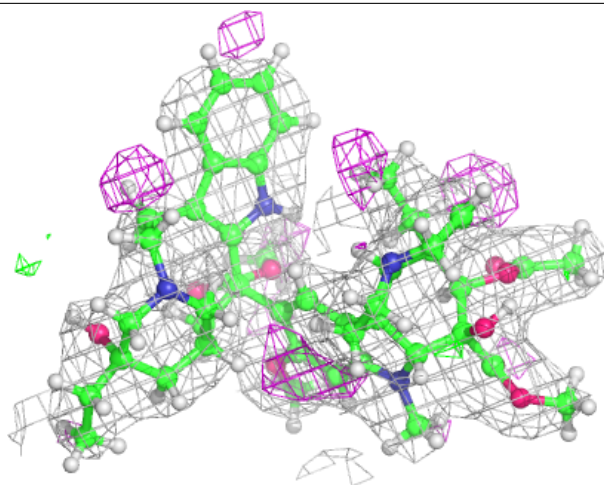
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MES	B	503	12/12	0.77	0.18	53,75,130,134	0
6	MG	C	502	1/1	0.90	0.21	42,42,42,42	0
7	CA	A	503	1/1	0.90	0.05	96,96,96,96	0
6	MG	B	502	1/1	0.92	0.55	85,85,85,85	0
9	GDP	D	501	28/28	0.94	0.11	54,69,83,97	0
8	VLB	C	503	59/59	0.96	0.10	30,48,64,84	0
6	MG	A	502	1/1	0.97	0.12	56,56,56,56	0
5	GTP	C	501	32/32	0.97	0.16	32,41,49,67	0
5	GTP	A	501	32/32	0.98	0.19	41,47,53,64	0
9	GDP	B	501	28/28	0.99	0.19	32,39,45,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



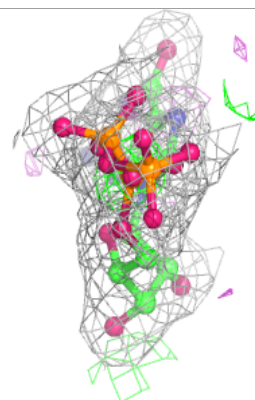
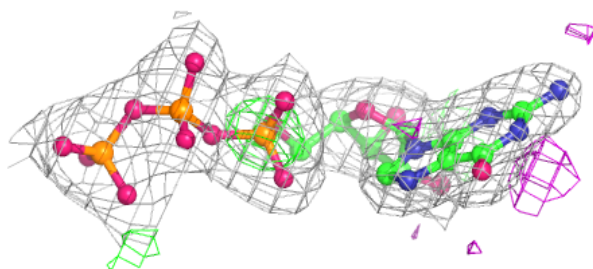
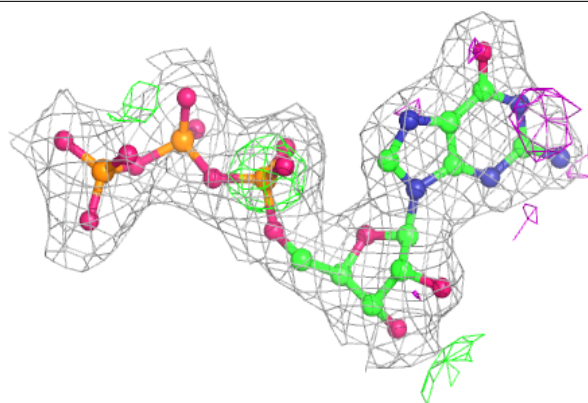
**Electron density around VLB C 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

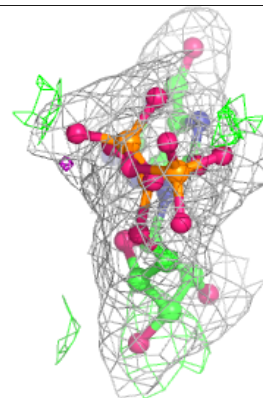
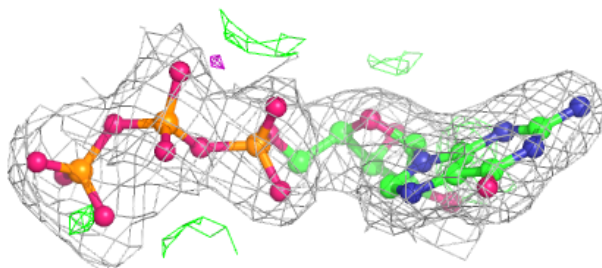
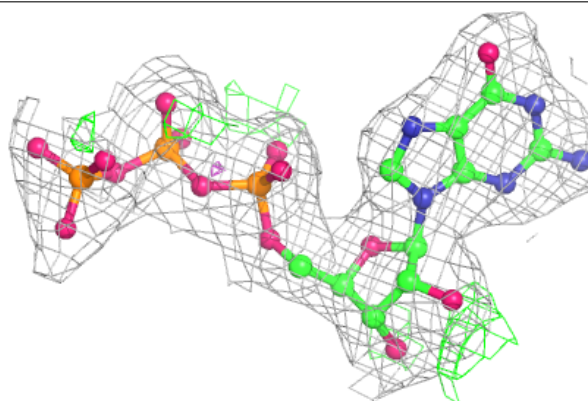


**Electron density around GTP C 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

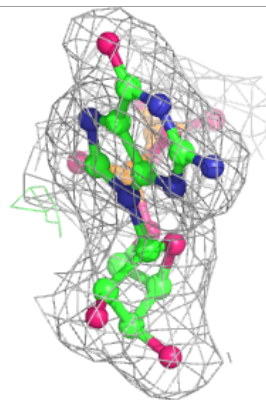
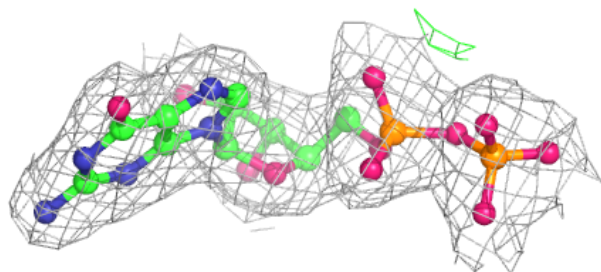
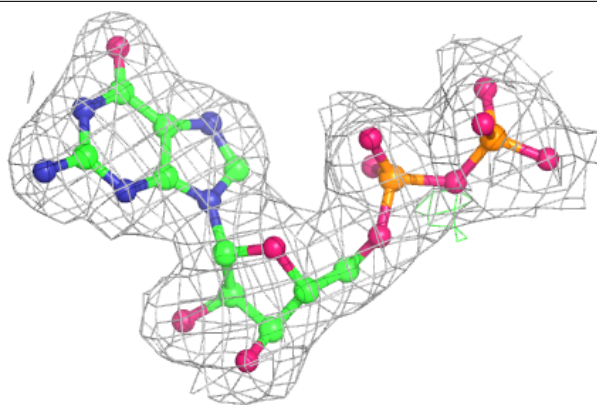
**Electron density around GTP A 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GDP B 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.