



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:27 AM UTC

PDB ID : 6BBN / pdb_00006bbn
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

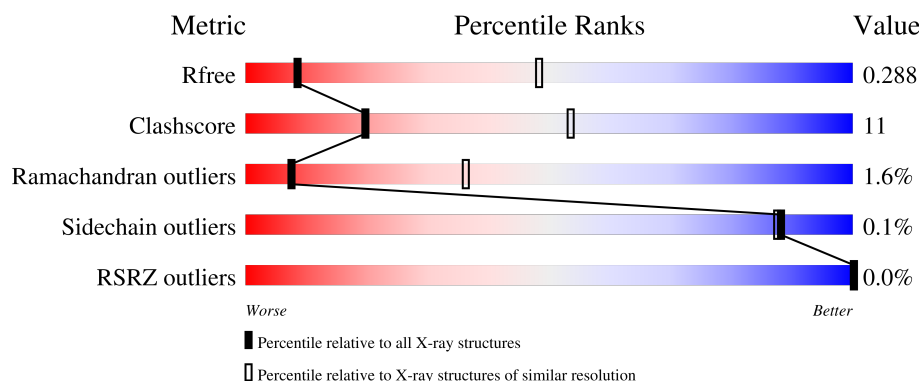
1 Overall quality at a glance

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}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	69% 27% ..
1	C	451	73% 23% .
2	B	445	71% 25% .
2	D	445	71% 26% .
3	P	168	63% 29% 8%

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Mol	Chain	Length	Quality of chain
4	E	420	 A horizontal bar chart showing the quality of chain E. The bar is divided into three segments: green (65%), yellow (24%), and orange (10%). The percentages are labeled below the bar.

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:

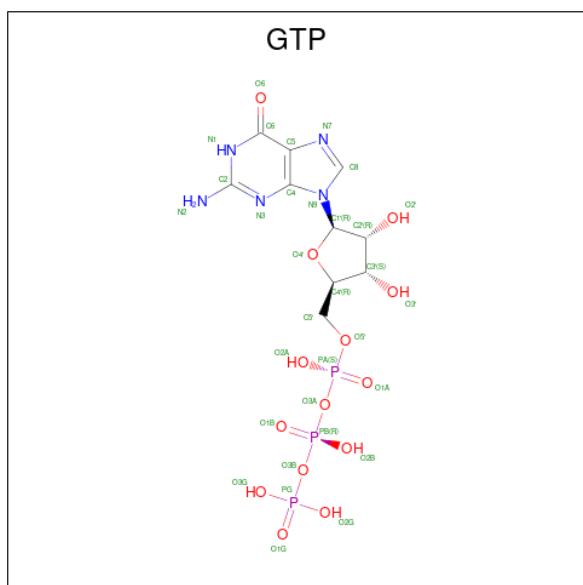
Chain	Residue	Modelled	Actual	Comment	Reference
E	134	MET	-	expression tag	UNP O00139
E	135	GLY	-	expression tag	UNP O00139
E	136	SER	-	expression tag	UNP O00139
E	137	SER	-	expression tag	UNP O00139

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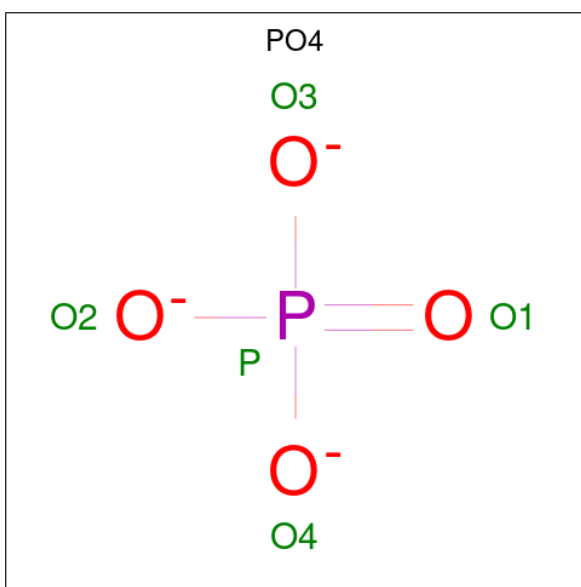
Chain	Residue	Modelled	Actual	Comment	Reference
E	138	HIS	-	expression tag	UNP O00139
E	139	HIS	-	expression tag	UNP O00139
E	140	HIS	-	expression tag	UNP O00139
E	141	HIS	-	expression tag	UNP O00139
E	142	HIS	-	expression tag	UNP O00139
E	143	HIS	-	expression tag	UNP O00139
E	144	SER	-	expression tag	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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



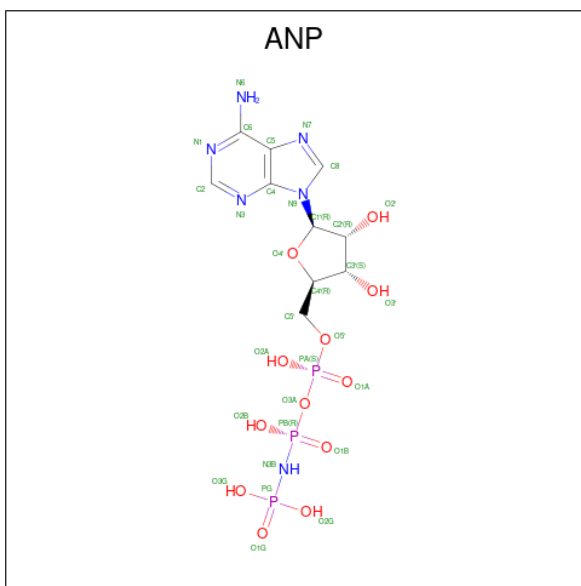
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).



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

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

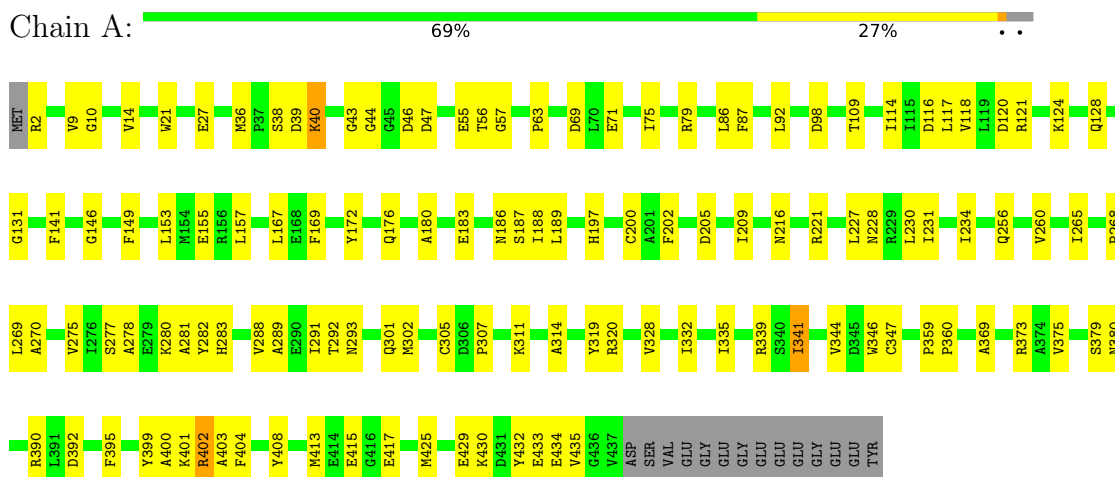


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

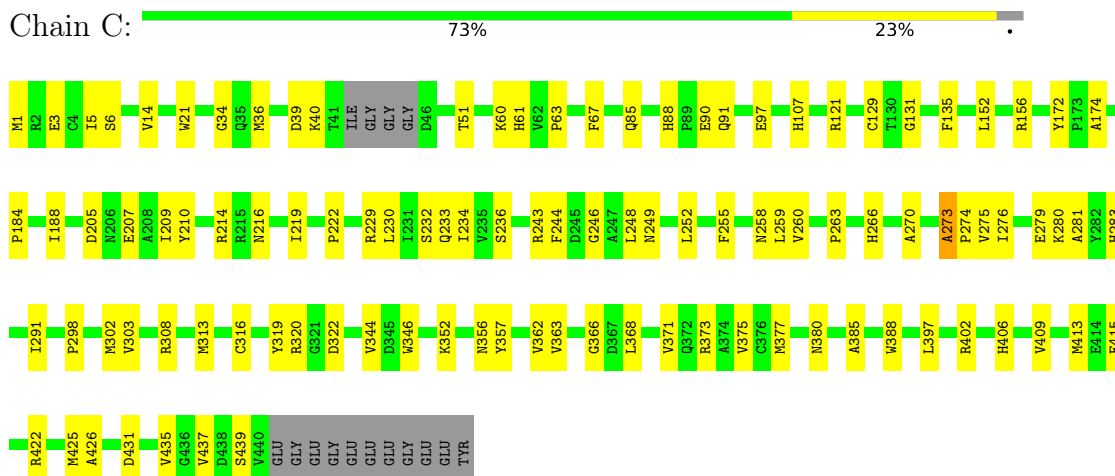
3 Residue-property plots

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

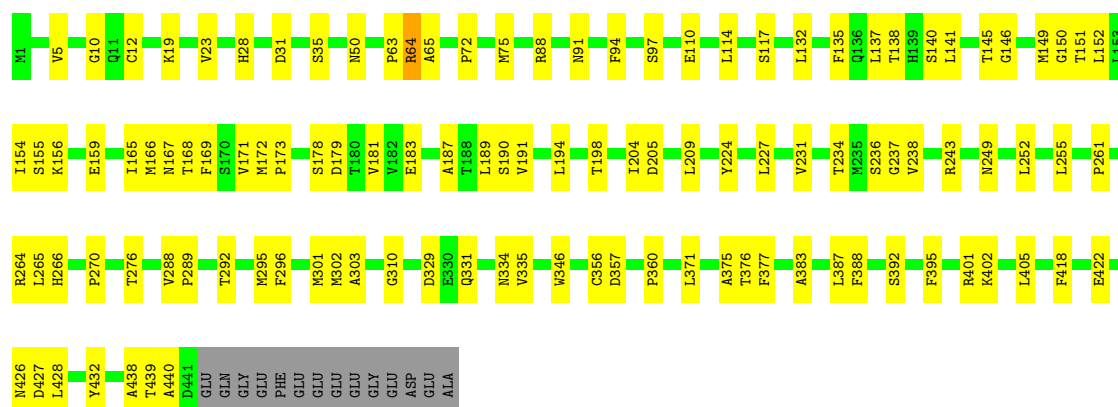


- Molecule 1: Tubulin alpha-1B chain



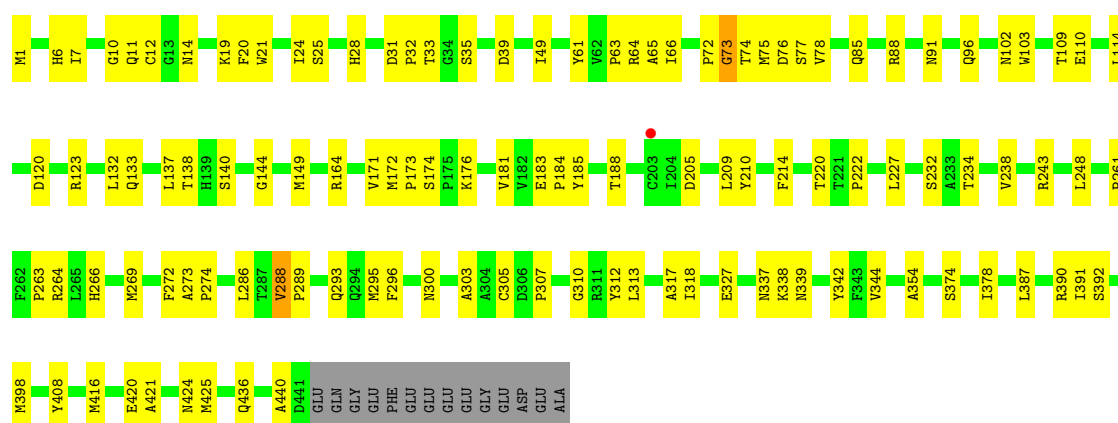
- Molecule 2: Tubulin beta-2B chain





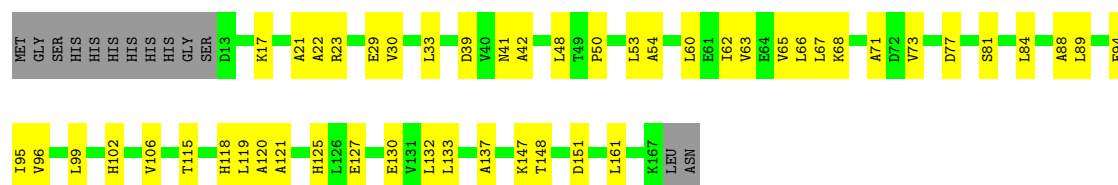
• Molecule 2: Tubulin beta-2B chain

Chain D: 71% 26% .



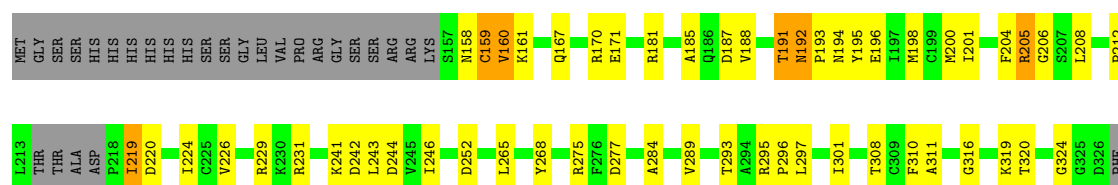
• Molecule 3: DARPin

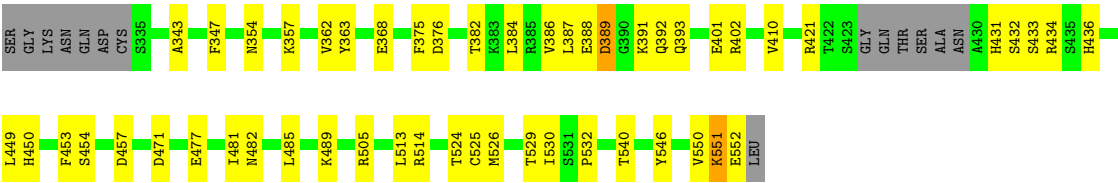
Chain P: 63% 29% 8%



• Molecule 4: Kinesin-like protein KIF2A

Chain E: 65% 24% 10%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 96.7 (49.22-3.51)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.236 , 0.287 0.243 , 0.288	Depositor DCC
R_{free} test set	1964 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	117.0	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.068 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17794	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, PO4, MG, ANP, GDP

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	0.17	0/3469	0.39	0/4711
1	C	0.19	0/3462	0.41	0/4705
2	B	0.17	0/3446	0.38	0/4670
2	D	0.17	0/3451	0.37	0/4678
3	P	0.18	0/1143	0.39	0/1556
4	E	0.25	0/3025	0.53	2/4067 (0.0%)
All	All	0.19	0/17996	0.41	2/24387 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	191	THR	CA-C-N	5.01	134.02	121.80
4	E	191	THR	C-N-CA	5.01	134.02	121.80

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	84	0
1	C	3386	0	3274	77	0
2	B	3372	0	3237	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3376	0	3237	82	0
3	P	1128	0	1110	32	0
4	E	2980	0	2962	79	0
5	A	32	0	12	1	0
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	0	0
All	All	17794	0	17178	402	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 (402) 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	0.88
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.59	0.84
4:E:200:MET:HE1	4:E:268:TYR:HA	1.62	0.81
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:7:ILE:HG12	2:D:66:ILE:HB	1.70	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:120:ASP:OD1	2:D:123:ARG:NH1	2.21	0.72
4:E:159:CYS:SG	4:E:160:VAL:N	2.63	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:172:MET:HE3	2:B:387:LEU:HD21	1.77	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
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
2:D:392:SER:HB2	2:D:425:MET:HE3	1.80	0.63
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.80	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:354:ASN:HA	4:E:357:LYS:HG2	1.82	0.61
1:C:258:ASN:CG	1:C:352:LYS:HE2	2.25	0.60
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
2:B:295:MET:HE3	2:B:296:PHE:HE1	1.66	0.60
3:P:89:LEU:HD13	3:P:119:LEU:HB3	1.84	0.60
4:E:550:VAL:O	4:E:552:GLU:N	2.33	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
2:B:50:ASN:OD1	2:B:50:ASN:N	2.35	0.59
3:P:84:LEU:HD11	3:P:96:VAL:HG13	1.85	0.59
4:E:167:GLN:NE2	4:E:171:GLU:OE2	2.36	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
2:D:295:MET:HE1	2:D:317:ALA:HB1	1.86	0.57
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.69	0.57
1:C:216:ASN:ND2	1:C:275:VAL:HG23	2.20	0.57
1:C:233:GLN:HG3	1:C:368:LEU:HD22	1.86	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: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:114:LEU:HB3	2:D:149:MET:HE1	1.87	0.56
2:D:420:GLU:HG3	4:E:387:LEU:HD22	1.88	0.56
1:A:189:LEU:HD11	1:A:413:MET:HE1	1.88	0.55
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
1:A:430:LYS:O	1:A:434:GLU:CD	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:234:ILE:HD13	1:C:302:MET:SD	2.48	0.54
2:B:356:CYS:SG	2:B:357:ASP:N	2.81	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.53
1:C:275:VAL:C	1:C:276:ILE:HG13	2.33	0.53
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:376:ASP:HB2	4:E:384:LEU:HD11	1.92	0.52
2:B:237:GLY:C	2:B:376:THR:HG21	2.34	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
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
2:B:388:PHE:CE2	2:B:428:LEU:HD23	2.45	0.51
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.74	0.51
1:A:40:LYS:HZ2	1:A:47:ASP:H	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:MET:HE3	2:B:296:PHE:CE1	2.45	0.51
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.92	0.51
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
1:C:3:GLU:CD	1:C:129:CYS:HB3	2.37	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
2:B:114:LEU:O	2:B:117:SER:OG	2.28	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
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:191:THR:OG1	4:E:192:ASN:N	2.42	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
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.94	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
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
3:P:77:ASP:OD1	3:P:81:SER:N	2.40	0.48
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.49	0.48
1:A:40:LYS:HZ3	1:A:47:ASP:H	1.62	0.48
2:B:151:THR:HA	2:B:154:ILE:HD12	1.96	0.48
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.32	0.48
2:D:85:GLN:CD	2:D:85:GLN:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:40:LYS:HZ2	1:A:46:ASP:H	1.62	0.47
2:D:185:TYR:OH	2:D:398:MET:O	2.32	0.47
1:A:69:ASP:C	1:A:71:GLU:H	2.22	0.47
1:C:248:LEU:HD23	1:C:357:TYR:HE2	1.78	0.47
2:B:189:LEU:HD11	2:B:418:PHE:CE1	2.49	0.47
2:B:439:THR:OG1	2:B:440:ALA:N	2.46	0.47
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
2:B:179:ASP:OD1	2:B:224:TYR:OH	2.33	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: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
4:E:289:VAL:O	4:E:293:THR:OG1	2.28	0.47
4:E:550:VAL:C	4:E:552:GLU:H	2.23	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
4:E:388:GLU:HG3	4:E:389:ASP:N	2.29	0.46
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.46
1:A:346:TRP:CD1	1:A:347:CYS:HG	2.33	0.46
1:A:392:ASP:HA	1:A:395:PHE:HB3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:O	1:A:120:ASP:HB2	2.15	0.46
2:D:75:MET:HE3	2:D:75:MET:HB3	1.82	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
2:D:269:MET:HE1	2:D:307:PRO:HG3	1.98	0.45
4:E:192:ASN:O	4:E:194:ASN:N	2.49	0.45
2:D:295:MET:HE3	2:D:296:PHE:CE1	2.51	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
1:C:1:MET:HE2	1:C:51:THR:HG23	1.98	0.45
2:D:295:MET:HE3	2:D:296:PHE:HE1	1.80	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: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
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
1:C:409:VAL:HG13	4:E:482:ASN:HB3	1.99	0.45
4:E:308:THR:HG22	4:E:454:SER:HB2	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:43:GLY:HA2	1:A:55:GLU:HB2	2.00	0.44
1:A:221:ARG:NH2	2:B:329:ASP:OD2	2.50	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
4:E:200:MET:CE	4:E:268:TYR:HA	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:249:ASN:CG	2:B:255:LEU:HD13	2.43	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
1:C:388:TRP:CE3	1:C:425:MET:HE1	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:79:ARG:HD3	1:A:92:LEU:HD13	2.00	0.43
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.53	0.43
2:B:152:LEU:O	2:B:155:SER:OG	2.34	0.43
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.53	0.43
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
1:A:404:PHE:CZ	2:B:261:PRO:HB3	2.54	0.43
2:B:168:THR:HG21	2:B:194:LEU:HD22	2.00	0.43
1:C:219:ILE:HB	1:C:222:PRO:HG3	2.00	0.43
3:P:65:VAL:HG13	3:P:68:LYS:HE2	1.99	0.43
4:E:229:ARG:HB3	4:E:529:THR:HG22	2.00	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
3:P:48:LEU:HD13	3:P:53:LEU:HD21	2.01	0.43
3:P:73:VAL:HG21	3:P:102:HIS:HB2	2.00	0.43
3:P:60:LEU:HD11	3:P:94:GLU:HB2	2.01	0.43
4:E:295:ARG:C	4:E:297:LEU:H	2.27	0.43
2:D:303:ALA:O	2:D:305:CYS:N	2.52	0.43
2:D:317:ALA:C	2:D:318:ILE:HD12	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:HE2	1:A:38:SER:OG	2.18	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:311:LYS:HZ2	1:A:344:VAL:HG12	1.84	0.42
2:D:174:SER:C	2:D:176:LYS:H	2.27	0.42
3:P:42:ALA:O	3:P:50:PRO:HD3	2.19	0.42
4:E:402:ARG:HD2	4:E:402:ARG:N	2.33	0.42
4:E:433:SER:O	4:E:433:SER:OG	2.36	0.42
1:A:39:ASP:OD1	1:A:40:LYS:N	2.51	0.42
1:A:359:PRO:HA	1:A:360:PRO:HD3	1.89	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
4:E:275:ARG:O	4:E:551:LYS:NZ	2.52	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:B:346:TRP:CD1	2:B:346:TRP:H	2.38	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
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
1:C:97:GLU:HA	2:D:1:MET:H3	1.84	0.42
2:D:32:PRO:C	2:D:85:GLN:HE21	2.26	0.42
3:P:67:LEU:HB3	3:P:102:HIS:CE1	2.54	0.42
1:A:275:VAL:HG13	1:A:275:VAL:O	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:N	2:D:39:ASP:OD1	2.53	0.41
4:E:489:LYS:HD3	4:E:546:TYR:CZ	2.55	0.41
2:B:19:LYS:O	2:B:23:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:ALA:O	2:B:191:VAL:HG23	2.20	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
1:C:366:GLY:C	1:C:368:LEU:H	2.28	0.41
2:D:11:GLN:HG3	8:D:502:PO4:O2	2.21	0.41
2:D:28:HIS:NE2	2:D:243:ARG:HB3	2.35	0.41
2:D:102:ASN:H	2:D:144:GLY:HA3	1.84	0.41
2:D:310:GLY:HA2	2:D:436:GLN:NE2	2.34	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
1:A:288:VAL:HG11	1:A:328:VAL:HG22	2.02	0.41
2:B:205:ASP:HB2	2:B:303:ALA:HA	2.03	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
1:C:302:MET:HE3	1:C:302:MET:HB3	1.86	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
2:D:264:ARG:O	2:D:266:HIS:ND1	2.54	0.41
2:D:272:PHE:CE1	2:D:374:SER:HB2	2.55	0.41
2:D:288:VAL:HG11	2:D:327:GLU:HG2	2.03	0.41
3:P:17:LYS:O	3:P:21:ALA:HB2	2.21	0.41
4:E:311:ALA:HB3	4:E:457:ASP:HA	2.02	0.41
1:A:292:THR:HG1	1:A:319:TYR:HH	1.69	0.41
2:B:132:LEU:HD21	2:B:135:PHE:CZ	2.55	0.41
1:C:90:GLU:CD	1:C:90:GLU:H	2.29	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
2:D:416:MET:HB2	4:E:389:ASP:CG	2.46	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:VAL:HG12	1:A:146:GLY:HA2	2.02	0.40
1:A:40:LYS:HD3	1:A:47:ASP:OD2	2.20	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:HD12	4:E:449:LEU:HA	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
2:D:75:MET:O	2:D:78:VAL:HB	2.22	0.40
2:D:234:THR:O	2:D:238:VAL:HG13	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%)	6	34
1	C	432/451 (96%)	392 (91%)	35 (8%)	5 (1%)	10	42
2	B	429/445 (96%)	397 (92%)	29 (7%)	3 (1%)	18	52
2	D	429/445 (96%)	378 (88%)	46 (11%)	5 (1%)	10	42
3	P	153/168 (91%)	132 (86%)	21 (14%)	0	100	100
4	E	371/420 (88%)	309 (83%)	47 (13%)	15 (4%)	2	19
All	All	2248/2380 (94%)	1992 (89%)	220 (10%)	36 (2%)	7	36

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
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%)	363 (100%)	0	100	100
1	C	363/379 (96%)	363 (100%)	0	100	100
2	B	369/383 (96%)	369 (100%)	0	100	100
2	D	369/383 (96%)	369 (100%)	0	100	100
3	P	113/131 (86%)	113 (100%)	0	100	100
4	E	320/370 (86%)	318 (99%)	2 (1%)	78	80
All	All	1897/2025 (94%)	1895 (100%)	2 (0%)	88	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	450[A]	HIS
4	E	450[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	133	GLN
1	A	256	GLN
1	A	301	GLN
1	A	358	GLN
2	B	249	ASN
2	B	294	GLN
2	B	349	ASN
2	B	385	GLN
2	B	394	GLN
2	B	424	ASN
2	B	433	GLN
1	C	61	HIS
1	C	192	HIS
1	C	226	ASN
1	C	256	GLN
1	C	393	HIS
2	D	15	GLN
2	D	91	ASN
2	D	229	HIS
4	E	167	GLN

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Mol	Chain	Res	Type
4	E	178	GLN
4	E	194	ASN
4	E	354	ASN
4	E	361	GLN
4	E	482	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 oligosaccharides 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	$\# Z > 2$
5	GTP	A	501	6	33,34,34	1.00	2 (6%)	50,54,54	1.61	8 (16%)
7	GDP	B	501	6	29,30,30	1.21	3 (10%)	45,47,47	1.66	5 (11%)
7	GDP	D	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
5	GTP	C	501	6	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
8	PO4	D	502	-	4,4,4	0.91	0	6,6,6	0.96	0
9	ANP	E	601	6	33,33,33	1.57	5 (15%)	45,52,52	0.72	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	3/22/38/38	0/3/3/3
7	GDP	B	501	6	-	3/16/32/32	0/3/3/3
7	GDP	D	501	-	-	4/16/32/32	0/3/3/3
5	GTP	C	501	6	-	5/22/38/38	0/3/3/3
9	ANP	E	601	6	-	6/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	601	ANP	PB-O1B	6.79	1.56	1.46
7	B	501	GDP	C5-C4	3.25	1.47	1.38
7	D	501	GDP	C5-C4	3.16	1.47	1.38
9	E	601	ANP	PB-O2B	-2.79	1.49	1.56
7	B	501	GDP	C6-N1	-2.67	1.33	1.38
9	E	601	ANP	PG-N3B	2.50	1.69	1.63
9	E	601	ANP	PB-O3A	-2.48	1.56	1.59
7	D	501	GDP	C6-N1	-2.45	1.34	1.38
5	A	501	GTP	PA-O3A	2.44	1.62	1.59
9	E	601	ANP	PG-O1G	2.44	1.49	1.46
5	A	501	GTP	C2-N3	2.22	1.38	1.33
5	C	501	GTP	C2-N3	2.19	1.38	1.33
7	B	501	GDP	C5-N7	-2.19	1.34	1.39
7	D	501	GDP	C5-N7	-2.01	1.35	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	GDP	C5-C4-N3	-6.19	118.54	128.39
7	D	501	GDP	C5-C4-N3	-6.06	118.74	128.39
5	C	501	GTP	C5-C4-N3	-5.12	120.24	128.39
7	D	501	GDP	C2-N3-C4	5.02	120.94	112.30
5	A	501	GTP	C5-C4-N3	-5.01	120.42	128.39
5	A	501	GTP	C2-N3-C4	4.82	120.61	112.30
5	C	501	GTP	C2-N3-C4	4.77	120.51	112.30
7	B	501	GDP	C2-N3-C4	4.55	120.14	112.30
7	D	501	GDP	N9-C4-N3	4.45	134.85	125.95
7	B	501	GDP	N9-C4-N3	4.42	134.80	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	501	GDP	C6-C5-N7	3.33	136.36	130.29
5	A	501	GTP	N9-C4-N3	3.30	132.56	125.95
5	C	501	GTP	N9-C4-N3	3.15	132.25	125.95
5	C	501	GTP	C2-N1-C6	-3.04	119.59	125.11
7	B	501	GDP	C6-C5-N7	3.03	135.80	130.29
5	A	501	GTP	C2-N1-C6	-2.81	120.01	125.11
7	B	501	GDP	C4-C5-N7	-2.70	106.39	110.67
5	A	501	GTP	N9-C8-N7	-2.70	108.40	113.40
7	D	501	GDP	C4-C5-N7	-2.64	106.48	110.67
5	A	501	GTP	C5-C6-N1	2.59	119.84	113.25
5	C	501	GTP	C5-C6-N1	2.58	119.81	113.25
5	A	501	GTP	O6-C6-C5	-2.53	119.86	126.53
5	A	501	GTP	C8-N7-C5	2.45	108.62	104.26
5	C	501	GTP	N9-C8-N7	-2.42	108.91	113.40
5	C	501	GTP	O6-C6-C5	-2.40	120.21	126.53
5	C	501	GTP	C8-N7-C5	2.36	108.47	104.26
9	E	601	ANP	O2G-PG-O1G	-2.33	107.60	113.45
7	D	501	GDP	C3'-C2'-C1'	2.29	105.79	101.46
5	C	501	GTP	C3'-C2'-C1'	2.02	105.29	101.46

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

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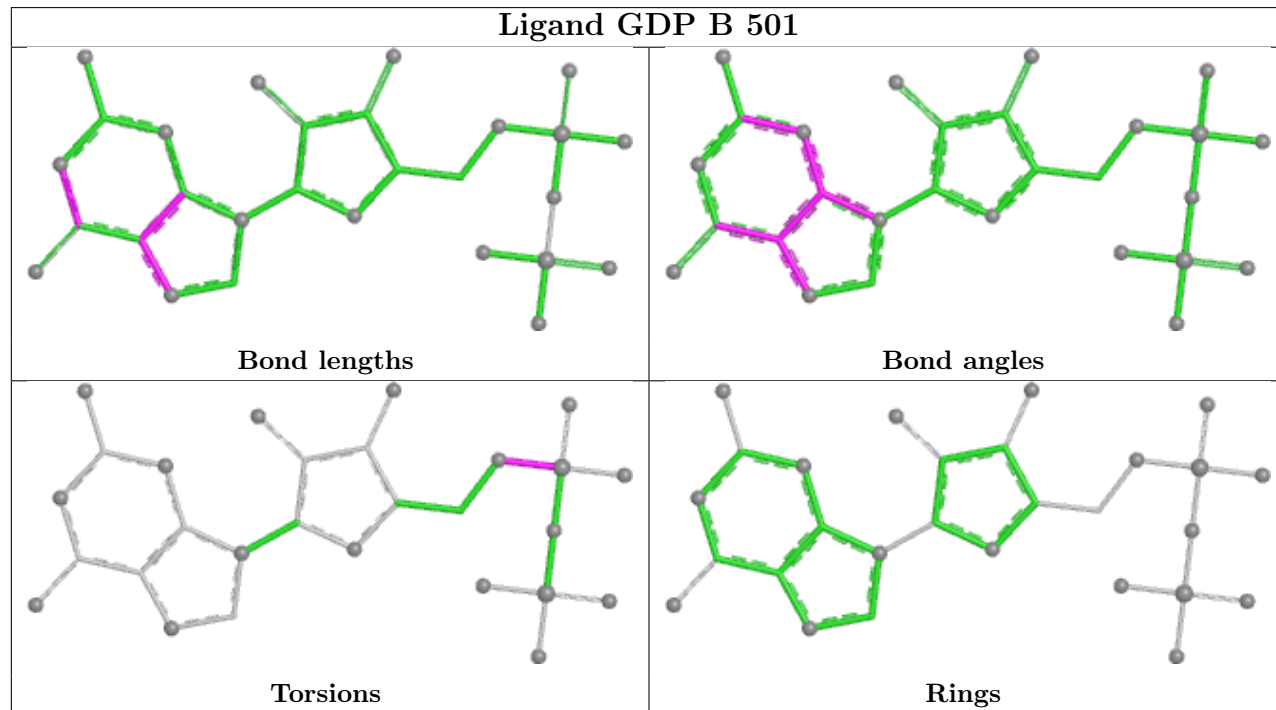
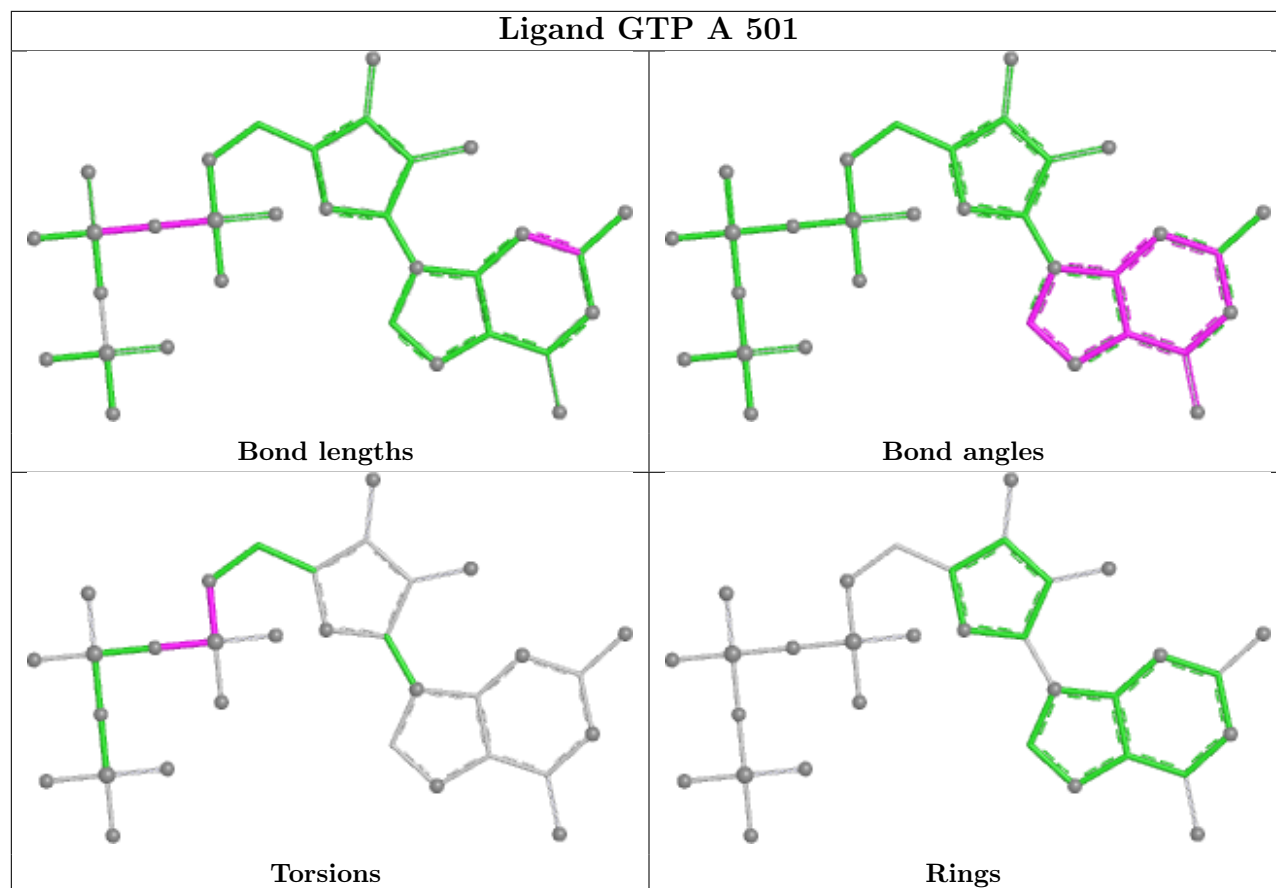
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A

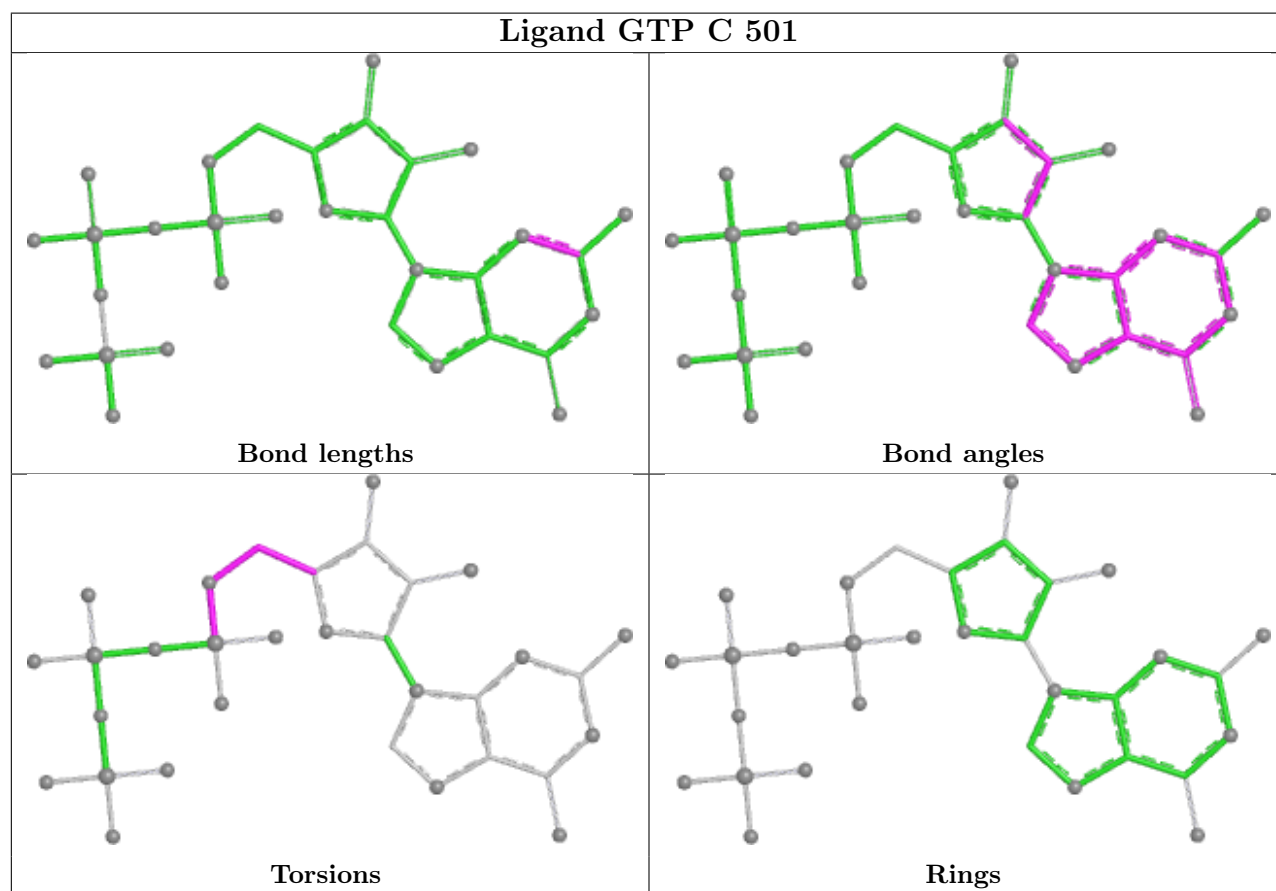
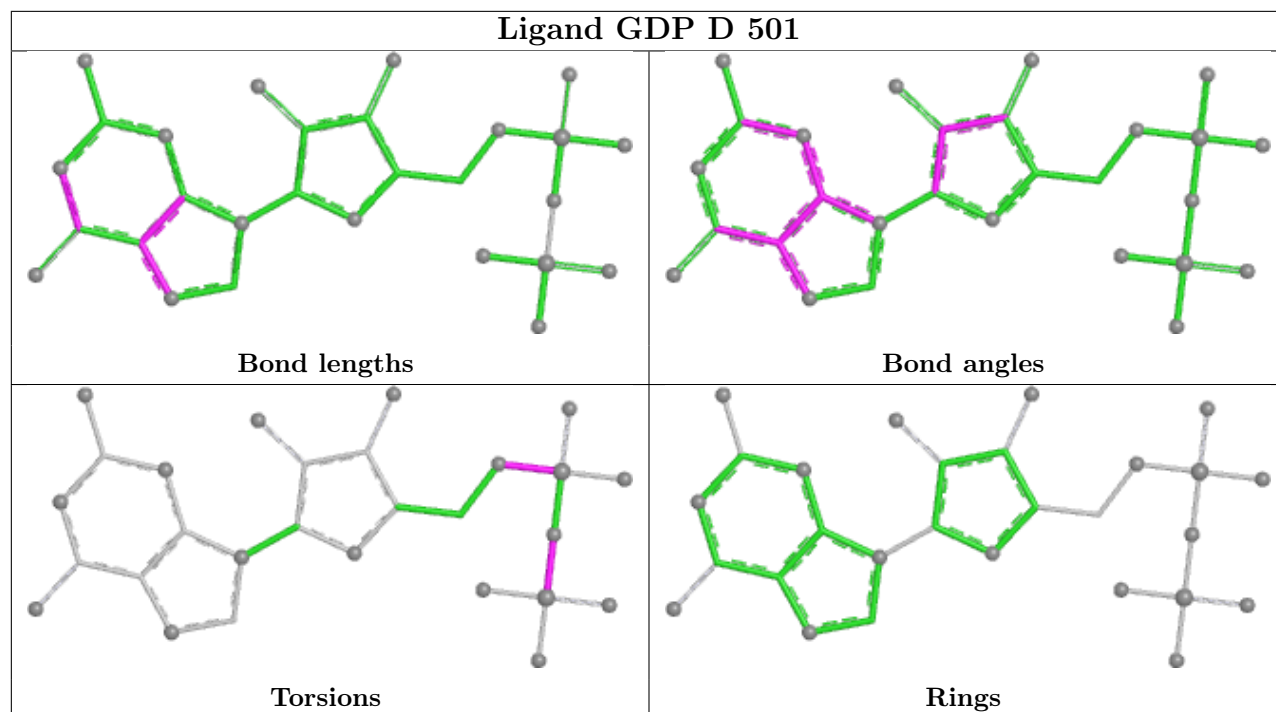
There are no ring outliers.

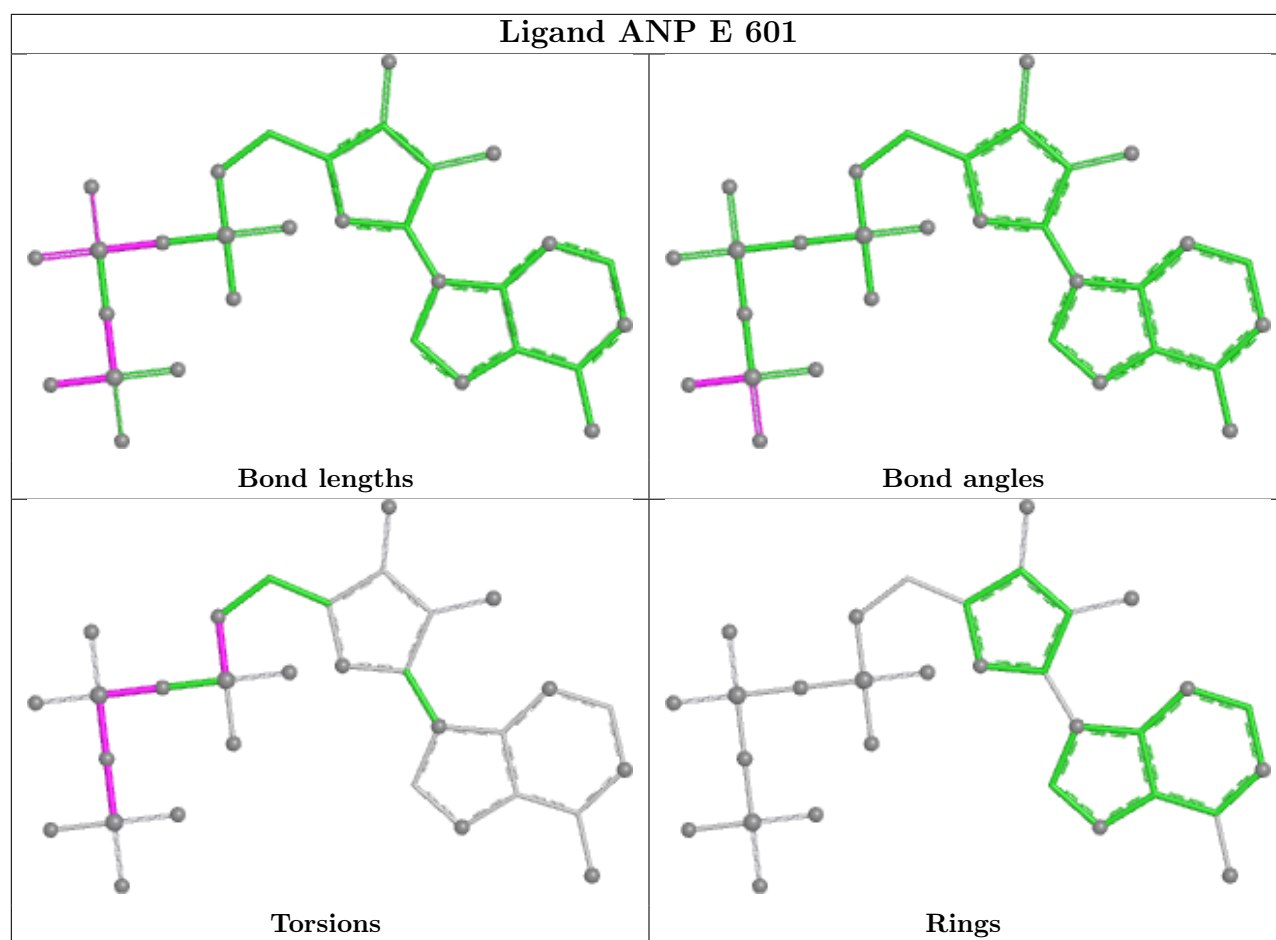
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/451 (96%)	-0.64	0 100 100	103, 146, 179, 213	0
1	C	436/451 (96%)	-0.67	0 100 100	86, 126, 162, 195	0
2	B	431/445 (96%)	-0.70	0 100 100	79, 122, 170, 200	0
2	D	431/445 (96%)	-0.54	1 (0%) 91 81	108, 162, 191, 215	0
3	P	155/168 (92%)	-0.60	0 100 100	172, 233, 252, 258	0
4	E	378/420 (90%)	-0.67	0 100 100	95, 140, 169, 189	1 (0%)
All	All	2267/2380 (95%)	-0.64	1 (0%) 100 100	79, 142, 224, 258	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	203	CYS	2.3

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](#)

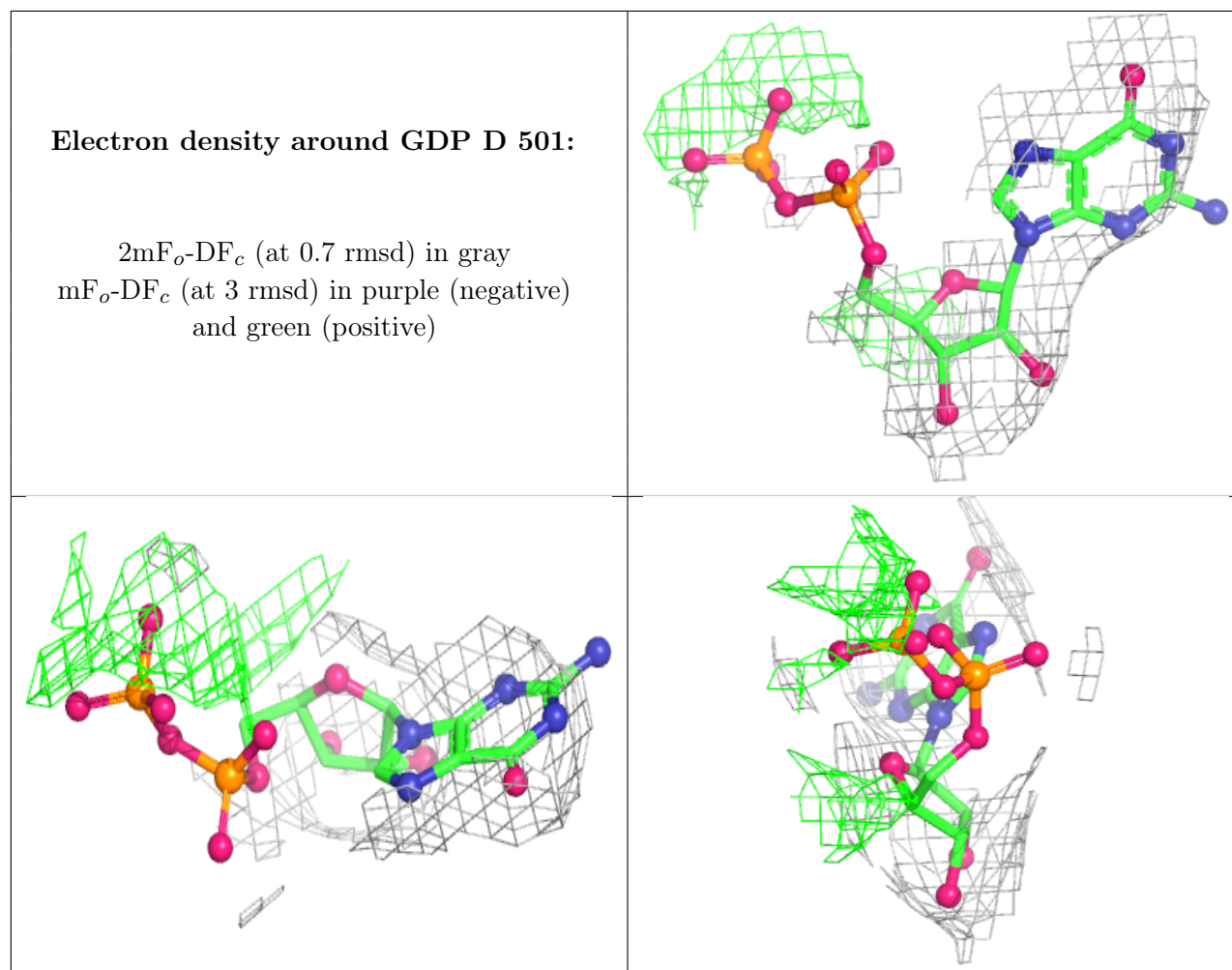
There are no oligosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

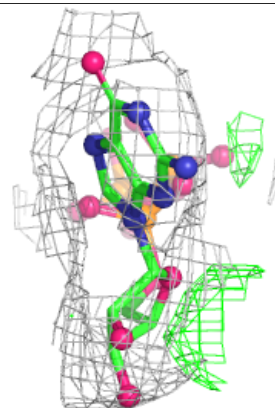
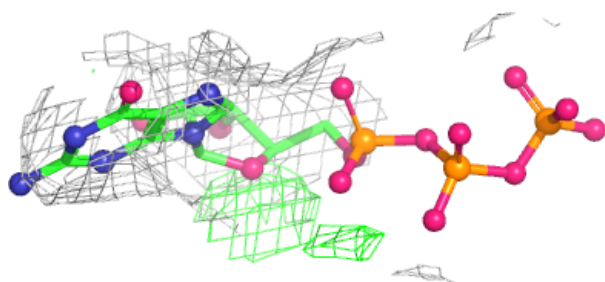
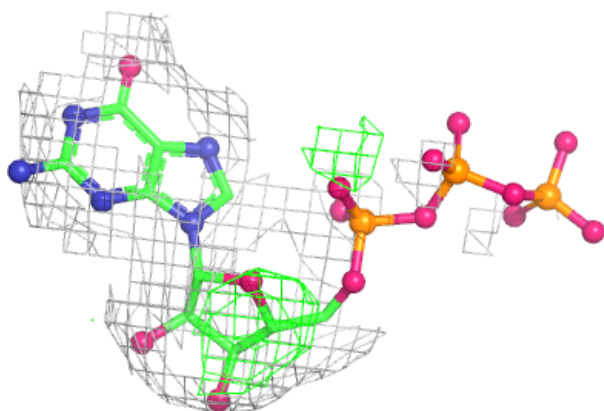
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	502	1/1	0.86	0.09	113,113,113,113	0
8	PO4	D	502	5/5	0.90	0.05	173,174,180,181	0
6	MG	C	502	1/1	0.94	0.07	102,102,102,102	0
7	GDP	D	501	28/28	0.94	0.07	168,177,182,184	0
6	MG	A	502	1/1	0.94	0.10	205,205,205,205	0
5	GTP	C	501	32/32	0.95	0.06	91,123,133,140	0
5	GTP	A	501	32/32	0.95	0.07	114,126,136,137	0
9	ANP	E	601	31/31	0.96	0.04	108,131,139,142	0
7	GDP	B	501	28/28	0.97	0.06	99,115,124,133	0
6	MG	E	602	1/1	0.99	0.03	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.

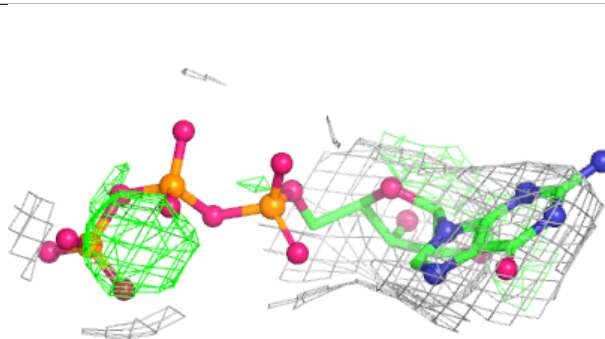
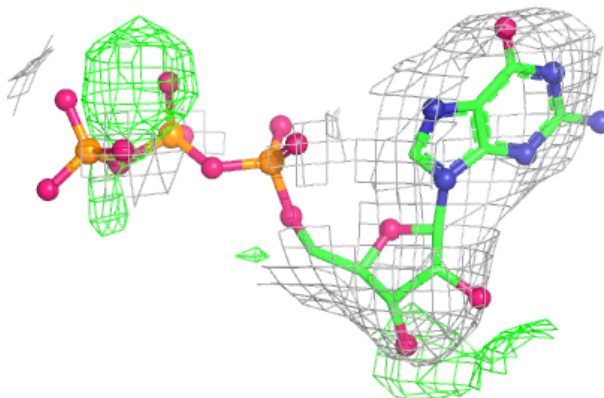


Electron density around GTP C 501:

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

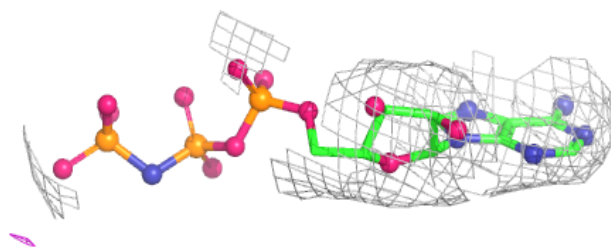
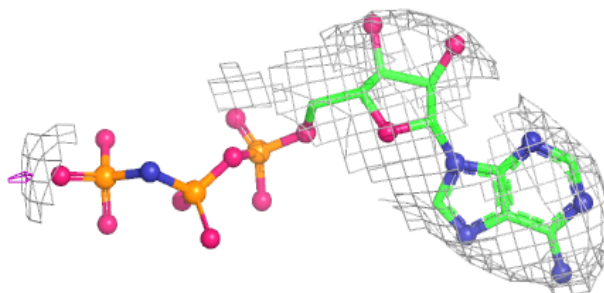
**Electron density around GTP A 501:**

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

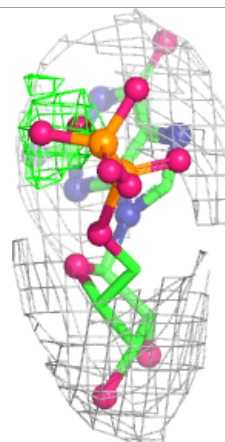
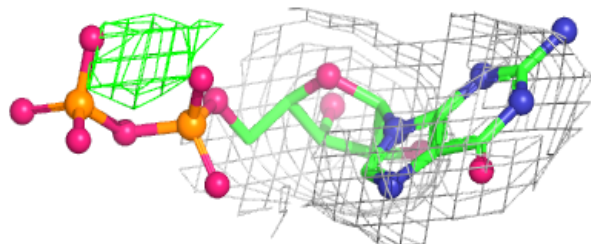
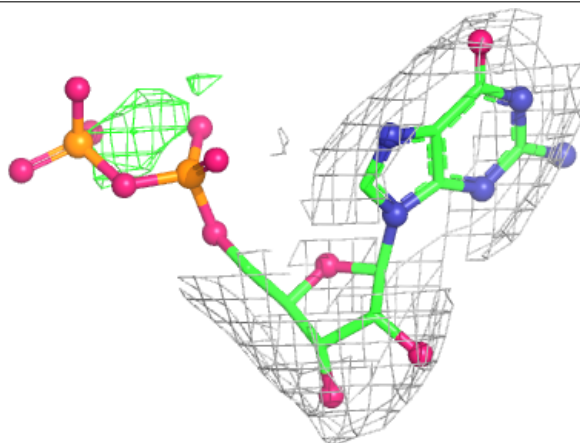


Electron density around ANP E 601:

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

**Electron density around 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.