



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:50 PM BST

PDB ID : 6BBN  
Title : Crystal structure of a curved tubulin complex induced by the kinesin-13 Kif2A  
Authors : Allingham, J.S.; Trofimova, D.  
Deposited on : 2017-10-19  
Resolution : 3.51 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.

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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 : 1.8.5 (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

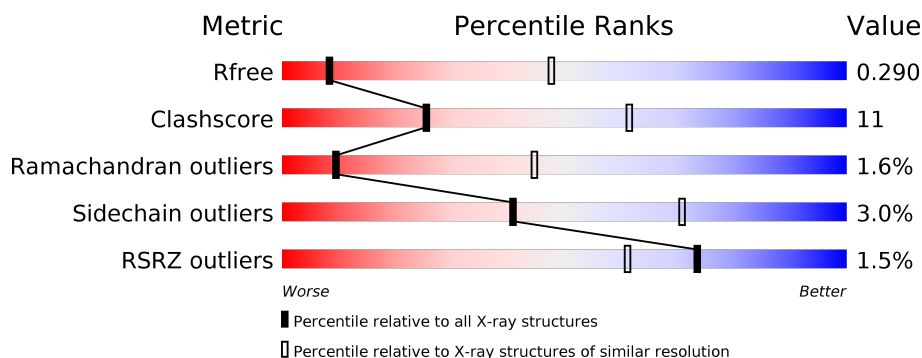
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.51 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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>70%</div> <div>26%</div> <div>• •</div> </div>
1	C	451	<div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
2	B	445	<div> <div>72%</div> <div>24%</div> <div>• •</div> </div>
2	D	445	<div> <div>2%</div> <div>71%</div> <div>25%</div> <div>• •</div> </div>
3	P	168	<div> <div>11%</div> <div>62%</div> <div>29%</div> <div>• 8%</div> </div>
4	E	420	<div> <div>62%</div> <div>25%</div> <div>• 10%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17794 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3392	2148	578	645	21			
1	C	436	Total	C	N	O	S	0	0	0
			3386	2142	576	646	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3372	2114	576	655	27			
2	D	431	Total	C	N	O	S	0	0	0
			3376	2118	576	656	26			

- Molecule 3 is a protein called DARPin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	155	Total	C	N	O	S	0	0	0
			1128	710	194	221	3			

- Molecule 4 is a protein called Kinesin-like protein KIF2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	378	Total	C	N	O	S	0	1	0
			2980	1859	544	557	20			

There are 19 discrepancies between the modelled and reference sequences:

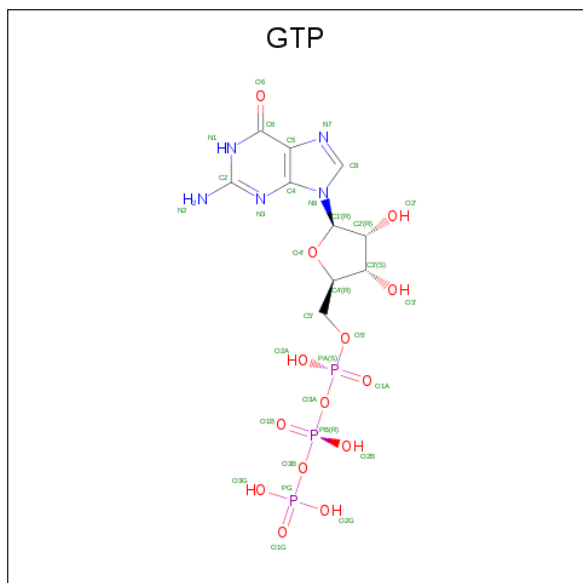
Chain	Residue	Modelled	Actual	Comment	Reference
E	134	MET	-	expression tag	UNP O00139
E	135	GLY	-	expression tag	UNP O00139
E	136	SER	-	expression tag	UNP O00139
E	137	SER	-	expression tag	UNP O00139

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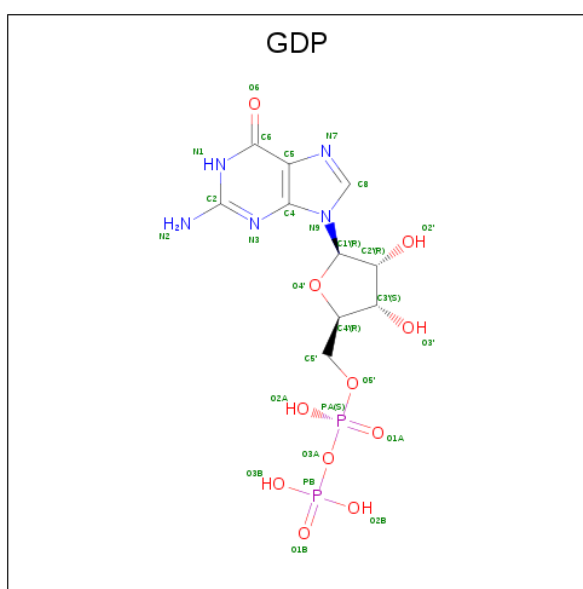
Chain	Residue	Modelled	Actual	Comment	Reference
E	138	HIS	-	expression tag	UNP O00139
E	139	HIS	-	expression tag	UNP O00139
E	140	HIS	-	expression tag	UNP O00139
E	141	HIS	-	expression tag	UNP O00139
E	142	HIS	-	expression tag	UNP O00139
E	143	HIS	-	expression tag	UNP O00139
E	144	SER	-	expression tag	UNP O00139
E	145	SER	-	expression tag	UNP O00139
E	146	GLY	-	expression tag	UNP O00139
E	147	LEU	-	expression tag	UNP O00139
E	148	VAL	-	expression tag	UNP O00139
E	149	PRO	-	expression tag	UNP O00139
E	150	ARG	-	expression tag	UNP O00139
E	151	GLY	-	expression tag	UNP O00139
E	152	SER	-	expression tag	UNP O00139

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



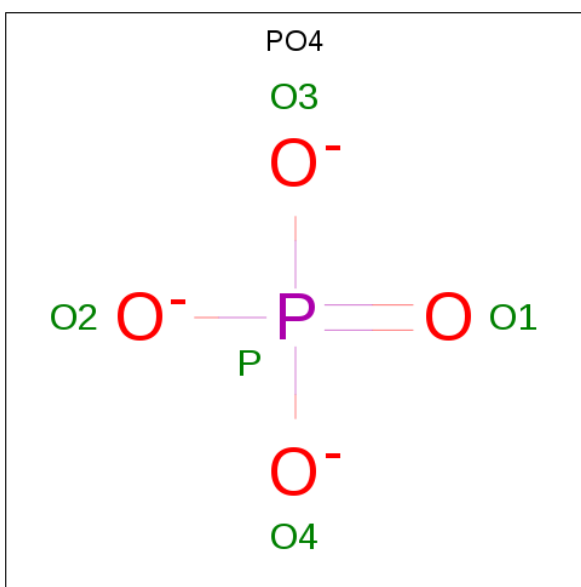
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	A	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	E	1	Total Mg 1 1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



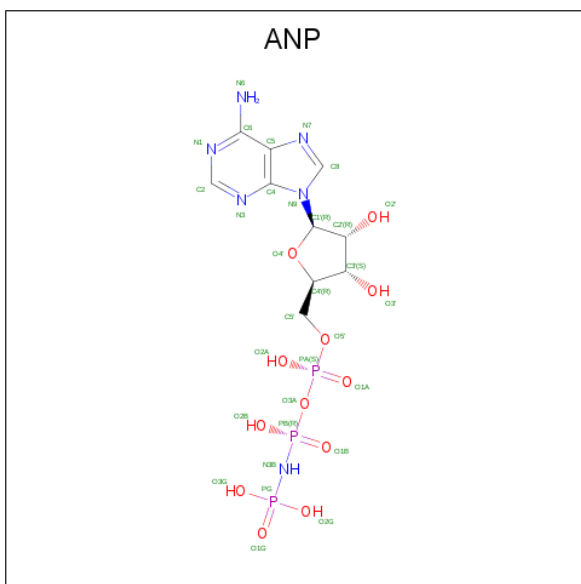
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 28 10 5 11 2	0	0
7	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$ ).

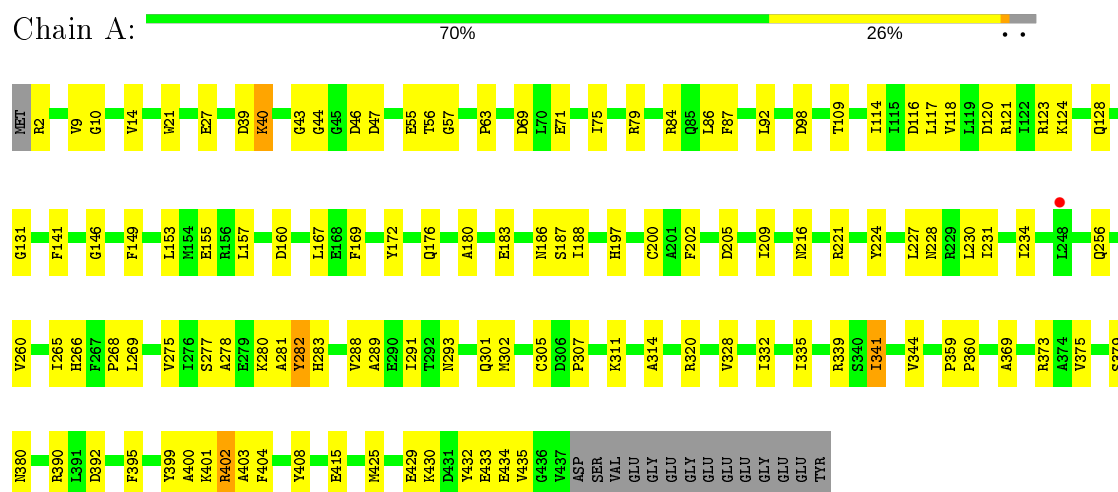


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

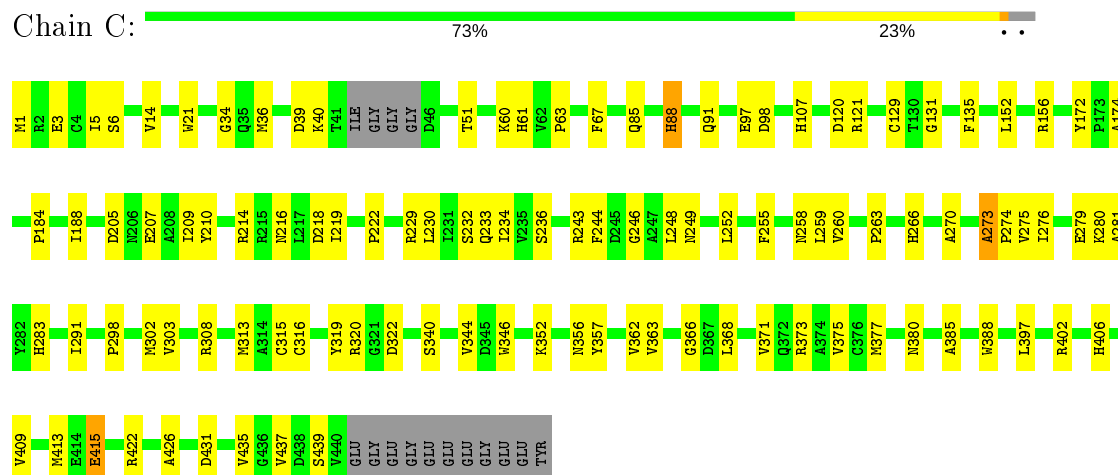
### 3 Residue-property plots

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

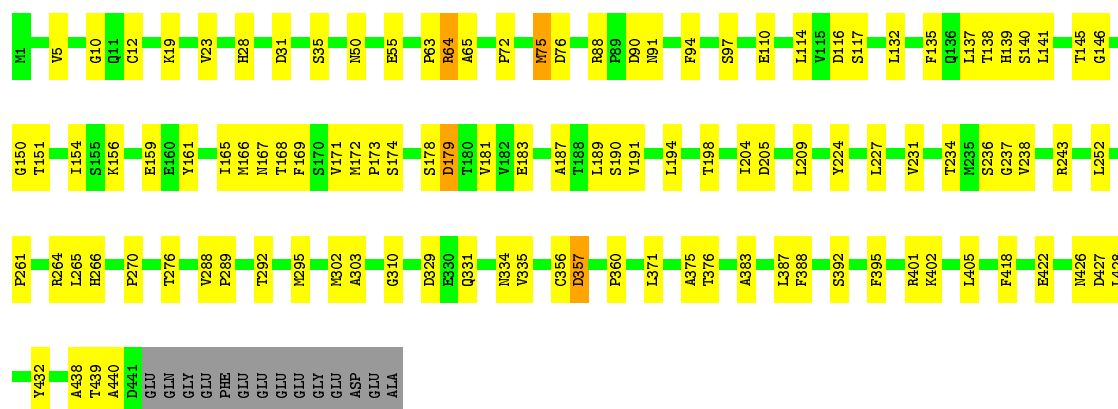


#### • Molecule 1: Tubulin alpha-1B chain

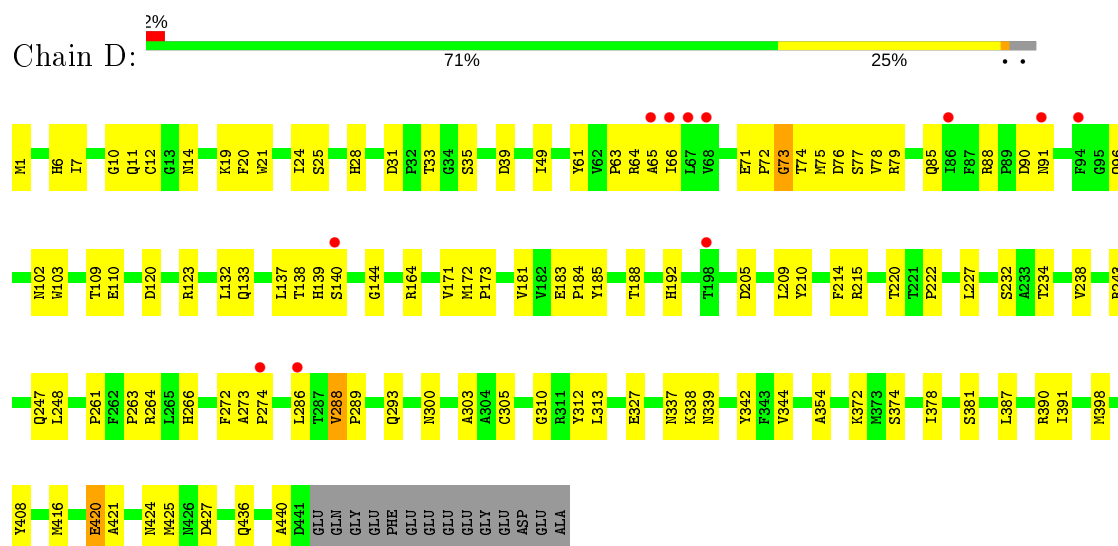


#### • Molecule 2: Tubulin beta-2B chain

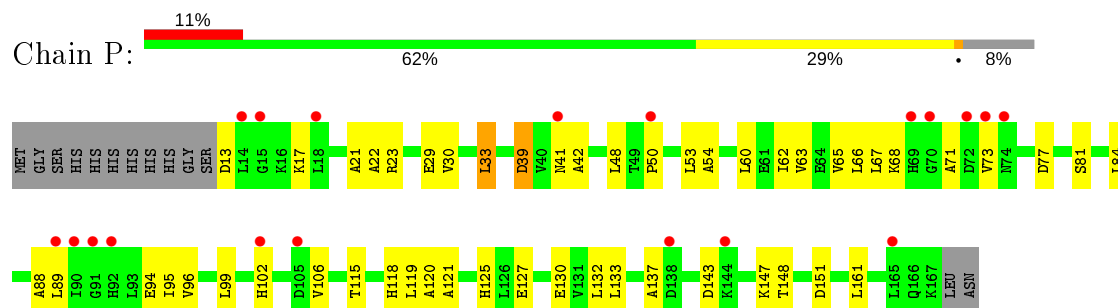




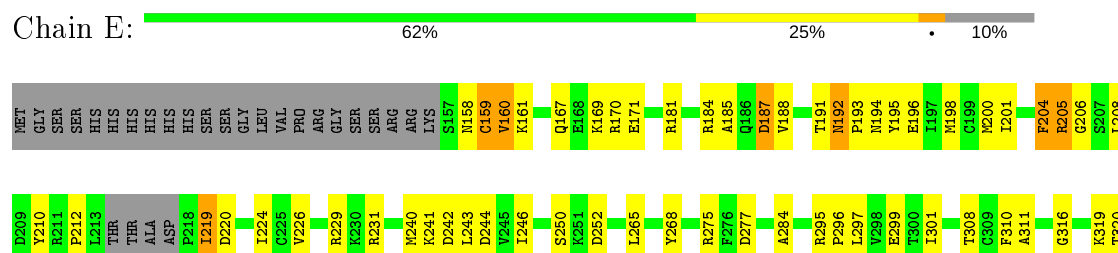
• Molecule 2: Tubulin beta-2B chain



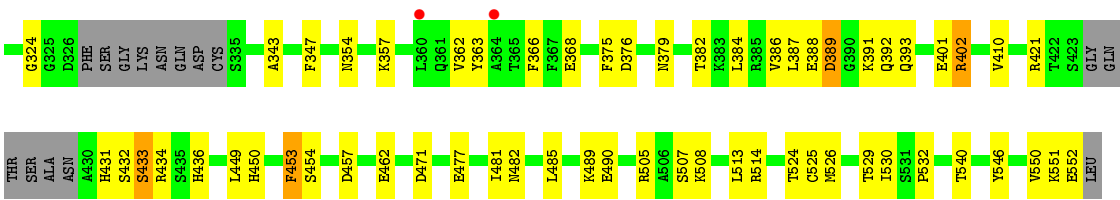
• Molecule 3: DARPin



• Molecule 4: Kinesin-like protein KIF2A







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.05Å 82.19Å 147.66Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	49.22 – 3.51 49.22 – 3.51	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.22-3.51) 96.8 (49.22-3.51)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.236 , 0.287 0.242 , 0.290	Depositor DCC
$R_{free}$ test set	1964 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	117.0	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.068 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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, GTP, PO4, ANP, MG

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	0.27	0/3469	0.45	0/4711
1	C	0.29	0/3462	0.47	0/4705
2	B	0.28	0/3446	0.45	0/4670
2	D	0.27	0/3451	0.44	0/4678
3	P	0.24	0/1143	0.43	0/1556
4	E	0.33	0/3025	0.53	0/4067
All	All	0.28	0/17996	0.47	0/24387

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	3392	0	3297	78	0
1	C	3386	0	3274	74	0
2	B	3372	0	3237	61	0
2	D	3376	0	3237	72	0
3	P	1128	0	1110	32	0
4	E	2980	0	2962	75	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	B	28	0	12	0	0
7	D	28	0	12	0	0
8	D	5	0	0	1	0
9	E	31	0	13	1	0
All	All	17794	0	17178	372	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 11.

All (372) 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:A:430:LYS:O	1:A:434:GLU:OE2	1.56	1.21
4:E:181:ARG:O	4:E:185:ALA:N	2.05	0.90
1:A:430:LYS:C	1:A:434:GLU:OE2	2.17	0.83
3:P:62:ILE:O	3:P:66:LEU:HB2	1.80	0.81
2:D:420:GLU:OE1	4:E:505:ARG:NH2	2.14	0.80
1:A:400:ALA:HB1	4:E:158:ASN:HD22	1.50	0.77
3:P:133:LEU:HD23	3:P:137:ALA:HB3	1.67	0.75
1:A:403:ALA:HB1	2:B:261:PRO:HB2	1.69	0.75
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.69	0.75
1:C:402:ARG:NH1	1:C:415:GLU:OE1	2.20	0.74
4:E:159:CYS:O	4:E:161:LYS:N	2.20	0.74
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.68	0.74
1:A:2:ARG:N	1:A:131:GLY:O	2.22	0.72
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.21	0.72
2:D:10:GLY:O	2:D:14:ASN:ND2	2.23	0.72
2:D:19:LYS:HB3	2:D:232:SER:HB3	1.72	0.72
2:D:7:ILE:HG12	2:D:66:ILE:HB	1.70	0.72
4:E:159:CYS:SG	4:E:160:VAL:N	2.63	0.71
2:B:166:MET:HG3	2:B:198:THR:HG22	1.72	0.71
3:P:39:ASP:HB3	3:P:42:ALA:HB2	1.72	0.71
1:A:27:GLU:OE1	1:A:320:ARG:NH1	2.22	0.70
4:E:246:ILE:HD13	4:E:532:PRO:HA	1.74	0.70
1:C:255:PHE:HA	1:C:258:ASN:HD22	1.55	0.70
1:A:153:LEU:O	1:A:157:LEU:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:NZ	1:A:47:ASP:H	1.90	0.69
2:D:73:GLY:O	2:D:75:MET:N	2.26	0.69
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.74	0.69
1:C:298:PRO:HG2	1:C:308:ARG:HH21	1.58	0.69
2:B:12:CYS:HB3	2:B:140:SER:HB3	1.74	0.69
2:B:427:ASP:OD1	4:E:170:ARG:NH2	2.25	0.69
1:A:289:ALA:O	1:A:293:ASN:ND2	2.26	0.69
3:P:88:ALA:HB1	3:P:120:ALA:HB2	1.75	0.69
3:P:121:ALA:HB1	3:P:161:LEU:HD21	1.75	0.68
1:A:216:ASN:HD22	1:A:275:VAL:HG13	1.58	0.68
2:B:173:PRO:HB3	2:B:183:GLU:HB3	1.75	0.68
1:A:320:ARG:HG3	1:A:360:PRO:HG3	1.75	0.67
4:E:310:PHE:HB2	4:E:526:MET:HA	1.77	0.67
2:B:236:SER:O	2:B:243:ARG:NH2	2.29	0.66
1:C:363:VAL:HB	1:C:366:GLY:HA3	1.78	0.66
2:B:401:ARG:NH2	1:C:437:VAL:O	2.29	0.66
2:D:188:THR:HG23	2:D:425:MET:HE2	1.79	0.65
1:C:60:LYS:NZ	1:C:85:GLN:O	2.30	0.65
2:D:172:MET:HB2	2:D:205:ASP:HA	1.79	0.65
4:E:368:GLU:HA	4:E:436:HIS:O	1.96	0.65
3:P:115:THR:OG1	3:P:118:HIS:ND1	2.27	0.65
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.79	0.64
3:P:17:LYS:HB2	3:P:33:LEU:HD11	1.77	0.64
4:E:311:ALA:HB1	4:E:319:LYS:HB3	1.79	0.64
2:D:289:PRO:O	2:D:293:GLN:HB2	1.98	0.63
2:B:140:SER:HA	2:B:171:VAL:HG22	1.79	0.63
1:C:216:ASN:ND2	1:C:275:VAL:O	2.26	0.63
4:E:158:ASN:OD1	4:E:159:CYS:N	2.32	0.62
4:E:320:THR:O	4:E:324:GLY:N	2.26	0.62
3:P:22:ALA:HB1	3:P:54:ALA:HB2	1.83	0.61
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.82	0.61
1:A:401:LYS:O	1:A:403:ALA:N	2.34	0.61
4:E:219:ILE:HG22	4:E:220:ASP:H	1.66	0.61
4:E:354:ASN:HA	4:E:357:LYS:HG2	1.82	0.61
2:D:72:PRO:HB3	2:D:96:GLN:HG2	1.83	0.60
2:D:339:ASN:HB3	2:D:342:TYR:HD1	1.67	0.60
4:E:550:VAL:O	4:E:552:GLU:N	2.33	0.60
3:P:89:LEU:HD13	3:P:119:LEU:HB3	1.84	0.60
1:C:259:LEU:O	1:C:380:ASN:ND2	2.34	0.60
4:E:170:ARG:HG3	4:E:171:GLU:N	2.15	0.60
1:A:402:ARG:HB2	4:E:161:LYS:HE3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ASN:N	2:B:50:ASN:OD1	2.35	0.59
4:E:167:GLN:NE2	4:E:171:GLU:OE2	2.36	0.59
3:P:84:LEU:HD11	3:P:96:VAL:HG13	1.85	0.59
4:E:242:ASP:OD1	4:E:243:LEU:N	2.36	0.59
4:E:301:ILE:HG21	4:E:453:PHE:HB2	1.85	0.58
2:D:31:ASP:OD1	2:D:35:SER:N	2.29	0.58
1:C:276:ILE:HD13	1:C:283:HIS:CE1	2.38	0.58
2:B:270:PRO:HD2	2:B:302:MET:HB2	1.85	0.58
2:B:360:PRO:HG2	2:B:371:LEU:HB2	1.86	0.58
1:C:322:ASP:OD2	1:C:373:ARG:NH2	2.37	0.58
3:P:106:VAL:HG23	3:P:132:LEU:HD22	1.86	0.58
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.69	0.57
1:C:233:GLN:HG3	1:C:368:LEU:HD22	1.86	0.57
1:C:216:ASN:ND2	1:C:275:VAL:HG23	2.20	0.57
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.86	0.56
2:B:88:ARG:NH1	2:B:91:ASN:OD1	2.39	0.56
1:C:210:TYR:HE1	1:C:214:ARG:HE	1.53	0.56
1:C:246:GLY:N	1:C:249:ASN:OD1	2.38	0.56
1:C:39:ASP:OD1	1:C:40:LYS:N	2.39	0.56
1:C:258:ASN:CG	1:C:352:LYS:HE2	2.25	0.56
1:A:186:ASN:OD1	1:A:408:TYR:OH	2.14	0.56
1:C:397:LEU:HD22	2:D:440:ALA:HB1	1.88	0.56
2:B:209:LEU:HB3	2:B:227:LEU:HD22	1.86	0.56
2:D:420:GLU:HG3	4:E:387:LEU:HD22	1.88	0.56
4:E:301:ILE:HD13	4:E:453:PHE:HB2	1.89	0.55
2:D:132:LEU:O	2:D:164:ARG:NH1	2.39	0.55
2:B:10:GLY:HA2	2:B:145:THR:HB	1.88	0.55
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.88	0.55
2:B:5:VAL:HG22	2:B:64:ARG:HD3	1.89	0.55
1:C:34:GLY:O	1:C:61:HIS:N	2.40	0.55
3:P:67:LEU:HA	3:P:71:ALA:HB3	1.89	0.54
2:D:339:ASN:HB3	2:D:342:TYR:CD1	2.42	0.54
1:A:301:GLN:HE22	1:A:307:PRO:HD3	1.72	0.54
2:B:276:THR:HG21	2:B:371:LEU:HD11	1.89	0.54
1:C:255:PHE:HA	1:C:258:ASN:ND2	2.22	0.54
2:D:140:SER:HA	2:D:171:VAL:HG22	1.89	0.54
4:E:546:TYR:O	4:E:550:VAL:HG23	2.07	0.54
1:A:344:VAL:HG11	1:A:435:VAL:HG12	1.90	0.54
2:B:356:CYS:SG	2:B:357:ASP:N	2.81	0.54
1:C:234:ILE:HD13	1:C:302:MET:SD	2.48	0.54
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:201:ILE:HG22	4:E:205:ARG:HG2	1.91	0.53
4:E:363:TYR:HB3	4:E:401:GLU:HG2	1.91	0.53
1:A:402:ARG:NH1	1:A:415:GLU:OE2	2.42	0.53
2:D:310:GLY:HA2	2:D:436:GLN:HE22	1.73	0.53
2:D:220:THR:O	2:D:222:PRO:HD3	2.10	0.52
4:E:181:ARG:NH2	4:E:196:GLU:OE1	2.42	0.52
1:C:319:TYR:CD1	1:C:375:VAL:HB	2.44	0.52
4:E:200:MET:CE	4:E:268:TYR:HA	2.39	0.52
4:E:376:ASP:HB2	4:E:384:LEU:HD11	1.92	0.52
2:D:273:ALA:HB2	2:D:300:ASN:HD22	1.75	0.52
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.90	0.52
2:D:248:LEU:HB3	2:D:354:ALA:HB2	1.89	0.52
1:A:40:LYS:HD2	1:A:44:GLY:HA3	1.92	0.52
1:A:40:LYS:HZ2	1:A:47:ASP:H	1.58	0.52
4:E:229:ARG:NH2	4:E:284:ALA:O	2.41	0.52
2:D:21:TRP:O	2:D:25:SER:HB2	2.10	0.52
2:D:188:THR:HG22	2:D:421:ALA:HB1	1.92	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.51
4:E:347:PHE:HE1	4:E:362:VAL:HG21	1.75	0.51
4:E:319:LYS:NZ	9:E:601:ANP:O1B	2.31	0.51
2:B:388:PHE:CE2	2:B:428:LEU:HD23	2.45	0.51
1:C:340:SER:OG	1:C:340:SER:O	2.29	0.51
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.74	0.51
1:A:117:LEU:O	1:A:121:ARG:HG2	2.10	0.51
2:B:264:ARG:O	2:B:266:HIS:ND1	2.44	0.51
2:D:420:GLU:HG2	4:E:387:LEU:HA	1.92	0.51
2:D:103:TRP:H	2:D:408:TYR:HE1	1.59	0.51
2:D:289:PRO:O	2:D:293:GLN:CB	2.59	0.51
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.93	0.51
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.46	0.51
2:D:305:CYS:SG	2:D:387:LEU:HB2	2.50	0.51
2:D:109:THR:HG22	2:D:110:GLU:HG3	1.93	0.51
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.92	0.51
1:A:430:LYS:O	1:A:434:GLU:CD	2.43	0.50
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.93	0.50
1:C:252:LEU:HD12	1:C:255:PHE:HE1	1.76	0.50
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.93	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.47	0.50
4:E:191:THR:OG1	4:E:192:ASN:N	2.42	0.50
2:B:75:MET:HG2	2:B:94:PHE:CD1	2.47	0.50
4:E:388:GLU:OE2	4:E:514:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD22	2:B:190:SER:HB3	1.94	0.50
3:P:127:GLU:HA	3:P:130:GLU:HB2	1.94	0.50
1:A:401:LYS:HE3	2:B:438:ALA:HB1	1.93	0.50
1:C:236:SER:O	1:C:243:ARG:NH2	2.44	0.49
4:E:310:PHE:CZ	4:E:513:LEU:HD13	2.46	0.49
2:B:5:VAL:HB	2:B:135:PHE:CD1	2.47	0.49
4:E:231:ARG:NE	4:E:316:GLY:O	2.42	0.49
1:C:263:PRO:HG2	4:E:265:LEU:HD21	1.95	0.49
3:P:29:GLU:HG3	3:P:33:LEU:HD12	1.95	0.49
4:E:530:ILE:HB	4:E:540:THR:HG23	1.93	0.49
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.95	0.49
4:E:224:ILE:HD13	4:E:524:THR:HG23	1.94	0.49
1:C:275:VAL:C	1:C:276:ILE:HG13	2.33	0.49
4:E:431:HIS:O	4:E:431:HIS:ND1	2.46	0.49
2:B:392:SER:OG	2:B:426:ASN:OD1	2.28	0.48
1:A:268:PRO:HA	1:A:380:ASN:HA	1.95	0.48
3:P:63:VAL:O	3:P:67:LEU:HB2	2.12	0.48
2:B:63:PRO:O	2:B:65:ALA:N	2.46	0.48
1:C:273:ALA:HB2	1:C:375:VAL:HG13	1.94	0.48
4:E:200:MET:HE2	4:E:268:TYR:HA	1.94	0.48
3:P:77:ASP:OD1	3:P:81:SER:N	2.40	0.48
2:B:151:THR:HA	2:B:154:ILE:HD12	1.96	0.48
2:B:237:GLY:C	2:B:376:THR:HG21	2.34	0.48
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.32	0.48
2:D:88:ARG:HB3	2:D:91:ASN:ND2	2.29	0.48
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.96	0.48
2:D:238:VAL:HG12	2:D:378:ILE:HD11	1.95	0.48
4:E:201:ILE:CG2	4:E:205:ARG:HE	2.27	0.48
4:E:297:LEU:HD11	4:E:525:CYS:HB2	1.96	0.48
1:C:88:HIS:CE1	1:C:91:GLN:HB2	2.48	0.47
2:D:20:PHE:O	2:D:24:ILE:HG23	2.14	0.47
4:E:388:GLU:HG3	4:E:389:ASP:N	2.29	0.47
3:P:65:VAL:HA	3:P:68:LYS:HE2	1.96	0.47
2:D:214:PHE:CD1	2:D:220:THR:HA	2.49	0.47
3:P:30:VAL:HG21	3:P:62:ILE:HG23	1.96	0.47
2:B:114:LEU:O	2:B:117:SER:OG	2.28	0.47
2:D:185:TYR:OH	2:D:398:MET:O	2.32	0.47
1:C:248:LEU:HD23	1:C:357:TYR:HE2	1.78	0.47
2:B:439:THR:OG1	2:B:440:ALA:N	2.46	0.47
1:A:40:LYS:HZ3	1:A:47:ASP:H	1.62	0.47
2:B:189:LEU:HD11	2:B:418:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:23:ARG:HD3	3:P:53:LEU:HD13	1.96	0.47
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.97	0.47
1:A:75:ILE:O	1:A:79:ARG:HG2	2.14	0.47
1:A:277:SER:HB3	1:A:280:LYS:HB2	1.95	0.47
1:A:429:GLU:O	1:A:433:GLU:HG3	2.15	0.47
2:B:179:ASP:OD1	2:B:224:TYR:OH	2.33	0.47
2:D:337:ASN:OD1	2:D:338:LYS:N	2.47	0.47
2:D:416:MET:HB2	4:E:389:ASP:OD2	2.15	0.47
2:D:424:ASN:HA	4:E:505:ARG:CD	2.45	0.47
2:B:156:LYS:O	2:B:159:GLU:HG2	2.15	0.46
2:B:172:MET:HG2	2:B:205:ASP:HA	1.96	0.46
1:C:260:VAL:HG12	1:C:266:HIS:HA	1.96	0.46
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.46
1:A:392:ASP:HA	1:A:395:PHE:HB3	1.97	0.46
1:A:40:LYS:HZ2	1:A:46:ASP:H	1.64	0.46
1:C:229:ARG:O	1:C:232:SER:OG	2.22	0.46
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.97	0.46
2:B:171:VAL:HG12	2:B:204:ILE:HB	1.97	0.46
2:D:272:PHE:HE1	2:D:374:SER:HB2	1.80	0.46
1:A:121:ARG:HA	1:A:124:LYS:HE3	1.98	0.46
1:A:227:LEU:O	1:A:231:ILE:HG13	2.16	0.46
1:A:256:GLN:O	1:A:260:VAL:HB	2.15	0.46
1:C:279:GLU:O	1:C:281:ALA:N	2.49	0.46
4:E:421:ARG:CZ	4:E:433:SER:HB2	2.46	0.46
1:A:116:ASP:O	1:A:120:ASP:HB2	2.15	0.46
2:D:173:PRO:O	2:D:390:ARG:NH2	2.49	0.46
4:E:295:ARG:HB3	4:E:296:PRO:HD3	1.98	0.46
4:E:386:VAL:O	4:E:387:LEU:HD23	2.16	0.46
1:C:252:LEU:HD12	1:C:255:PHE:CE1	2.51	0.45
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.29	0.45
2:D:63:PRO:O	2:D:65:ALA:N	2.49	0.45
4:E:192:ASN:O	4:E:194:ASN:N	2.49	0.45
2:B:146:GLY:O	2:B:150:GLY:HA3	2.16	0.45
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.45
4:E:192:ASN:O	4:E:195:TYR:N	2.49	0.45
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.98	0.45
2:D:72:PRO:HD3	2:D:96:GLN:HA	1.99	0.45
1:C:3:GLU:CD	1:C:129:CYS:HB3	2.37	0.45
1:C:5:ILE:HB	1:C:135:PHE:HD1	1.81	0.45
1:C:184:PRO:O	1:C:188:ILE:HG12	2.17	0.45
1:C:422:ARG:HH12	1:C:426:ALA:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:VAL:HG11	3:P:125:HIS:NE2	2.32	0.45
1:C:352:LYS:HB2	1:C:352:LYS:NZ	2.32	0.45
2:B:227:LEU:O	2:B:231:VAL:HG23	2.17	0.45
2:B:310:GLY:HA3	2:B:383:ALA:HB2	1.98	0.45
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.52	0.45
1:A:314:ALA:O	1:A:379:SER:HA	2.16	0.45
2:B:141:LEU:HD22	2:B:190:SER:CB	2.47	0.45
2:B:181:VAL:HG22	1:C:258:ASN:OD1	2.17	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.52	0.45
4:E:308:THR:HG22	4:E:454:SER:HB2	1.99	0.45
1:C:409:VAL:HG13	4:E:482:ASN:HB3	1.99	0.45
4:E:160:VAL:HG13	4:E:161:LYS:H	1.82	0.44
1:A:277:SER:OG	1:A:278:ALA:N	2.50	0.44
1:A:221:ARG:NH2	2:B:329:ASP:OD2	2.50	0.44
1:A:43:GLY:HA2	1:A:55:GLU:HB2	2.00	0.44
1:C:97:GLU:HA	2:D:1:MET:H3	1.81	0.44
4:E:205:ARG:NH1	4:E:244:ASP:O	2.49	0.44
1:A:328:VAL:O	1:A:332:ILE:HG13	2.16	0.44
2:D:137:LEU:HD12	2:D:138:THR:H	1.82	0.44
3:P:41:ASN:HD21	3:P:71:ALA:HA	1.81	0.44
1:C:244:PHE:HB2	1:C:356:ASN:OD1	2.17	0.44
2:B:137:LEU:N	2:B:167:ASN:O	2.51	0.44
2:D:390:ARG:HH21	2:D:391:ILE:HD11	1.81	0.44
3:P:62:ILE:HG22	3:P:66:LEU:HD12	1.98	0.44
1:A:86:LEU:HD23	1:A:87:PHE:CE1	2.53	0.44
1:C:174:ALA:HB2	1:C:207:GLU:N	2.32	0.44
2:D:49:ILE:HG12	2:D:61:TYR:CE2	2.53	0.44
2:D:76:ASP:OD1	2:D:77:SER:N	2.51	0.44
1:A:228:ASN:OD1	5:A:501:GTP:N1	2.40	0.44
4:E:226:VAL:O	4:E:277:ASP:HB2	2.18	0.44
4:E:382:THR:HG23	4:E:384:LEU:HD21	1.99	0.44
1:C:291:ILE:HD12	1:C:375:VAL:HG12	2.00	0.44
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.43
3:P:147:LYS:HD2	3:P:151:ASP:HB3	1.99	0.43
1:C:216:ASN:HD22	1:C:275:VAL:HG23	1.81	0.43
1:C:431:ASP:O	1:C:435:VAL:HG23	2.18	0.43
2:D:21:TRP:CZ3	2:D:24:ILE:HD11	2.53	0.43
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.53	0.43
1:A:79:ARG:HD3	1:A:92:LEU:HD13	2.00	0.43
1:C:1:MET:HE2	1:C:51:THR:HG23	2.00	0.43
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:GLN:O	2:D:293:GLN:NE2	2.51	0.43
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.34	0.43
2:B:168:THR:HG21	2:B:194:LEU:HD22	2.00	0.43
1:A:404:PHE:CZ	2:B:261:PRO:HB3	2.54	0.43
1:C:219:ILE:HB	1:C:222:PRO:HG3	2.00	0.43
4:E:229:ARG:HB3	4:E:529:THR:HG22	2.00	0.43
3:P:65:VAL:HG13	3:P:68:LYS:HE2	1.99	0.43
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.50	0.43
1:A:56:THR:HG22	1:A:57:GLY:H	1.84	0.43
2:D:85:GLN:H	2:D:85:GLN:CD	2.22	0.43
3:P:73:VAL:HG21	3:P:102:HIS:HB2	2.00	0.43
3:P:48:LEU:HD13	3:P:53:LEU:HD21	2.01	0.43
3:P:60:LEU:HD11	3:P:94:GLU:HB2	2.01	0.43
2:D:303:ALA:O	2:D:305:CYS:N	2.52	0.43
1:A:141:PHE:HB3	1:A:187:SER:OG	2.19	0.43
1:A:234:ILE:HG21	1:A:302:MET:SD	2.59	0.43
1:A:280:LYS:O	1:A:282:TYR:N	2.52	0.43
4:E:432:SER:O	4:E:434:ARG:HG2	2.18	0.43
1:A:291:ILE:HB	1:A:375:VAL:HG12	2.01	0.42
1:A:69:ASP:C	1:A:71:GLU:H	2.22	0.42
4:E:402:ARG:N	4:E:402:ARG:HD2	2.33	0.42
4:E:433:SER:OG	4:E:433:SER:O	2.36	0.42
3:P:42:ALA:O	3:P:50:PRO:HD3	2.19	0.42
1:A:359:PRO:HA	1:A:360:PRO:HD3	1.89	0.42
1:A:39:ASP:OD1	1:A:40:LYS:N	2.51	0.42
1:C:152:LEU:O	1:C:156:ARG:HG2	2.18	0.42
1:C:316:CYS:O	1:C:377:MET:HA	2.19	0.42
1:A:40:LYS:NZ	1:A:46:ASP:H	2.17	0.42
1:C:36:MET:SD	1:C:39:ASP:HB2	2.60	0.42
1:C:409:VAL:HA	1:C:413:MET:O	2.19	0.42
2:B:31:ASP:OD1	2:B:35:SER:N	2.52	0.42
1:C:1:MET:HB2	1:C:3:GLU:HG3	2.01	0.42
1:C:313:MET:SD	1:C:435:VAL:HG11	2.59	0.42
4:E:205:ARG:O	4:E:208:LEU:HD12	2.20	0.42
1:A:10:GLY:O	1:A:14:VAL:HG23	2.20	0.42
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.00	0.42
4:E:485:LEU:O	4:E:489:LYS:HB2	2.18	0.42
1:C:107:HIS:ND1	1:C:152:LEU:HB2	2.34	0.42
3:P:148:THR:N	3:P:151:ASP:HB2	2.34	0.42
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.02	0.42
2:B:265:LEU:HD22	2:B:432:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.02	0.42
1:A:205:ASP:OD2	1:A:390:ARG:NH2	2.53	0.42
3:P:67:LEU:HB3	3:P:102:HIS:CE1	2.54	0.42
1:A:275:VAL:O	1:A:275:VAL:HG13	2.20	0.42
2:D:312:TYR:O	2:D:344:VAL:HG22	2.20	0.42
4:E:204:PHE:O	4:E:206:GLY:N	2.53	0.42
2:B:97:SER:OG	2:B:110:GLU:HG2	2.20	0.41
1:C:91:GLN:OE1	1:C:121:ARG:HB3	2.20	0.41
2:D:39:ASP:OD1	2:D:39:ASP:N	2.53	0.41
4:E:489:LYS:HD3	4:E:546:TYR:CZ	2.55	0.41
2:B:187:ALA:O	2:B:191:VAL:HG23	2.20	0.41
2:B:19:LYS:O	2:B:23:VAL:HG23	2.19	0.41
1:C:406:HIS:ND1	2:D:263:PRO:HG3	2.35	0.41
4:E:477:GLU:O	4:E:481:ILE:HG13	2.21	0.41
1:A:277:SER:O	1:A:369:ALA:HB2	2.20	0.41
1:C:274:PRO:HG2	1:C:371:VAL:HG21	2.01	0.41
2:D:102:ASN:H	2:D:144:GLY:HA3	1.84	0.41
2:D:28:HIS:NE2	2:D:243:ARG:HB3	2.35	0.41
2:D:310:GLY:HA2	2:D:436:GLN:NE2	2.34	0.41
2:D:11:GLN:HG3	8:D:502:PO4:O2	2.21	0.41
1:A:339:ARG:HB3	1:A:341:ILE:HG13	2.02	0.41
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.01	0.41
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.01	0.41
3:P:95:ILE:HG22	3:P:99:LEU:HD12	2.02	0.41
1:A:169:PHE:HE1	1:A:202:PHE:CD2	2.39	0.41
1:A:305:CYS:O	1:A:307:PRO:HD3	2.20	0.41
2:B:28:HIS:NE2	2:B:243:ARG:HD2	2.36	0.41
2:B:205:ASP:HB2	2:B:303:ALA:HA	2.03	0.41
2:D:31:ASP:OD2	2:D:33:THR:OG1	2.38	0.41
2:D:248:LEU:HD23	2:D:354:ALA:HB2	2.02	0.41
4:E:311:ALA:HB3	4:E:457:ASP:HA	2.02	0.41
1:A:288:VAL:HG11	1:A:328:VAL:HG22	2.02	0.41
2:B:234:THR:O	2:B:238:VAL:HG13	2.21	0.41
2:B:331:GLN:O	2:B:334:ASN:HB3	2.21	0.41
2:D:264:ARG:O	2:D:266:HIS:ND1	2.54	0.41
2:D:288:VAL:HG11	2:D:327:GLU:HG2	2.03	0.41
2:D:272:PHE:CE1	2:D:374:SER:HB2	2.55	0.41
3:P:17:LYS:O	3:P:21:ALA:HB2	2.21	0.41
2:B:132:LEU:HD21	2:B:135:PHE:CZ	2.55	0.41
1:C:229:ARG:HD3	1:C:363:VAL:HG21	2.03	0.41
1:C:385:ALA:HA	1:C:388:TRP:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:219:ILE:HG22	4:E:220:ASP:N	2.35	0.41
4:E:391:LYS:O	4:E:393:GLN:N	2.54	0.41
1:A:128:GLN:H	1:A:128:GLN:HG3	1.74	0.40
1:C:6:SER:HB2	1:C:21:TRP:HZ2	1.86	0.40
4:E:198:MET:HB2	4:E:243:LEU:HD11	2.04	0.40
1:A:399:TYR:CD1	1:A:402:ARG:HD3	2.56	0.40
2:D:261:PRO:HG3	2:D:313:LEU:HD13	2.03	0.40
4:E:319:LYS:HB2	4:E:319:LYS:HE2	1.88	0.40
4:E:343:ALA:CB	4:E:410:VAL:HG11	2.51	0.40
1:A:40:LYS:HD3	1:A:47:ASP:OD2	2.20	0.40
1:A:9:VAL:HG12	1:A:146:GLY:HA2	2.02	0.40
2:D:274:PRO:HB3	2:D:286:LEU:HD22	2.02	0.40
4:E:204:PHE:CE1	4:E:208:LEU:HD11	2.57	0.40
4:E:449:LEU:HA	4:E:449:LEU:HD12	1.88	0.40
2:B:295:MET:SD	2:B:375:ALA:HB1	2.61	0.40
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.02	0.40
1:A:311:LYS:HZ3	1:A:344:VAL:HG12	1.86	0.40
2:D:234:THR:O	2:D:238:VAL:HG13	2.22	0.40
2:D:75:MET:O	2:D:78:VAL:HB	2.22	0.40
4:E:375:PHE:HA	4:E:382:THR:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/451 (96%)	384 (88%)	42 (10%)	8 (2%)	8	42
1	C	432/451 (96%)	392 (91%)	35 (8%)	5 (1%)	13	51
2	B	429/445 (96%)	397 (92%)	29 (7%)	3 (1%)	22	62
2	D	429/445 (96%)	378 (88%)	46 (11%)	5 (1%)	13	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	153/168 (91%)	132 (86%)	21 (14%)	0	100	100
4	E	371/420 (88%)	309 (83%)	47 (13%)	15 (4%)	3	25
All	All	2248/2380 (94%)	1992 (89%)	220 (10%)	36 (2%)	9	45

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
2	D	74	THR
2	D	133	GLN
4	E	160	VAL
4	E	241	LYS
1	A	114	ILE
1	A	176	GLN
1	A	281	ALA
1	C	280	LYS
2	D	64	ARG
4	E	187	ASP
4	E	188	VAL
4	E	205	ARG
4	E	212	PRO
4	E	392	GLN
4	E	551	LYS
2	D	73	GLY
4	E	252	ASP
4	E	471	ASP
1	A	283	HIS
2	B	64	ARG
1	C	273	ALA
1	C	439	SER
4	E	192	ASN
4	E	389	ASP
1	A	40	LYS
2	B	178	SER
2	D	288	VAL
4	E	159	CYS
1	A	109	THR
4	E	219	ILE
1	A	341	ILE
2	B	72	PRO
1	C	362	VAL

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Mol	Chain	Res	Type
1	C	131	GLY
4	E	193	PRO

### 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	363/379 (96%)	357 (98%)	6 (2%)	60	82
1	C	363/379 (96%)	357 (98%)	6 (2%)	60	82
2	B	369/383 (96%)	359 (97%)	10 (3%)	44	73
2	D	369/383 (96%)	358 (97%)	11 (3%)	41	71
3	P	113/131 (86%)	109 (96%)	4 (4%)	36	67
4	E	320/370 (86%)	300 (94%)	20 (6%)	18	51
All	All	1897/2025 (94%)	1840 (97%)	57 (3%)	41	71

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	123	ARG
1	A	160	ASP
1	A	224	TYR
1	A	266	HIS
1	A	282	TYR
2	B	55	GLU
2	B	75	MET
2	B	76	ASP
2	B	90	ASP
2	B	116	ASP
2	B	139	HIS
2	B	161	TYR
2	B	174	SER
2	B	179	ASP
2	B	357	ASP

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Mol	Chain	Res	Type
1	C	88	HIS
1	C	98	ASP
1	C	120	ASP
1	C	218	ASP
1	C	315	CYS
1	C	415	GLU
2	D	71	GLU
2	D	79	ARG
2	D	90	ASP
2	D	139	HIS
2	D	192	HIS
2	D	215	ARG
2	D	247	GLN
2	D	372	LYS
2	D	381	SER
2	D	420	GLU
2	D	427	ASP
3	P	13	ASP
3	P	33	LEU
3	P	39	ASP
3	P	143	ASP
4	E	169	LYS
4	E	184	ARG
4	E	187	ASP
4	E	204	PHE
4	E	210	TYR
4	E	240	MET
4	E	250	SER
4	E	275	ARG
4	E	299	GLU
4	E	366	PHE
4	E	379	ASN
4	E	402	ARG
4	E	433	SER
4	E	450[A]	HIS
4	E	450[B]	HIS
4	E	453	PHE
4	E	462	GLU
4	E	490	GLU
4	E	507	SER
4	E	508	LYS

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



sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
2	B	294	GLN
4	E	167	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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
7	GDP	B	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.81	8 (25%)
5	GTP	A	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.92	7 (21%)
7	GDP	D	501	-	24,30,30	1.19	2 (8%)	31,47,47	2.00	8 (25%)
9	ANP	E	601	6	29,33,33	1.67	5 (17%)	31,52,52	1.32	3 (9%)
8	PO4	D	502	-	4,4,4	0.88	0	6,6,6	0.91	0
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.89	7 (21%)

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
7	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
9	ANP	E	601	6	-	6/14/38/38	0/3/3/3
7	GDP	D	501	-	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	601	ANP	PB-O1B	6.49	1.56	1.46
7	D	501	GDP	C6-C5	4.30	1.48	1.41
7	B	501	GDP	C6-C5	4.23	1.48	1.41
5	C	501	GTP	C6-N1	3.21	1.38	1.33
5	A	501	GTP	C6-N1	3.07	1.38	1.33
9	E	601	ANP	PB-O2B	-2.73	1.49	1.56
7	B	501	GDP	C5-C4	2.56	1.47	1.40
9	E	601	ANP	PG-N3B	2.50	1.69	1.63
7	D	501	GDP	C5-C4	2.46	1.47	1.40
9	E	601	ANP	PB-O3A	-2.44	1.56	1.59
9	E	601	ANP	PG-O1G	2.35	1.49	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.66	119.68	127.22
5	C	501	GTP	N3-C2-N1	-5.24	120.24	127.22
9	E	601	ANP	PA-O3A-PB	-5.06	114.79	132.62
7	D	501	GDP	C2-N3-C4	4.89	120.94	115.36
5	C	501	GTP	PB-O3B-PG	-4.80	116.36	132.83
5	A	501	GTP	C2-N3-C4	4.60	120.61	115.36
5	C	501	GTP	C2-N3-C4	4.51	120.51	115.36
7	B	501	GDP	C5-C6-N1	-4.36	117.47	123.43
5	A	501	GTP	PB-O3B-PG	-4.19	118.45	132.83
7	B	501	GDP	C2-N3-C4	4.19	120.14	115.36
7	D	501	GDP	C6-N1-C2	4.09	122.43	115.93
7	D	501	GDP	C5-C6-N1	-4.03	117.92	123.43
7	B	501	GDP	C6-N1-C2	3.90	122.12	115.93
7	D	501	GDP	C6-C5-C4	-3.81	117.16	120.80
7	B	501	GDP	PA-O3A-PB	-3.34	121.38	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	501	GDP	N3-C2-N1	-3.31	122.81	127.22
7	D	501	GDP	C3'-C2'-C1'	3.19	105.79	100.98
7	B	501	GDP	C6-C5-C4	-3.13	117.81	120.80
7	D	501	GDP	PA-O3A-PB	-3.12	122.12	132.83
5	A	501	GTP	PA-O3A-PB	-3.08	122.26	132.83
7	B	501	GDP	C4-C5-N7	-2.89	106.39	109.40
5	C	501	GTP	C3'-C2'-C1'	2.86	105.29	100.98
7	D	501	GDP	C4-C5-N7	-2.80	106.48	109.40
5	C	501	GTP	PA-O3A-PB	-2.75	123.38	132.83
5	C	501	GTP	C5-C6-N1	-2.65	119.81	123.43
5	A	501	GTP	C5-C6-N1	-2.63	119.84	123.43
5	A	501	GTP	C6-N1-C2	2.57	120.01	115.93
5	A	501	GTP	C3'-C2'-C1'	2.57	104.84	100.98
7	B	501	GDP	N3-C2-N1	-2.48	123.92	127.22
7	B	501	GDP	C3'-C2'-C1'	2.46	104.68	100.98
9	E	601	ANP	C5-C6-N6	2.42	124.03	120.35
9	E	601	ANP	O2G-PG-O1G	-2.33	107.60	113.45
5	C	501	GTP	C6-N1-C2	2.31	119.59	115.93

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
7	D	501	GDP	C5'-O5'-PA-O3A
7	D	501	GDP	C5'-O5'-PA-O1A
9	E	601	ANP	PB-N3B-PG-O1G
9	E	601	ANP	PG-N3B-PB-O1B
9	E	601	ANP	PA-O3A-PB-O2B
9	E	601	ANP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
7	D	501	GDP	PA-O3A-PB-O2B
7	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
9	E	601	ANP	C5'-O5'-PA-O1A
9	E	601	ANP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
7	D	501	GDP	PA-O3A-PB-O3B
5	C	501	GTP	C5'-O5'-PA-O3A

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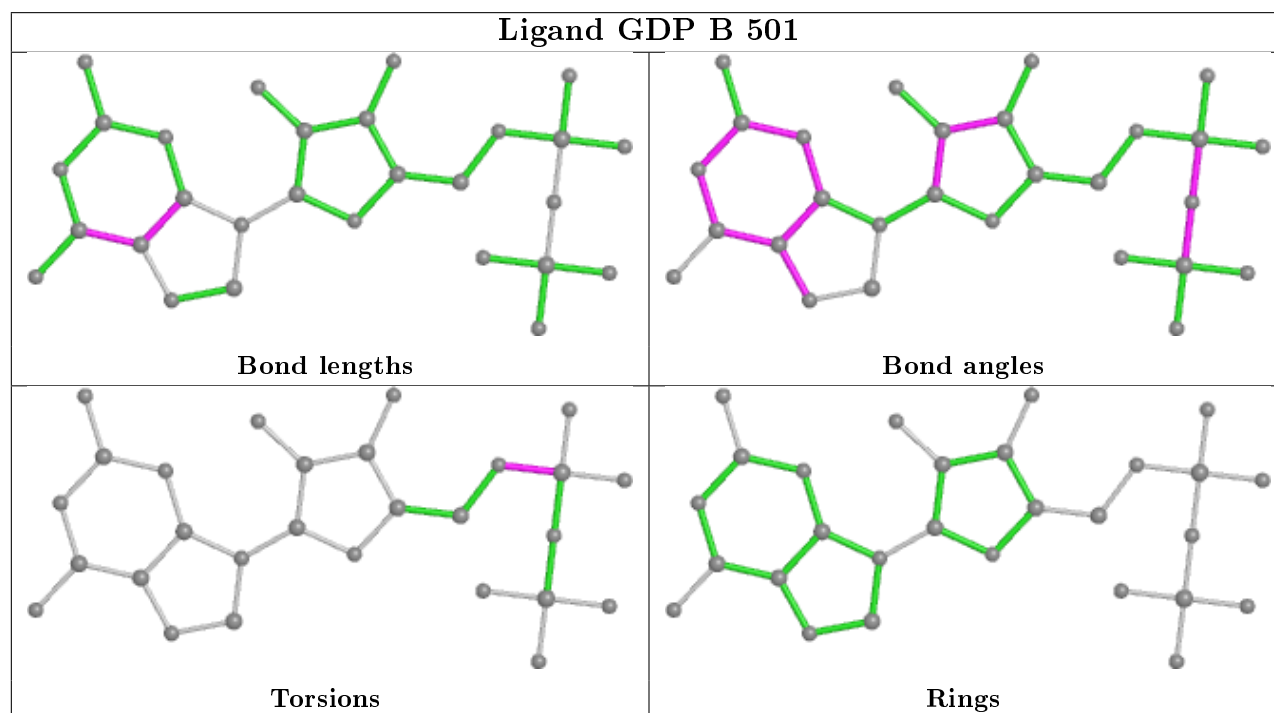
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O1A
7	D	501	GDP	C5'-O5'-PA-O2A

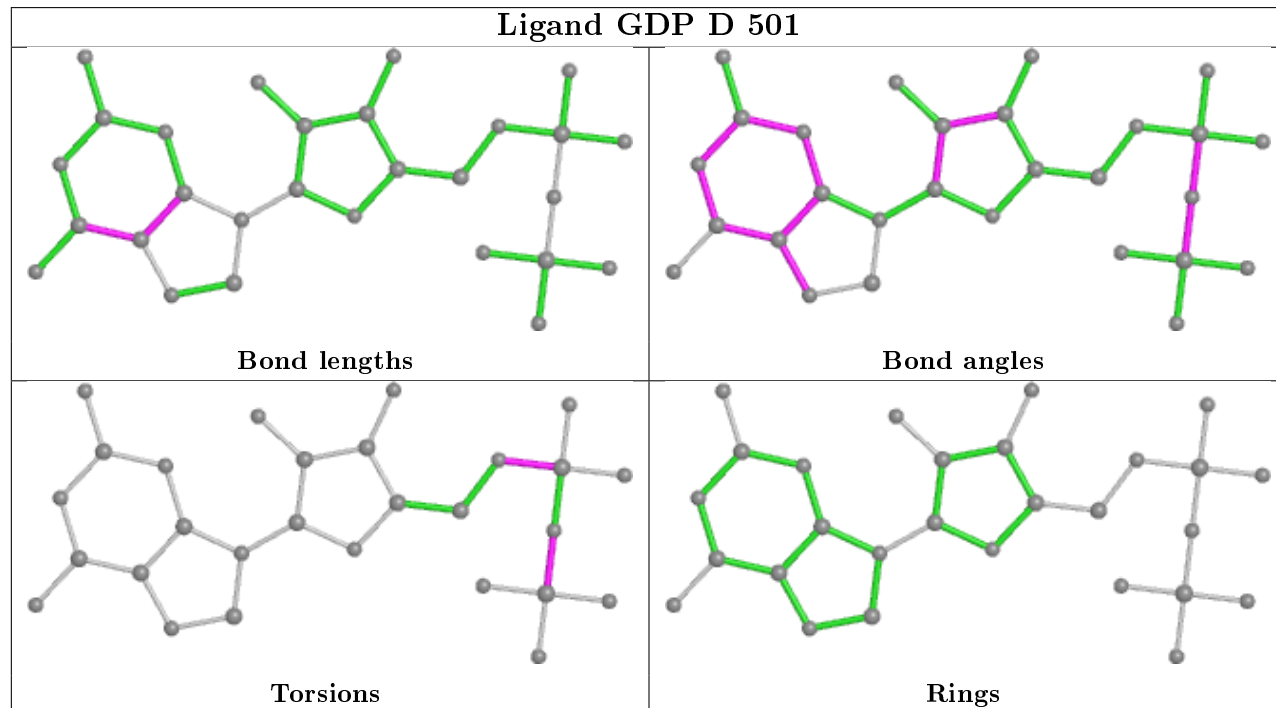
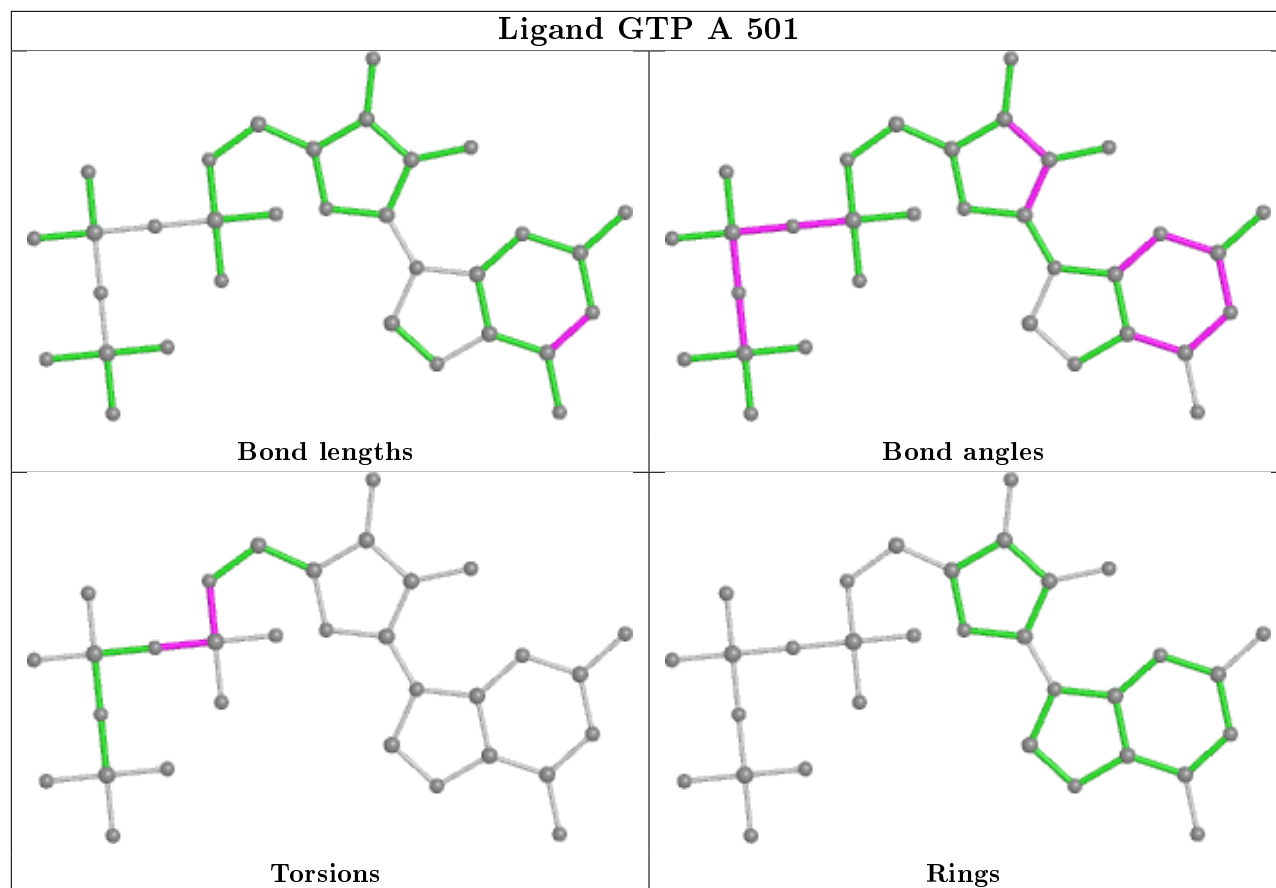
There are no ring outliers.

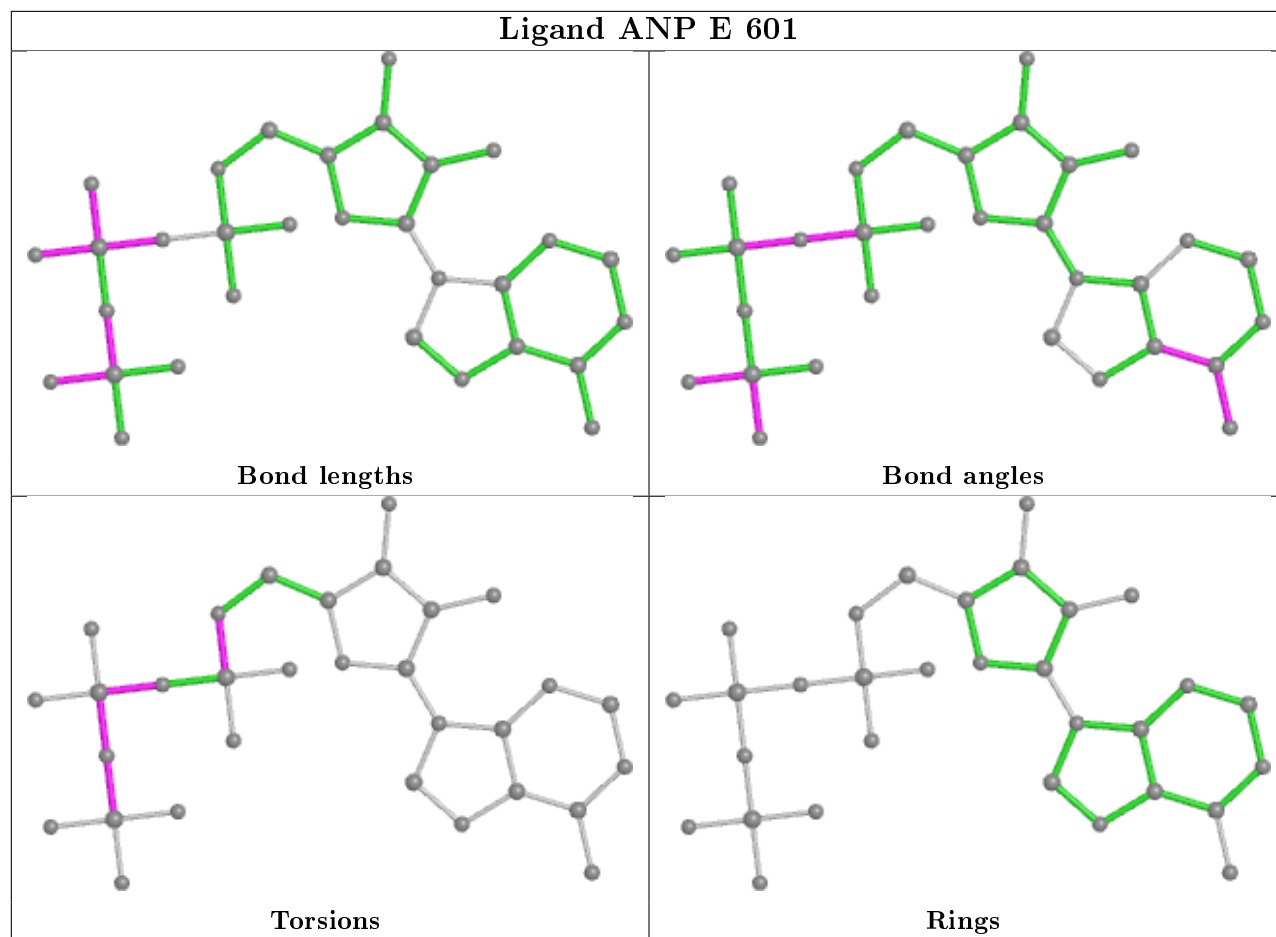
3 monomers are involved in 3 short contacts:

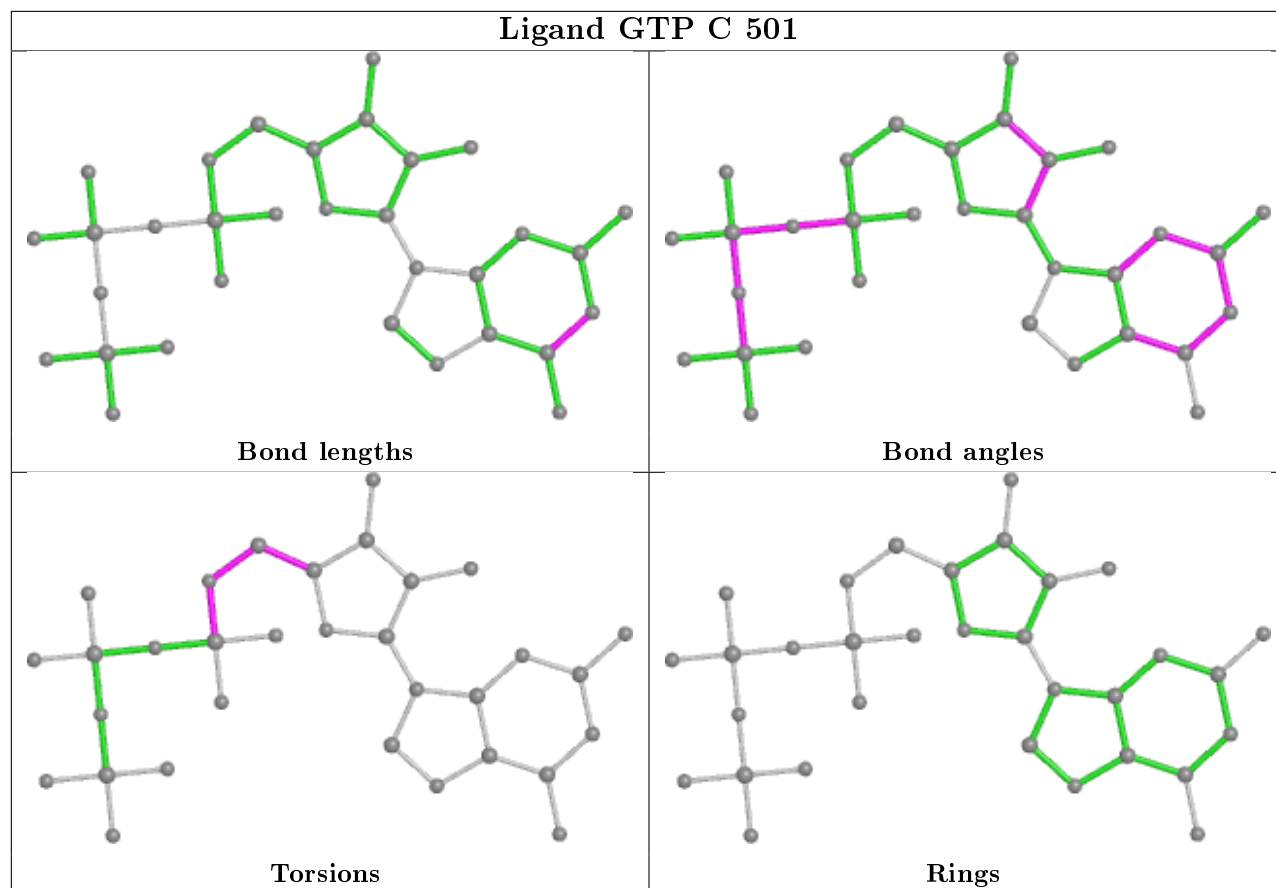
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	E	601	ANP	1	0
8	D	502	PO4	1	0

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 [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	436/451 (96%)	-0.31	1 (0%) 95 91	103, 146, 179, 213	0
1	C	436/451 (96%)	-0.45	0 100 100	86, 126, 162, 195	0
2	B	431/445 (96%)	-0.42	0 100 100	79, 122, 170, 200	0
2	D	431/445 (96%)	-0.12	11 (2%) 56 43	108, 162, 191, 215	0
3	P	155/168 (92%)	0.76	19 (12%) 4 4	172, 233, 252, 258	0
4	E	378/420 (90%)	-0.49	2 (0%) 91 84	106, 140, 169, 189	0
All	All	2267/2380 (95%)	-0.28	33 (1%) 73 61	79, 142, 224, 258	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	72	ASP	7.2
3	P	91	GLY	5.2
3	P	90	ILE	4.0
2	D	67	LEU	3.9
2	D	66	ILE	3.6
1	A	248	LEU	3.1
3	P	69	HIS	3.1
3	P	18	LEU	3.0
3	P	92	HIS	3.0
3	P	165	LEU	3.0
2	D	274	PRO	2.8
3	P	41	ASN	2.7
3	P	50	PRO	2.7
3	P	102	HIS	2.4
3	P	105	ASP	2.4
4	E	364	ALA	2.4
2	D	65	ALA	2.4
2	D	286	LEU	2.3
3	P	14	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	P	74	ASN	2.3
3	P	15	GLY	2.2
3	P	70	GLY	2.2
2	D	198	THR	2.1
3	P	89	LEU	2.1
2	D	86	ILE	2.1
3	P	138	ASP	2.1
2	D	94	PHE	2.1
2	D	68	VAL	2.1
2	D	91	ASN	2.1
3	P	73	VAL	2.1
3	P	144	LYS	2.1
2	D	140	SER	2.0
4	E	360	LEU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	PO4	D	502	5/5	0.78	0.25	173,174,180,181	0
6	MG	C	502	1/1	0.84	0.27	102,102,102,102	0
7	GDP	D	501	28/28	0.92	0.34	168,177,182,184	0
6	MG	B	502	1/1	0.92	0.54	113,113,113,113	0
9	ANP	E	601	31/31	0.93	0.15	108,131,139,142	0
5	GTP	C	501	32/32	0.93	0.26	91,123,133,140	0
7	GDP	B	501	28/28	0.94	0.29	99,115,124,133	0
6	MG	A	502	1/1	0.95	0.53	205,205,205,205	0
5	GTP	A	501	32/32	0.95	0.40	114,126,136,137	0

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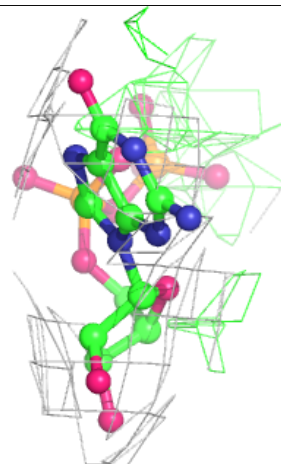
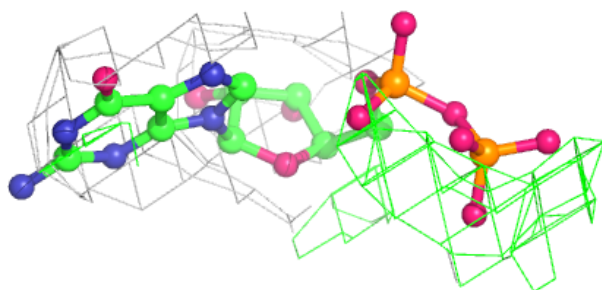
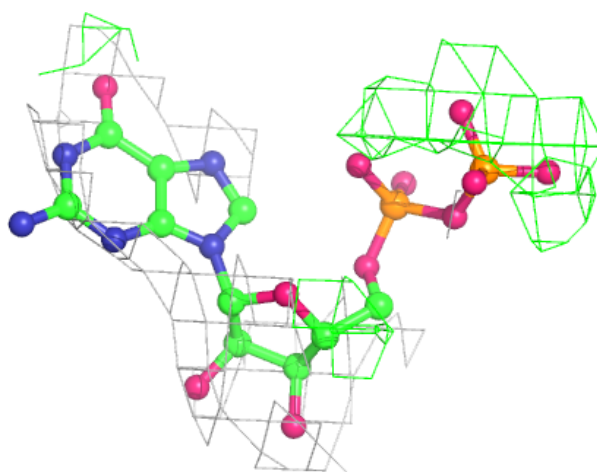
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	E	602	1/1	0.97	0.10	135,135,135,135	0

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.

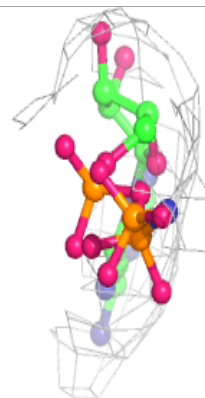
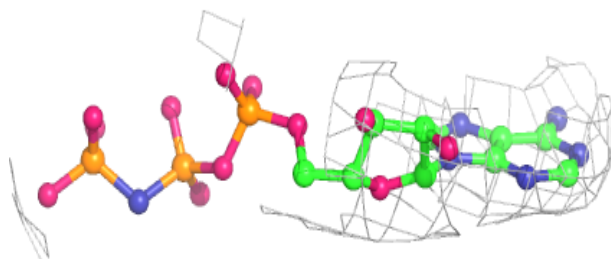
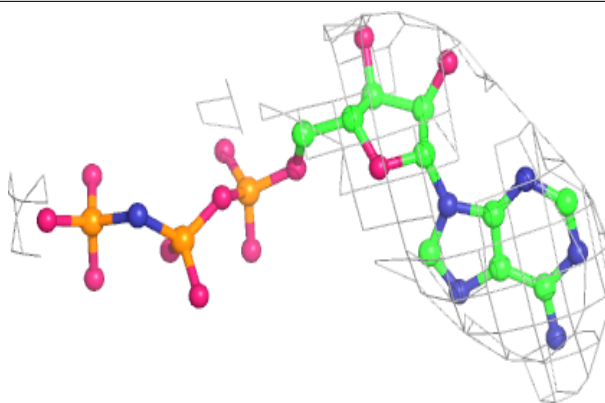
**Electron density around GDP D 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

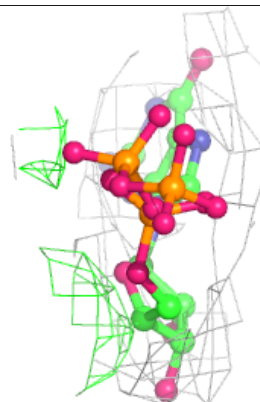
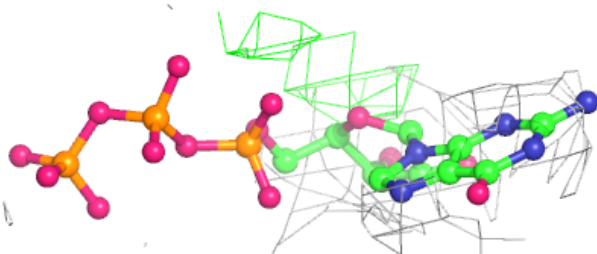
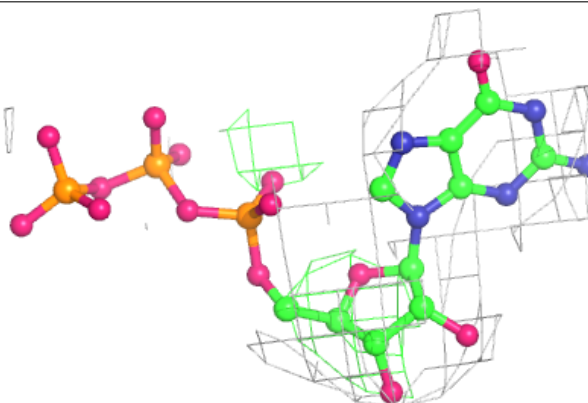


**Electron density around ANP E 601:**

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

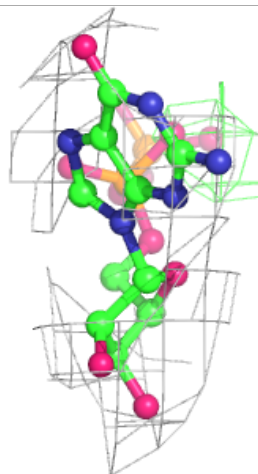
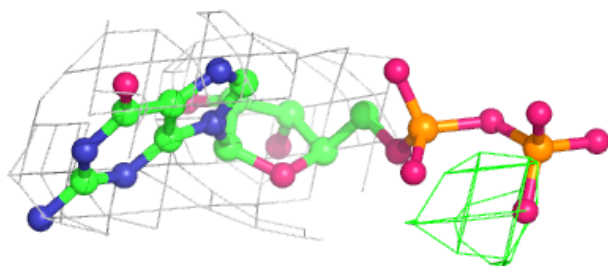
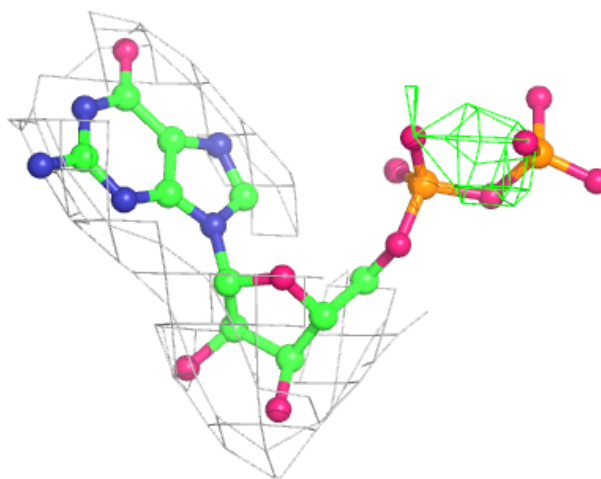
**Electron density around GTP C 501:**

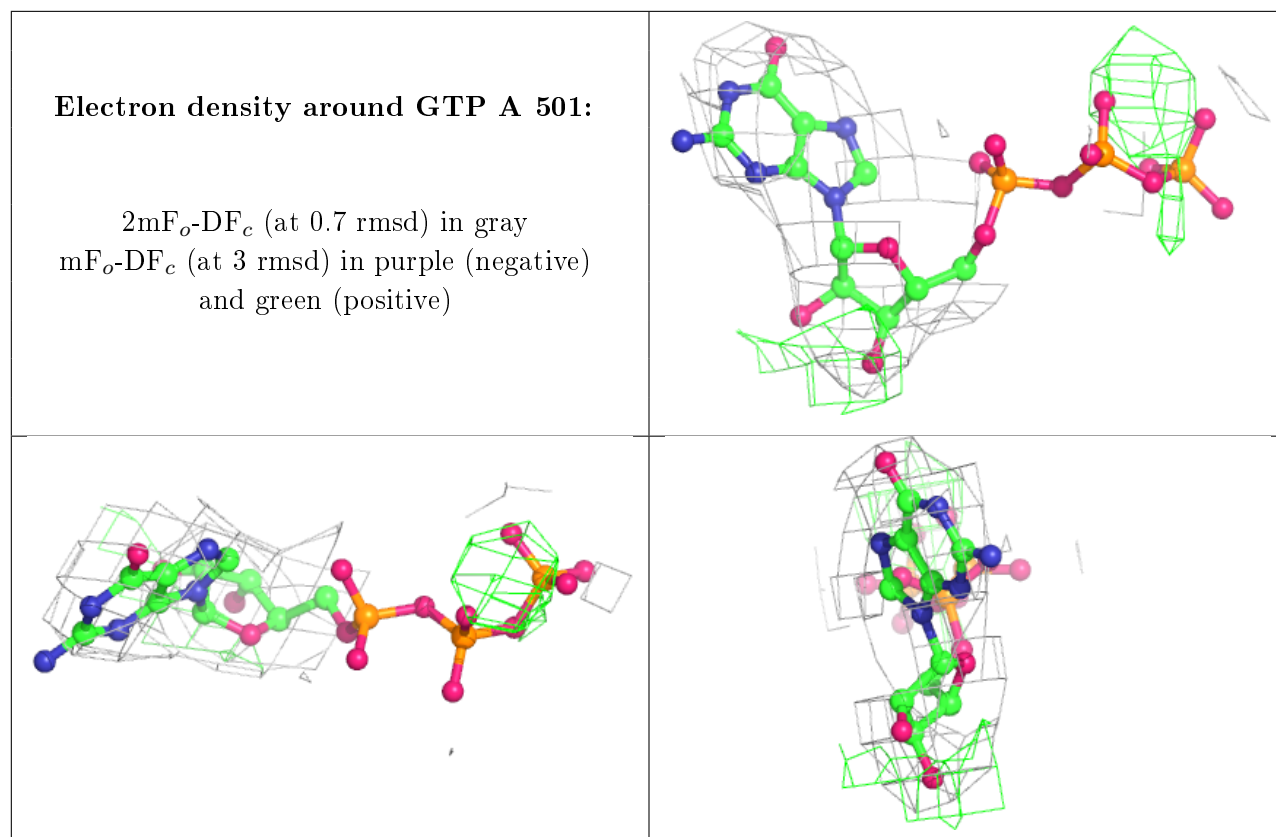
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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.