



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:49 AM UTC

PDB ID : 6MZG / pdb_00006mzg
Title : Structural Basis of Tubulin Recruitment and Assembly by Microtubule Polymerases with Tumor Overexpressed Gene (TOG) Domain Arrays
Authors : Nithianantham, S.; Al-Bassam, J.
Deposited on : 2018-11-05
Resolution : 3.21 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

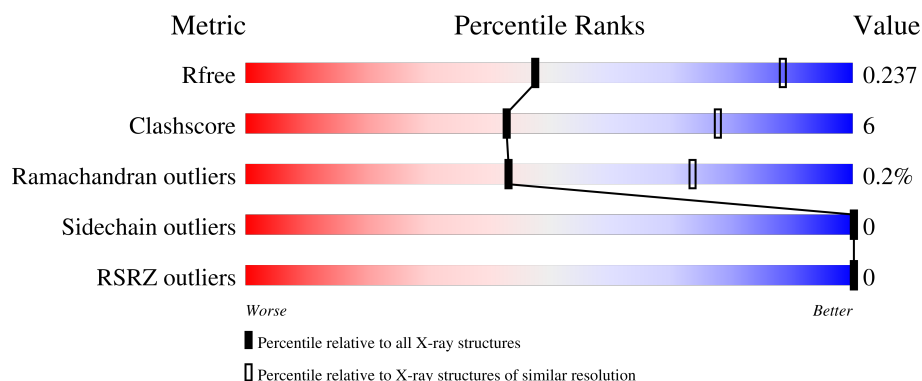
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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	 86% 9% 5%
1	C	451	 82% 15% .
1	G	451	 83% 11% 6%
1	I	451	 85% 12% .
2	B	445	 83% 13% .

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Mol	Chain	Length	Quality of chain
2	D	445	 82% 14% .
2	H	445	 80% 16% .
2	J	445	 84% 12% .
3	E	554	 64% 24% 12%
3	K	554	 69% 19% 12%
4	F	140	 79% 11% 11%
4	L	140	 76% 14% 11%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36853 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-1A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3338	2113	568	636	21			
1	C	434	Total	C	N	O	S	0	0	0
			3377	2134	575	647	21			
1	G	425	Total	C	N	O	S	0	0	0
			3322	2102	564	635	21			
1	I	436	Total	C	N	O	S	0	0	0
			3391	2144	577	649	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3378	2122	579	651	26			
2	D	428	Total	C	N	O	S	0	0	0
			3363	2112	575	650	26			
2	H	429	Total	C	N	O	S	0	0	0
			3375	2119	578	652	26			
2	J	428	Total	C	N	O	S	0	0	0
			3363	2112	575	650	26			

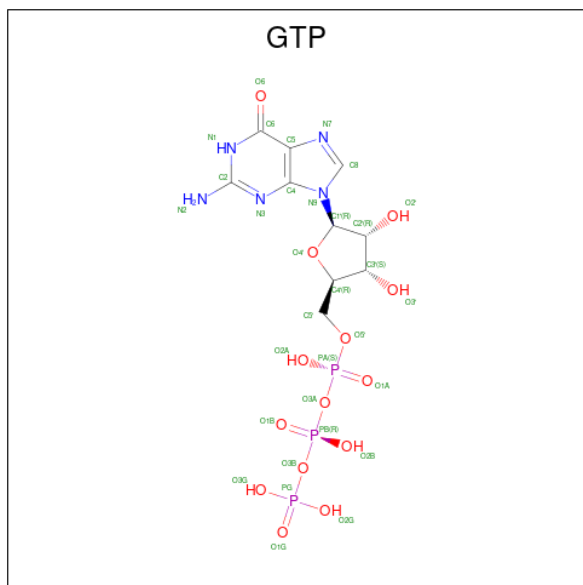
- Molecule 3 is a protein called Protein Stu2p/Alp14p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	487	Total	C	N	O	S	0	0	0
			3914	2506	662	730	16			
3	K	487	Total	C	N	O	S	0	0	0
			3914	2506	662	730	16			

- Molecule 4 is a protein called Truncated Darpin-D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	125	Total	C	N	O	S	0	0	0
			935	595	157	181	2			
4	L	125	Total	C	N	O	S	0	0	0
			935	595	157	181	2			

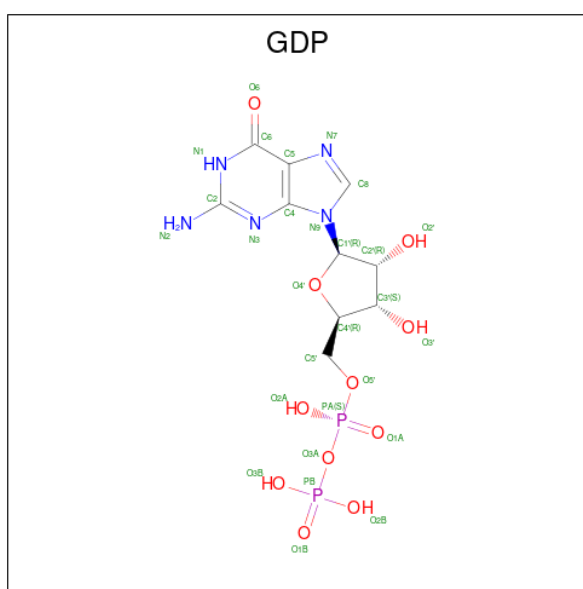
- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mg	0	0
			1	1		
6	H	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

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

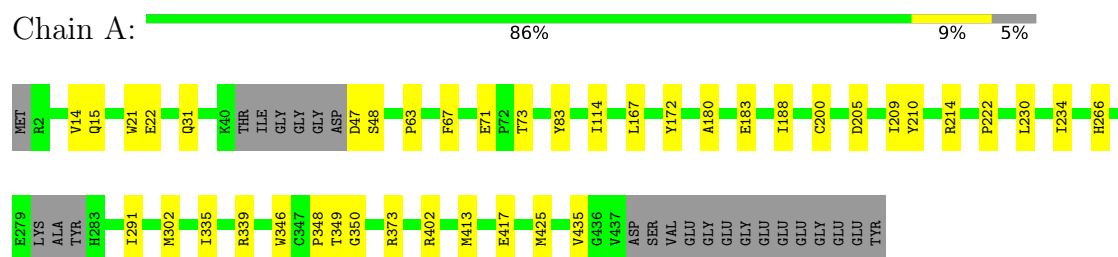


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	H	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	J	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

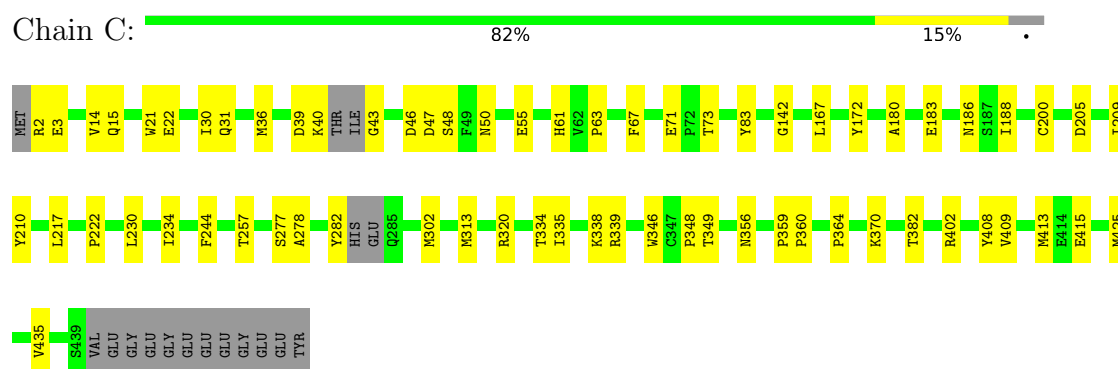
3 Residue-property plots [i](#)

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.

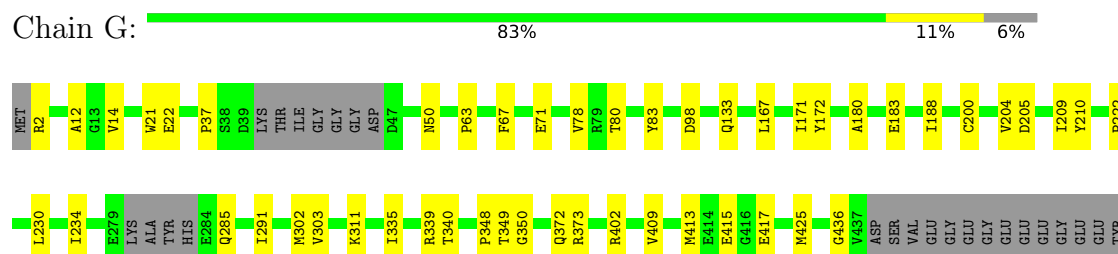
- Molecule 1: Tubulin alpha-1A chain



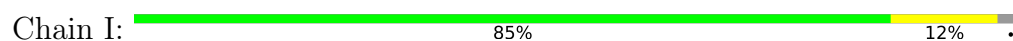
- Molecule 1: Tubulin alpha-1A chain

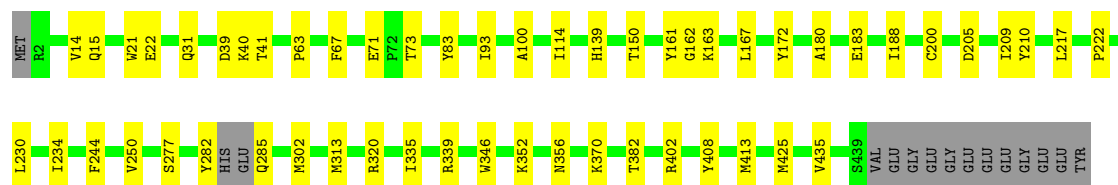


- Molecule 1: Tubulin alpha-1A chain



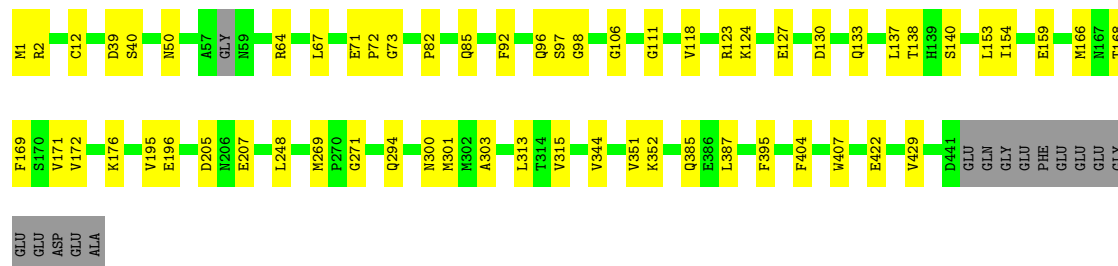
- Molecule 1: Tubulin alpha-1A chain





• Molecule 2: Tubulin beta chain

Chain B: 83% 13% .



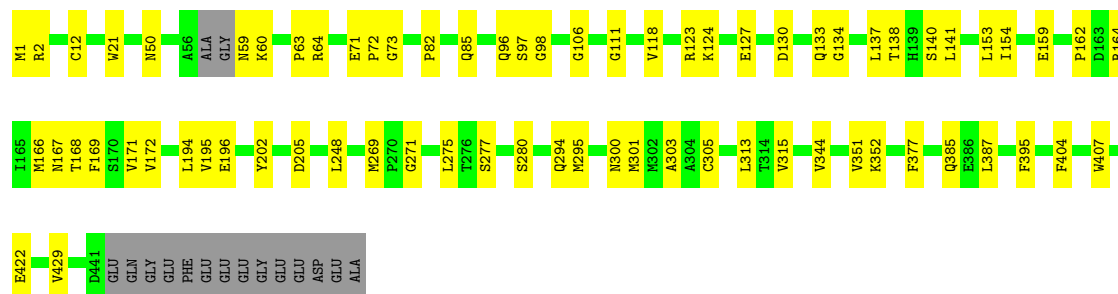
• Molecule 2: Tubulin beta chain

Chain D: 82% 14% .



• Molecule 2: Tubulin beta chain

Chain H: 80% 16% .



• Molecule 2: Tubulin beta chain

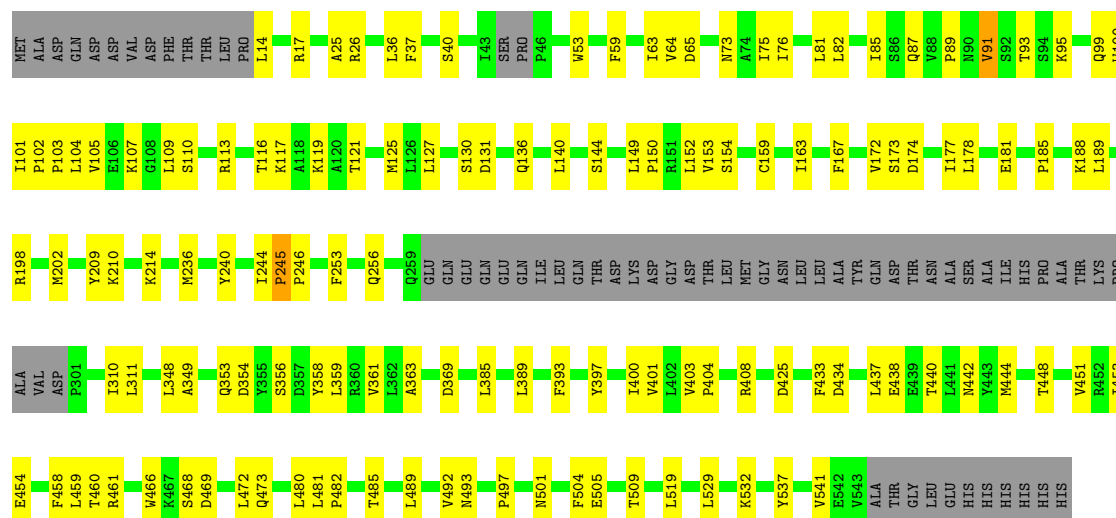
Chain J: 84% 12% .





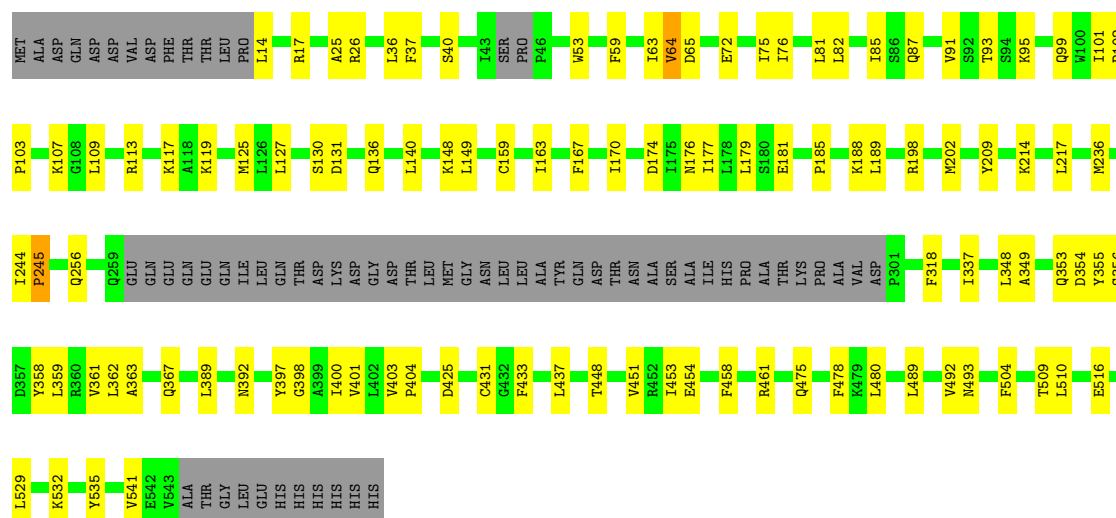
• Molecule 3: Protein Stu2p/Alp14p

Chain E: 64% 24% 12%



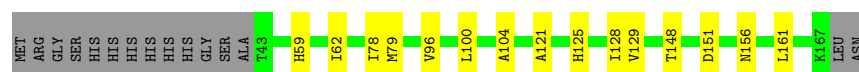
• Molecule 3: Protein Stu2p/Alp14p

Chain K: 69% 19% 12%



• Molecule 4: Truncated Darpin-D1

Chain F: 79% 11% 11%



• Molecule 4: Truncated Darpin-D1

Chain L:

76%

14%

11%

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	GLY	SER	ALA	T43	S46	G47	I78	M79	I90	G91	Y96	L100	A104	V112	A121	I122	M123	G124	H125	I128	V129	T148	D151	L161	K167	LEU	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.13Å 194.99Å 149.57Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	57.56 – 3.21 57.56 – 3.21	Depositor EDS
% Data completeness (in resolution range)	81.9 (57.56-3.21) 81.9 (57.56-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.175 , 0.234 0.178 , 0.237	Depositor DCC
R_{free} test set	4370 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 5.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.410 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	0 of 88337 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36853	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: GDP, GTP, 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	0.11	0/3411	0.28	0/4628
1	C	0.12	0/3445	0.30	0/4671
1	G	0.11	0/3396	0.29	0/4610
1	I	0.11	0/3463	0.29	0/4698
2	B	0.11	0/3452	0.29	0/4676
2	D	0.10	0/3437	0.27	0/4657
2	H	0.11	0/3449	0.30	0/4672
2	J	0.10	0/3437	0.27	0/4657
3	E	0.13	0/3986	0.35	1/5401 (0.0%)
3	K	0.13	0/3986	0.34	1/5401 (0.0%)
4	F	0.10	0/951	0.26	0/1296
4	L	0.09	0/951	0.25	0/1296
All	All	0.11	0/37364	0.30	2/50663 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	91	VAL	N-CA-C	-5.66	105.91	112.98
3	E	91	VAL	N-CA-C	-5.16	106.53	112.98

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	3338	0	3240	27	0
1	C	3377	0	3270	49	0
1	G	3322	0	3225	28	0
1	I	3391	0	3288	38	0
2	B	3378	0	3258	35	0
2	D	3363	0	3239	35	0
2	H	3375	0	3253	41	0
2	J	3363	0	3239	31	0
3	E	3914	0	4032	87	0
3	K	3914	0	4032	74	0
4	F	935	0	935	9	0
4	L	935	0	935	12	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
5	G	32	0	12	0	0
5	I	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
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	B	28	0	12	1	0
7	D	28	0	12	2	0
7	H	28	0	12	1	0
7	J	28	0	12	1	0
All	All	36853	0	36042	452	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (452) 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:I:31:GLN:C	1:I:31:GLN:CB	2.51	0.83
1:C:31:GLN:CG	1:C:31:GLN:NE2	2.42	0.83
1:I:31:GLN:CG	1:I:31:GLN:NE2	2.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:CG	1:A:31:GLN:NE2	2.42	0.83
1:C:47:ASP:CB	1:C:47:ASP:N	2.44	0.81
2:H:172:VAL:HG11	2:H:387:LEU:HD11	1.61	0.81
1:I:31:GLN:CB	1:I:31:GLN:N	2.43	0.80
2:J:172:VAL:HG11	2:J:387:LEU:HD11	1.64	0.80
2:D:172:VAL:HG11	2:D:387:LEU:HD11	1.63	0.79
3:E:403:VAL:HG13	3:E:404:PRO:HD3	1.64	0.77
3:K:480:LEU:HD11	3:K:510:LEU:HD21	1.67	0.75
1:I:31:GLN:C	1:I:31:GLN:N	2.45	0.74
2:B:172:VAL:HG11	2:B:387:LEU:HD11	1.70	0.72
3:K:125:MET:HE1	3:K:163:ILE:HG22	1.70	0.72
1:C:46:ASP:OD2	1:C:46:ASP:CB	2.38	0.71
1:C:31:GLN:CG	1:C:31:GLN:OE1	2.39	0.71
3:K:76:ILE:HG22	3:K:119:LYS:HG3	1.73	0.70
1:I:31:GLN:NE2	1:I:31:GLN:OE1	2.25	0.70
1:C:31:GLN:NE2	1:C:31:GLN:OE1	2.25	0.70
1:I:31:GLN:CG	1:I:31:GLN:OE1	2.39	0.70
1:A:31:GLN:CG	1:A:31:GLN:OE1	2.39	0.70
1:A:31:GLN:NE2	1:A:31:GLN:OE1	2.25	0.69
1:C:46:ASP:CB	1:C:46:ASP:OD1	2.39	0.69
1:C:47:ASP:O	1:C:48:SER:N	2.25	0.69
3:E:17:ARG:HD3	3:E:25:ALA:HB1	1.76	0.68
3:E:125:MET:HE1	3:E:163:ILE:HG22	1.76	0.68
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.75	0.68
2:H:277:SER:HB3	2:H:280:SER:HB3	1.76	0.68
2:B:71:GLU:HG3	2:B:73:GLY:H	1.58	0.66
3:K:403:VAL:HG13	3:K:404:PRO:HD3	1.77	0.66
3:E:64:VAL:HG13	3:E:107:LYS:HD3	1.77	0.66
3:E:458:PHE:HA	3:E:461:ARG:HD2	1.78	0.66
1:I:172:TYR:HB3	1:I:205:ASP:HA	1.76	0.66
3:E:393:PHE:HA	3:E:397:TYR:HB2	1.79	0.65
3:K:458:PHE:HA	3:K:461:ARG:HD2	1.79	0.65
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.79	0.64
2:H:295:MET:HG3	2:H:377:PHE:HB2	1.79	0.64
2:D:71:GLU:HG3	2:D:73:GLY:H	1.62	0.64
3:E:460:THR:HG23	3:E:509:THR:HG21	1.79	0.63
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.80	0.63
2:H:313:LEU:HD23	2:H:344:VAL:HG21	1.80	0.63
4:L:46:SER:O	4:L:78:ILE:N	2.31	0.63
3:K:95:LYS:NZ	3:K:99:GLN:OE1	2.32	0.63
3:K:170:ILE:HD11	3:K:256:GLN:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:ILE:HG23	1:G:339:ARG:HD2	1.81	0.62
2:B:72:PRO:HD3	2:B:96:GLN:HA	1.79	0.62
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.80	0.62
3:E:489:LEU:O	3:E:493:ASN:ND2	2.33	0.62
2:J:118:VAL:HG11	2:J:153:LEU:HD11	1.80	0.62
3:E:95:LYS:NZ	3:E:99:GLN:OE1	2.33	0.61
3:E:82:LEU:HD21	3:E:127:LEU:HG	1.81	0.61
3:K:489:LEU:O	3:K:493:ASN:ND2	2.34	0.61
2:H:159:GLU:HA	3:K:149:LEU:HD13	1.83	0.61
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.81	0.61
1:C:46:ASP:OD2	1:C:46:ASP:OD1	2.19	0.61
2:H:71:GLU:HG3	2:H:73:GLY:H	1.65	0.60
2:J:248:LEU:HD21	2:J:352:LYS:HB3	1.82	0.60
2:B:313:LEU:HD23	2:B:344:VAL:HG21	1.82	0.60
1:I:346:TRP:HZ2	1:I:435:VAL:HG13	1.66	0.60
3:K:363:ALA:HB1	3:K:404:PRO:HG2	1.83	0.60
1:G:172:TYR:HB3	1:G:205:ASP:HA	1.83	0.59
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.84	0.59
2:H:269:MET:HG3	2:H:303:ALA:HB3	1.85	0.59
2:J:313:LEU:HD23	2:J:344:VAL:HG21	1.84	0.59
2:H:118:VAL:HG11	2:H:153:LEU:HD11	1.83	0.59
3:E:81:LEU:O	3:E:85:ILE:HG23	2.03	0.59
1:G:409:VAL:O	3:K:198:ARG:NH2	2.36	0.59
1:C:335:ILE:HG23	1:C:339:ARG:HD2	1.85	0.59
3:E:172:VAL:HG21	3:E:178:LEU:HD22	1.84	0.59
3:K:529:LEU:HD23	3:K:532:LYS:HE3	1.85	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.83	0.58
1:G:2:ARG:HH12	1:G:50:ASN:HB3	1.68	0.58
3:K:81:LEU:O	3:K:85:ILE:HG23	2.03	0.58
3:K:64:VAL:HG13	3:K:107:LYS:HD3	1.85	0.58
1:C:348:PRO:O	1:C:349:THR:HG22	2.03	0.58
3:E:363:ALA:HB1	3:E:404:PRO:HG2	1.84	0.58
2:D:313:LEU:HD23	2:D:344:VAL:HG21	1.86	0.58
1:I:335:ILE:HG23	1:I:339:ARG:HD2	1.86	0.58
2:H:50:ASN:O	2:H:64:ARG:NH2	2.36	0.58
1:G:285:GLN:NE2	1:G:372:GLN:OE1	2.35	0.58
1:C:15:GLN:NE2	5:C:600:GTP:O6	2.37	0.58
1:C:217:LEU:HA	1:C:277:SER:HB2	1.86	0.58
3:E:433:PHE:CE2	3:E:466:TRP:HD1	2.21	0.58
1:I:39:ASP:OD1	1:I:40:LYS:N	2.37	0.57
2:D:1:MET:HE3	2:D:133:GLN:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:349:ALA:HB3	3:E:353:GLN:HG3	1.86	0.57
3:K:82:LEU:HD21	3:K:127:LEU:HG	1.84	0.57
2:B:294:GLN:O	2:B:300:ASN:ND2	2.36	0.57
1:C:409:VAL:HG12	3:E:497:PRO:HB3	1.87	0.57
3:K:101:ILE:HG22	3:K:127:LEU:HD13	1.85	0.57
3:E:433:PHE:HB3	3:E:437:LEU:HB2	1.87	0.57
2:H:154:ILE:HG23	2:H:166:MET:HG2	1.87	0.56
2:H:72:PRO:HD3	2:H:96:GLN:HA	1.87	0.56
2:B:39:ASP:HB3	3:K:478:PHE:HB3	1.85	0.56
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.41	0.56
2:D:195:VAL:HG13	2:D:196:GLU:HG2	1.87	0.56
4:F:100:LEU:HD23	4:F:104:ALA:HB3	1.87	0.56
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.89	0.55
1:A:71:GLU:HG2	1:A:73:THR:H	1.71	0.55
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.89	0.55
3:E:468:SER:OG	3:E:469:ASP:N	2.39	0.55
2:J:195:VAL:HG13	2:J:196:GLU:HG2	1.88	0.55
2:J:1:MET:HE3	2:J:133:GLN:HG3	1.88	0.55
3:E:101:ILE:HG22	3:E:127:LEU:HD13	1.88	0.55
3:E:400:ILE:HG23	3:E:401:VAL:HG13	1.88	0.54
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.88	0.54
2:B:172:VAL:HB	2:B:205:ASP:HA	1.89	0.54
2:D:172:VAL:HG21	2:D:387:LEU:HD21	1.90	0.54
3:K:389:LEU:HD12	3:K:392:ASN:HB3	1.90	0.54
4:F:148:THR:OG1	4:F:151:ASP:OD1	2.23	0.54
3:E:481:LEU:HA	3:E:485:THR:HG22	1.90	0.54
1:I:161:TYR:O	1:I:163:LYS:N	2.40	0.54
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.90	0.54
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.89	0.54
3:E:244:ILE:HB	3:E:245:PRO:HD3	1.88	0.54
3:K:348:LEU:HB2	3:K:389:LEU:HD22	1.89	0.54
3:E:509:THR:HA	3:E:541:VAL:HG11	1.90	0.54
2:J:71:GLU:HG3	2:J:73:GLY:H	1.72	0.53
3:K:14:LEU:O	3:K:17:ARG:HG2	2.09	0.53
2:B:123:ARG:O	2:B:127:GLU:HG2	2.08	0.53
3:K:53:TRP:HE1	3:K:85:ILE:HB	1.74	0.53
2:H:195:VAL:HG13	2:H:196:GLU:HG2	1.90	0.53
2:B:50:ASN:O	2:B:64:ARG:NH2	2.42	0.53
3:E:403:VAL:CG1	3:E:404:PRO:HD3	2.36	0.53
2:H:1:MET:HE3	2:H:133:GLN:HG3	1.91	0.53
2:J:123:ARG:O	2:J:127:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:148:THR:OG1	4:L:151:ASP:OD1	2.25	0.53
1:I:180:ALA:HB3	1:I:183:GLU:HG3	1.91	0.53
1:C:71:GLU:HG2	1:C:73:THR:H	1.73	0.52
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.90	0.52
3:E:150:PRO:O	3:E:154:SER:OG	2.22	0.52
3:K:37:PHE:CD2	3:K:81:LEU:HB2	2.44	0.52
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.44	0.52
2:J:172:VAL:HG21	2:J:387:LEU:HD21	1.91	0.52
2:H:82:PRO:O	2:H:85:GLN:NE2	2.42	0.52
2:D:123:ARG:O	2:D:127:GLU:HG2	2.10	0.52
4:F:59:HIS:HB3	4:F:62:ILE:HD13	1.92	0.52
2:H:172:VAL:HG21	2:H:387:LEU:HD21	1.91	0.52
2:J:188:THR:HG23	2:J:425:MET:HE2	1.91	0.52
3:K:198:ARG:O	3:K:202:MET:HG2	2.08	0.52
2:D:188:THR:HG23	2:D:425:MET:HE2	1.92	0.52
3:E:209:TYR:HE1	3:E:214:LYS:HB2	1.75	0.52
2:J:154:ILE:HG23	2:J:166:MET:HG2	1.90	0.52
3:K:244:ILE:HB	3:K:245:PRO:HD3	1.92	0.52
2:B:159:GLU:HA	3:E:149:LEU:HD13	1.91	0.52
1:C:364:PRO:HG3	3:K:177:ILE:HG23	1.91	0.52
3:K:101:ILE:HD11	3:K:140:LEU:HB2	1.92	0.52
1:C:39:ASP:OD2	1:C:43:GLY:N	2.42	0.52
3:K:509:THR:HA	3:K:541:VAL:HG11	1.91	0.52
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.75	0.52
2:H:97:SER:OG	2:H:98:GLY:N	2.43	0.52
2:B:1:MET:HE3	2:B:133:GLN:HG3	1.92	0.51
3:E:101:ILE:HD11	3:E:140:LEU:HB2	1.92	0.51
1:G:234:ILE:HG21	1:G:302:MET:HE1	1.93	0.51
2:D:145:THR:N	7:D:600:GDP:O3B	2.30	0.51
3:E:102:PRO:HB2	3:E:103:PRO:HD3	1.92	0.51
1:C:188:ILE:HD12	1:C:425:MET:HG3	1.91	0.51
3:E:109:LEU:HA	3:E:117:LYS:HG3	1.92	0.51
1:I:217:LEU:HA	1:I:277:SER:HB2	1.92	0.51
3:K:202:MET:HB3	3:K:236:MET:HE1	1.93	0.51
2:H:123:ARG:O	2:H:127:GLU:HG2	2.11	0.51
2:H:385:GLN:HB2	2:H:429:VAL:HG13	1.92	0.51
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.90	0.51
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.92	0.51
3:E:311:LEU:HD12	3:E:353:GLN:HE21	1.76	0.51
1:G:413:MET:HE3	1:G:417:GLU:HB3	1.93	0.51
3:E:76:ILE:HG22	3:E:119:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:529:LEU:HD23	3:E:532:LYS:HE3	1.93	0.51
1:G:340:THR:O	1:G:340:THR:OG1	2.25	0.51
2:H:271:GLY:HA3	2:H:301:MET:HE2	1.93	0.51
3:E:310:ILE:HG12	3:E:348:LEU:HD22	1.92	0.50
3:E:480:LEU:HD21	3:E:519:LEU:HD11	1.92	0.50
2:H:404:PHE:HD2	2:H:407:TRP:HZ3	1.59	0.50
1:I:188:ILE:HD12	1:I:425:MET:HG3	1.92	0.50
1:C:364:PRO:HG3	3:K:177:ILE:HD12	1.93	0.50
3:E:348:LEU:HB2	3:E:389:LEU:HG	1.93	0.50
2:J:176:LYS:HD2	2:J:207:GLU:HG3	1.92	0.50
3:K:185:PRO:HB2	3:K:189:LEU:HD23	1.93	0.50
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.94	0.50
3:K:318:PHE:CE1	3:K:337:ILE:HD13	2.46	0.50
1:C:370:LYS:HZ2	3:K:181:GLU:HG2	1.77	0.50
3:E:63:ILE:HD12	3:E:75:ILE:HG12	1.93	0.50
1:G:188:ILE:HG23	1:G:425:MET:HG3	1.93	0.49
1:A:210:TYR:CE2	1:A:222:PRO:HD2	2.47	0.49
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.93	0.49
3:E:53:TRP:HE1	3:E:85:ILE:HB	1.77	0.49
3:E:174:ASP:O	3:E:177:ILE:HG22	2.12	0.49
3:E:185:PRO:HB2	3:E:189:LEU:HD23	1.93	0.49
2:J:12:CYS:HB2	7:J:600:GDP:C8	2.47	0.49
3:K:36:LEU:O	3:K:40:SER:HB2	2.11	0.49
3:K:63:ILE:HD12	3:K:75:ILE:HG12	1.94	0.49
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.95	0.49
3:E:110:SER:HB2	3:E:152:LEU:HD13	1.95	0.49
2:J:141:LEU:HD22	2:J:190:SER:HB3	1.94	0.49
3:K:159:CYS:O	3:K:163:ILE:HG23	2.11	0.49
3:K:174:ASP:OD1	3:K:174:ASP:N	2.43	0.49
1:A:15:GLN:NE2	5:A:600:GTP:O6	2.43	0.49
2:B:315:VAL:HB	2:B:351:VAL:HG22	1.93	0.49
2:H:137:LEU:HB3	2:H:168:THR:HG22	1.95	0.49
2:H:294:GLN:O	2:H:300:ASN:ND2	2.44	0.49
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.93	0.48
2:B:271:GLY:HA3	2:B:301:MET:HE2	1.94	0.48
1:G:167:LEU:HG	1:G:200:CYS:HB3	1.95	0.48
3:K:26:ARG:NH1	3:K:65:ASP:OD1	2.46	0.48
1:G:210:TYR:CE2	1:G:222:PRO:HD2	2.48	0.48
3:E:492:VAL:HG13	3:E:504:PHE:HE1	1.79	0.48
3:K:59:PHE:O	3:K:63:ILE:HG12	2.13	0.48
2:D:75:MET:HB2	2:D:94:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ASP:OD1	1:C:40:LYS:N	2.47	0.48
1:I:244:PHE:HB2	1:I:356:ASN:HD21	1.79	0.48
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.96	0.48
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.95	0.48
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.94	0.48
1:G:180:ALA:HB3	1:G:183:GLU:HG3	1.95	0.48
3:K:176:ASN:N	3:K:176:ASN:OD1	2.46	0.48
2:B:82:PRO:O	2:B:85:GLN:NE2	2.47	0.48
2:J:172:VAL:HB	2:J:205:ASP:HA	1.96	0.48
3:K:433:PHE:CE1	3:K:475:GLN:HB3	2.49	0.48
2:D:140:SER:HA	2:D:171:VAL:HG22	1.95	0.48
2:D:172:VAL:HB	2:D:205:ASP:HA	1.96	0.48
1:I:40:LYS:HG2	1:I:41:THR:H	1.79	0.48
3:E:14:LEU:O	3:E:17:ARG:HG2	2.12	0.47
3:E:481:LEU:HG	3:E:482:PRO:HD3	1.95	0.47
1:I:14:VAL:HG13	1:I:67:PHE:HD2	1.77	0.47
2:J:75:MET:HB2	2:J:94:PHE:CD1	2.49	0.47
3:K:318:PHE:HE1	3:K:337:ILE:HD13	1.78	0.47
3:K:425:ASP:OD2	3:K:461:ARG:NH1	2.46	0.47
1:G:209:ILE:HG23	1:G:230:LEU:HD23	1.95	0.47
2:H:172:VAL:HB	2:H:205:ASP:HA	1.96	0.47
1:I:210:TYR:CE2	1:I:222:PRO:HD2	2.50	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
1:I:188:ILE:HG23	1:I:425:MET:HG3	1.95	0.47
3:K:163:ILE:O	3:K:167:PHE:HB2	2.15	0.47
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.96	0.47
3:E:26:ARG:NH1	3:E:65:ASP:OD1	2.47	0.47
2:H:248:LEU:HD21	2:H:352:LYS:HB3	1.96	0.47
1:I:71:GLU:HG2	1:I:73:THR:H	1.80	0.47
3:E:37:PHE:CD2	3:E:81:LEU:HB2	2.50	0.47
3:E:210:LYS:HE3	3:E:240:TYR:CE1	2.50	0.47
3:E:210:LYS:O	3:E:246:PRO:HD3	2.14	0.47
3:K:102:PRO:HB2	3:K:103:PRO:HD3	1.96	0.47
3:E:198:ARG:O	3:E:202:MET:HG2	2.14	0.47
3:E:425:ASP:OD2	3:E:461:ARG:NH1	2.47	0.47
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.96	0.47
3:E:59:PHE:O	3:E:63:ILE:HG12	2.14	0.47
1:G:2:ARG:N	1:G:133:GLN:HG3	2.29	0.47
2:B:124:LYS:HB2	2:B:124:LYS:HE3	1.68	0.47
2:J:138:THR:HG22	2:J:169:PHE:HB2	1.96	0.47
4:L:100:LEU:HD23	4:L:104:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:163:ILE:O	3:E:167:PHE:HB2	2.14	0.47
2:J:137:LEU:HB3	2:J:168:THR:HG22	1.97	0.47
3:E:501:ASN:OD1	3:E:537:TYR:OH	2.33	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.97	0.46
3:E:159:CYS:O	3:E:163:ILE:HG23	2.14	0.46
2:H:124:LYS:HE3	2:H:124:LYS:HB2	1.73	0.46
3:K:349:ALA:HB3	3:K:353:GLN:HG3	1.97	0.46
4:L:78:ILE:HG23	4:L:79:MET:HE2	1.96	0.46
2:B:97:SER:OG	2:B:98:GLY:N	2.49	0.46
1:I:167:LEU:HG	1:I:200:CYS:HB3	1.96	0.46
2:J:70:LEU:HD12	2:J:99:ALA:HB2	1.96	0.46
3:E:185:PRO:HA	3:E:188:LYS:HE3	1.97	0.46
3:E:253:PHE:HD2	3:E:256:GLN:HE22	1.63	0.46
3:E:311:LEU:HD12	3:E:353:GLN:NE2	2.31	0.46
1:I:100:ALA:HA	2:J:254:LYS:HG2	1.98	0.46
1:I:282:TYR:OH	1:I:370:LYS:O	2.32	0.46
2:H:2:ARG:HH21	2:H:130:ASP:HB3	1.80	0.46
2:H:162:PRO:HD2	3:K:148:LYS:HE3	1.96	0.46
2:D:50:ASN:O	2:D:64:ARG:NH2	2.49	0.46
1:I:250:VAL:HG11	1:I:352:LYS:HE3	1.98	0.46
3:K:403:VAL:CG1	3:K:404:PRO:HD3	2.46	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.98	0.46
2:H:12:CYS:HB2	7:H:600:GDP:C8	2.51	0.46
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.97	0.46
1:G:171:ILE:HA	1:G:204:VAL:HG23	1.98	0.46
1:I:139:HIS:CD2	1:I:150:THR:HG21	2.50	0.46
3:K:433:PHE:HB2	3:K:437:LEU:HB2	1.97	0.46
2:B:172:VAL:HG21	2:B:387:LEU:HD21	1.98	0.46
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.98	0.46
3:E:93:THR:HG21	3:E:130:SER:HB3	1.97	0.46
1:I:93:ILE:HG22	1:I:114:ILE:HD11	1.98	0.46
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.81	0.45
1:G:205:ASP:HB2	1:G:303:VAL:HA	1.98	0.45
2:D:12:CYS:HB2	7:D:600:GDP:C8	2.51	0.45
1:G:21:TRP:CZ3	1:G:63:PRO:HB3	2.51	0.45
3:K:17:ARG:HD3	3:K:25:ALA:HB1	1.97	0.45
3:K:93:THR:HG21	3:K:130:SER:HB3	1.97	0.45
2:H:315:VAL:HB	2:H:351:VAL:HG22	1.98	0.45
1:I:282:TYR:O	1:I:285:GLN:N	2.49	0.45
3:E:354:ASP:OD2	3:E:356:SER:OG	2.23	0.45
4:F:121:ALA:HB1	4:F:161:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.82	0.45
1:C:50:ASN:ND2	1:C:55:GLU:OE1	2.50	0.45
1:G:14:VAL:HG13	1:G:67:PHE:HD2	1.82	0.45
3:K:516:GLU:OE2	3:K:535:TYR:OH	2.28	0.45
1:C:313:MET:SD	1:C:435:VAL:HG11	2.57	0.45
2:J:269:MET:HG3	2:J:303:ALA:HB3	1.98	0.45
3:K:209:TYR:HE1	3:K:214:LYS:HB2	1.81	0.45
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.82	0.44
2:H:395:PHE:CE2	2:H:422:GLU:HB2	2.52	0.44
2:B:137:LEU:HB3	2:B:168:THR:HG22	2.00	0.44
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.52	0.44
1:C:408:TYR:HB3	1:C:413:MET:HE2	1.98	0.44
1:G:291:ILE:HD13	1:G:373:ARG:HG3	1.99	0.44
1:I:313:MET:HE2	1:I:382:THR:HG23	1.99	0.44
3:K:72:GLU:OE1	3:K:113:ARG:NH2	2.47	0.44
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.98	0.44
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.83	0.44
2:D:106:GLY:O	2:D:111:GLY:HA3	2.17	0.44
2:J:181:VAL:HG11	4:L:90:ILE:HA	2.00	0.44
3:K:131:ASP:OD2	3:K:136:GLN:HB2	2.16	0.44
2:B:395:PHE:CE2	2:B:422:GLU:HB2	2.53	0.44
3:E:472:LEU:O	3:E:473:GLN:HG2	2.18	0.44
3:E:492:VAL:HG13	3:E:504:PHE:CE1	2.53	0.44
1:I:402:ARG:HA	1:I:402:ARG:HD3	1.88	0.44
1:C:402:ARG:NH1	1:C:415:GLU:OE2	2.49	0.44
2:D:393:GLU:OE2	4:F:156:ASN:ND2	2.49	0.44
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.99	0.44
2:J:165:ILE:HG21	2:J:252:LEU:HB3	1.99	0.44
3:K:367:GLN:HB2	3:K:404:PRO:HB3	2.00	0.44
1:A:348:PRO:O	1:A:350:GLY:N	2.50	0.44
2:B:39:ASP:OD1	2:B:40:SER:N	2.50	0.44
1:G:402:ARG:NH1	1:G:415:GLU:OE2	2.47	0.44
2:J:395:PHE:CE2	2:J:422:GLU:HB2	2.53	0.44
3:K:354:ASP:OD2	3:K:356:SER:OG	2.28	0.44
1:C:402:ARG:HA	1:C:402:ARG:HD3	1.86	0.43
2:H:138:THR:HG22	2:H:169:PHE:HB2	2.00	0.43
2:H:167:ASN:HD21	2:H:202:TYR:HE1	1.66	0.43
1:I:15:GLN:NE2	5:I:600:GTP:O6	2.51	0.43
1:I:313:MET:SD	1:I:435:VAL:HG11	2.58	0.43
1:I:408:TYR:HB3	1:I:413:MET:HE2	1.99	0.43
2:H:106:GLY:O	2:H:111:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:ARG:HA	1:I:356:ASN:O	2.19	0.43
3:K:109:LEU:HA	3:K:117:LYS:HG3	2.00	0.43
1:C:22:GLU:HG3	1:C:83:TYR:OH	2.18	0.43
3:E:101:ILE:HA	3:E:104:LEU:HB2	2.00	0.43
4:L:96:VAL:HG21	4:L:128:ILE:HD13	2.01	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.53	0.43
3:E:36:LEU:O	3:E:40:SER:HB2	2.19	0.43
3:E:358:TYR:CE2	3:E:385:LEU:HD11	2.53	0.43
4:F:96:VAL:HG21	4:F:128:ILE:HD13	2.00	0.43
2:H:140:SER:HA	2:H:171:VAL:HG22	2.01	0.43
1:I:22:GLU:HG3	1:I:83:TYR:OH	2.18	0.43
3:K:358:TYR:O	3:K:361:VAL:HG22	2.17	0.43
3:E:73:ASN:HA	3:E:76:ILE:HG12	2.01	0.43
1:I:21:TRP:CZ3	1:I:63:PRO:HB3	2.53	0.43
1:C:142:GLY:HA3	1:C:183:GLU:HG2	2.00	0.43
1:C:320:ARG:HA	1:C:356:ASN:O	2.19	0.43
3:E:177:ILE:O	3:E:181:GLU:HB2	2.19	0.43
1:G:12:ALA:HB1	1:G:171:ILE:HG13	1.99	0.43
1:C:278:ALA:HA	1:C:282:TYR:OH	2.19	0.43
3:E:444:MET:HE1	3:E:459:LEU:HD22	2.00	0.43
1:G:348:PRO:O	1:G:350:GLY:N	2.51	0.43
3:K:85:ILE:C	3:K:87:GLN:H	2.27	0.43
1:C:30:ILE:HG12	1:C:36:MET:SD	2.59	0.43
3:E:440:THR:O	3:E:444:MET:HG3	2.18	0.43
3:E:481:LEU:HA	3:E:485:THR:CG2	2.49	0.43
3:K:217:LEU:H	3:K:217:LEU:HD23	1.83	0.43
1:I:230:LEU:O	1:I:234:ILE:HD12	2.18	0.43
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.54	0.42
2:B:12:CYS:HB2	7:B:600:GDP:C8	2.53	0.42
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.53	0.42
1:G:402:ARG:HA	1:G:402:ARG:HD3	1.86	0.42
3:E:505:GLU:O	3:E:509:THR:HG23	2.18	0.42
2:H:59:ASN:HB2	2:H:60:LYS:HG3	2.01	0.42
3:K:425:ASP:OD1	3:K:461:ARG:HD3	2.19	0.42
2:B:404:PHE:HD2	2:B:407:TRP:HZ3	1.67	0.42
3:E:359:LEU:HD22	3:E:401:VAL:HG11	2.02	0.42
1:G:78:VAL:C	1:G:80:THR:H	2.28	0.42
3:K:453:ILE:HG13	3:K:454:GLU:N	2.34	0.42
2:D:141:LEU:HD22	2:D:190:SER:OG	2.20	0.42
2:D:395:PHE:CE2	2:D:422:GLU:HB2	2.54	0.42
3:K:355:TYR:HB2	3:K:397:TYR:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:123:MET:HB2	4:L:125:HIS:CD2	2.54	0.42
2:B:140:SER:HA	2:B:171:VAL:HG22	2.01	0.42
2:H:134:GLY:HA2	2:H:164:ARG:HB3	2.01	0.42
4:L:121:ALA:HB1	4:L:161:LEU:HD21	2.01	0.42
1:A:234:ILE:HG21	1:A:302:MET:SD	2.59	0.42
1:C:142:GLY:O	1:C:186:ASN:ND2	2.43	0.42
3:E:91:VAL:C	3:E:93:THR:H	2.28	0.42
2:B:407:TRP:CH2	1:C:257:THR:HA	2.55	0.42
1:C:2:ARG:HB2	1:C:3:GLU:OE1	2.19	0.42
1:C:334:THR:O	1:C:338:LYS:HB2	2.20	0.42
3:K:359:LEU:HD23	3:K:362:LEU:HD12	2.02	0.42
1:C:234:ILE:HG21	1:C:302:MET:SD	2.60	0.42
3:E:438:GLU:O	3:E:442:ASN:ND2	2.52	0.42
1:G:22:GLU:HG3	1:G:83:TYR:OH	2.20	0.42
1:I:209:ILE:HG23	1:I:230:LEU:HD23	2.02	0.42
2:J:270:PRO:HG2	2:J:302:MET:HB2	2.02	0.42
3:E:144:SER:O	3:E:153:VAL:HG12	2.19	0.42
3:E:369:ASP:O	3:E:408:ARG:NH2	2.53	0.42
1:G:71:GLU:HB2	1:G:98:ASP:HB3	2.02	0.42
3:K:448:THR:HB	3:K:451:VAL:HG22	2.02	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.02	0.41
1:A:402:ARG:HA	1:A:402:ARG:HD3	1.86	0.41
2:J:400:ARG:HD2	4:L:112:TRP:NE1	2.34	0.41
3:K:363:ALA:HB2	3:K:401:VAL:HG12	2.01	0.41
4:L:91:GLY:HA2	4:L:128:ILE:HD12	2.02	0.41
3:E:131:ASP:OD2	3:E:136:GLN:HB2	2.19	0.41
4:F:125:HIS:O	4:F:129:VAL:HG23	2.20	0.41
2:J:106:GLY:O	2:J:111:GLY:HA3	2.20	0.41
2:J:140:SER:HA	2:J:171:VAL:HG22	2.01	0.41
3:K:359:LEU:HD23	3:K:359:LEU:HA	1.86	0.41
3:K:398:GLY:HA3	3:K:431:CYS:SG	2.60	0.41
3:E:100:TRP:C	3:E:103:PRO:HD2	2.46	0.41
3:E:358:TYR:O	3:E:361:VAL:HG22	2.19	0.41
3:E:453:ILE:HG13	3:E:454:GLU:N	2.35	0.41
2:D:50:ASN:OD1	2:D:50:ASN:N	2.54	0.41
4:F:78:ILE:HG23	4:F:79:MET:HE2	2.02	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.21	0.41
1:G:409:VAL:HA	1:G:413:MET:O	2.20	0.41
1:A:22:GLU:HG3	1:A:83:TYR:OH	2.21	0.41
2:D:176:LYS:HD2	2:D:207:GLU:HG3	2.01	0.41
3:E:202:MET:HB3	3:E:236:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:TRP:CZ3	2:H:63:PRO:HB3	2.54	0.41
1:A:47:ASP:OD1	1:A:48:SER:N	2.46	0.41
1:A:266:HIS:O	1:A:266:HIS:ND1	2.51	0.41
2:D:323:MET:HE2	2:D:373:MET:HE3	2.03	0.41
2:B:2:ARG:HH21	2:B:130:ASP:HB3	1.85	0.41
1:C:313:MET:HE2	1:C:382:THR:HG23	2.02	0.41
3:E:448:THR:HB	3:E:451:VAL:HG22	2.03	0.41
3:K:179:LEU:HD23	3:K:179:LEU:HA	1.91	0.41
3:K:397:TYR:O	3:K:400:ILE:HG22	2.20	0.41
3:K:401:VAL:C	3:K:404:PRO:HD2	2.45	0.41
1:C:55:GLU:HG2	1:C:61:HIS:HD2	1.86	0.41
3:E:82:LEU:O	3:E:85:ILE:HG12	2.20	0.41
3:E:105:VAL:HA	3:E:109:LEU:HG	2.03	0.41
2:H:205:ASP:HB2	2:H:303:ALA:HA	2.03	0.41
2:H:275:LEU:HD23	2:H:275:LEU:HA	1.96	0.41
2:H:303:ALA:O	2:H:305:CYS:N	2.53	0.41
2:J:141:LEU:HD21	2:J:194:LEU:HD11	2.02	0.41
2:J:405:LEU:HD21	2:J:415:GLU:HG3	2.03	0.41
4:L:43:THR:HB	4:L:47:GLY:HA2	2.02	0.41
2:D:405:LEU:HD21	2:D:415:GLU:HG3	2.02	0.41
2:H:141:LEU:HD21	2:H:194:LEU:HD11	2.03	0.41
3:E:85:ILE:C	3:E:87:GLN:H	2.29	0.40
4:F:59:HIS:HB3	4:F:62:ILE:HB	2.03	0.40
3:K:82:LEU:O	3:K:85:ILE:HG12	2.20	0.40
3:K:185:PRO:HA	3:K:188:LYS:HE3	2.03	0.40
2:D:295:MET:HE3	2:D:375:ALA:HB1	2.03	0.40
3:E:113:ARG:HB2	3:E:116:THR:HB	2.03	0.40
3:E:425:ASP:OD1	3:E:461:ARG:HD3	2.21	0.40
1:G:311:LYS:HE2	1:G:436:GLY:O	2.21	0.40
1:A:230:LEU:O	1:A:234:ILE:HD12	2.21	0.40
1:A:348:PRO:C	1:A:350:GLY:H	2.30	0.40
1:C:359:PRO:HA	1:C:360:PRO:HD3	1.98	0.40
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.04	0.40
3:K:492:VAL:HG13	3:K:504:PHE:CE1	2.56	0.40
2:D:158:ARG:HH22	2:D:199:ASP:CG	2.28	0.40
3:E:109:LEU:HD22	3:E:121:THR:HG23	2.03	0.40
1:I:234:ILE:HG21	1:I:302:MET:SD	2.61	0.40
2:J:83:PHE:O	2:J:86:ILE:HG22	2.22	0.40
4:L:125:HIS:O	4:L:129:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/451 (93%)	407 (97%)	12 (3%)	2 (0%)	24	59
1	C	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
1	G	419/451 (93%)	403 (96%)	14 (3%)	2 (0%)	24	59
1	I	431/451 (96%)	416 (96%)	14 (3%)	1 (0%)	43	73
2	B	426/445 (96%)	405 (95%)	21 (5%)	0	100	100
2	D	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
2	H	425/445 (96%)	406 (96%)	19 (4%)	0	100	100
2	J	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
3	E	481/554 (87%)	442 (92%)	35 (7%)	4 (1%)	16	50
3	K	481/554 (87%)	449 (93%)	30 (6%)	2 (0%)	30	62
4	F	123/140 (88%)	118 (96%)	5 (4%)	0	100	100
4	L	123/140 (88%)	116 (94%)	7 (6%)	0	100	100
All	All	4604/4972 (93%)	4385 (95%)	208 (4%)	11 (0%)	43	73

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	THR
1	G	349	THR
1	I	162	GLY
3	E	173	SER
3	E	89	PRO
3	E	245	PRO
3	E	434	ASP
3	K	245	PRO
1	G	37	PRO
1	A	114	ILE
3	K	64	VAL

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	358/377 (95%)	358 (100%)	0	100	100
1	C	360/377 (96%)	360 (100%)	0	100	100
1	G	358/377 (95%)	358 (100%)	0	100	100
1	I	363/377 (96%)	363 (100%)	0	100	100
2	B	369/381 (97%)	369 (100%)	0	100	100
2	D	368/381 (97%)	368 (100%)	0	100	100
2	H	370/381 (97%)	370 (100%)	0	100	100
2	J	368/381 (97%)	368 (100%)	0	100	100
3	E	447/504 (89%)	447 (100%)	0	100	100
3	K	447/504 (89%)	447 (100%)	0	100	100
4	F	99/111 (89%)	99 (100%)	0	100	100
4	L	99/111 (89%)	99 (100%)	0	100	100
All	All	4006/4262 (94%)	4006 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	HIS
1	A	101	ASN
1	A	342	GLN
1	A	393	HIS
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	167	ASN
2	B	247	GLN
2	B	331	GLN

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Mol	Chain	Res	Type
2	B	336	GLN
2	B	433	GLN
2	B	436	GLN
1	C	133	GLN
1	C	197	HIS
1	C	256	GLN
1	C	380	ASN
1	C	393	HIS
2	D	6	HIS
2	D	15	GLN
2	D	167	ASN
2	D	294	GLN
2	D	331	GLN
2	D	406	HIS
3	E	79	HIS
3	E	171	ASN
3	E	230	GLN
3	E	249	GLN
3	E	340	ASN
3	E	353	GLN
3	E	392	ASN
3	E	464	GLN
4	F	102	HIS
4	F	125	HIS
1	G	11	GLN
1	G	88	HIS
1	G	342	GLN
1	G	393	HIS
2	H	6	HIS
2	H	8	GLN
2	H	136	GLN
2	H	167	ASN
2	H	247	GLN
2	H	331	GLN
2	H	385	GLN
2	H	433	GLN
2	H	436	GLN
1	I	11	GLN
1	I	342	GLN
1	I	380	ASN
1	I	393	HIS
2	J	6	HIS

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Mol	Chain	Res	Type
2	J	15	GLN
2	J	136	GLN
2	J	247	GLN
2	J	331	GLN
3	K	73	ASN
3	K	135	GLN
3	K	171	ASN
3	K	230	GLN
3	K	340	ASN
3	K	442	ASN
3	K	464	GLN
4	L	125	HIS

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	600	6	33,34,34	0.96	2 (6%)	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GDP	B	600	6	29,30,30	1.14	2 (6%)	45,47,47	1.75	6 (13%)
7	GDP	H	600	6	29,30,30	1.16	2 (6%)	45,47,47	1.71	6 (13%)
5	GTP	I	600	6	33,34,34	0.98	3 (9%)	50,54,54	1.57	9 (18%)
5	GTP	C	600	6	33,34,34	0.99	3 (9%)	50,54,54	1.59	8 (16%)
5	GTP	G	600	6	33,34,34	0.99	3 (9%)	50,54,54	1.55	8 (16%)
7	GDP	J	600	6	29,30,30	1.15	2 (6%)	45,47,47	1.74	6 (13%)
7	GDP	D	600	6	29,30,30	1.14	2 (6%)	45,47,47	1.75	6 (13%)

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	600	6	-	6/22/38/38	0/3/3/3
7	GDP	B	600	6	-	5/16/32/32	0/3/3/3
7	GDP	H	600	6	-	5/16/32/32	0/3/3/3
5	GTP	I	600	6	-	8/22/38/38	0/3/3/3
5	GTP	C	600	6	-	8/22/38/38	0/3/3/3
5	GTP	G	600	6	-	6/22/38/38	0/3/3/3
7	GDP	J	600	6	-	5/16/32/32	0/3/3/3
7	GDP	D	600	6	-	4/16/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	600	GDP	C5-C4	3.21	1.47	1.38
7	D	600	GDP	C5-C4	3.13	1.47	1.38
7	J	600	GDP	C5-C4	3.12	1.47	1.38
7	B	600	GDP	C5-C4	3.11	1.47	1.38
7	H	600	GDP	C6-N1	-2.40	1.34	1.38
5	G	600	GTP	PA-O3A	2.36	1.62	1.59
7	J	600	GDP	C6-N1	-2.33	1.34	1.38
5	G	600	GTP	C2-N3	2.26	1.38	1.33
7	B	600	GDP	C6-N1	-2.26	1.34	1.38
5	C	600	GTP	C2-N3	2.25	1.38	1.33
7	D	600	GDP	C6-N1	-2.22	1.34	1.38
5	A	600	GTP	C2-N3	2.21	1.38	1.33
5	C	600	GTP	PA-O3A	2.20	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	600	GTP	C2-N3	2.19	1.38	1.33
5	C	600	GTP	PB-O3A	2.16	1.61	1.59
5	I	600	GTP	PB-O3A	2.10	1.61	1.59
5	I	600	GTP	PA-O3A	2.07	1.61	1.59
5	A	600	GTP	PA-O3A	2.03	1.61	1.59
5	G	600	GTP	PB-O3A	2.01	1.61	1.59

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	GDP	C5-C4-N3	-6.04	118.78	128.39
7	J	600	GDP	C5-C4-N3	-5.97	118.89	128.39
7	H	600	GDP	C5-C4-N3	-5.95	118.92	128.39
7	D	600	GDP	C5-C4-N3	-5.91	118.98	128.39
5	C	600	GTP	C5-C4-N3	-5.12	120.25	128.39
5	A	600	GTP	C5-C4-N3	-5.10	120.28	128.39
7	J	600	GDP	C2-N3-C4	5.08	121.06	112.30
5	G	600	GTP	C5-C4-N3	-5.08	120.30	128.39
7	B	600	GDP	C2-N3-C4	5.07	121.03	112.30
7	D	600	GDP	C2-N3-C4	5.04	120.98	112.30
5	I	600	GTP	C5-C4-N3	-5.03	120.39	128.39
7	H	600	GDP	C2-N3-C4	4.96	120.85	112.30
5	C	600	GTP	C2-N3-C4	4.69	120.38	112.30
5	I	600	GTP	C2-N3-C4	4.68	120.36	112.30
5	A	600	GTP	C2-N3-C4	4.67	120.34	112.30
5	G	600	GTP	C2-N3-C4	4.65	120.30	112.30
7	D	600	GDP	N9-C4-N3	4.44	134.83	125.95
7	B	600	GDP	N9-C4-N3	4.43	134.81	125.95
7	H	600	GDP	N9-C4-N3	4.42	134.79	125.95
7	J	600	GDP	N9-C4-N3	4.41	134.77	125.95
7	H	600	GDP	C6-C5-N7	3.39	136.45	130.29
7	J	600	GDP	C6-C5-N7	3.35	136.39	130.29
7	B	600	GDP	C6-C5-N7	3.32	136.33	130.29
5	C	600	GTP	N9-C4-N3	3.29	132.53	125.95
7	D	600	GDP	C6-C5-N7	3.28	136.25	130.29
5	A	600	GTP	N9-C4-N3	3.26	132.48	125.95
5	G	600	GTP	N9-C4-N3	3.25	132.46	125.95
5	I	600	GTP	N9-C4-N3	3.21	132.36	125.95
5	G	600	GTP	C2-N1-C6	-2.97	119.72	125.11
5	I	600	GTP	C2-N1-C6	-2.89	119.87	125.11
5	A	600	GTP	C2-N1-C6	-2.89	119.87	125.11
5	C	600	GTP	C2-N1-C6	-2.88	119.88	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	600	GTP	N9-C8-N7	-2.75	108.31	113.40
5	G	600	GTP	N9-C8-N7	-2.68	108.44	113.40
5	C	600	GTP	N9-C8-N7	-2.67	108.44	113.40
7	H	600	GDP	C4-C5-N7	-2.63	106.50	110.67
5	I	600	GTP	C8-N7-C5	2.62	108.92	104.26
7	B	600	GDP	C4-C5-N7	-2.59	106.56	110.67
5	C	600	GTP	C8-N7-C5	2.57	108.83	104.26
5	G	600	GTP	C5-C6-N1	2.56	119.78	113.25
5	G	600	GTP	C8-N7-C5	2.56	108.81	104.26
5	C	600	GTP	C5-C6-N1	2.53	119.70	113.25
5	A	600	GTP	N9-C8-N7	-2.52	108.72	113.40
7	J	600	GDP	C4-C5-N7	-2.52	106.67	110.67
5	I	600	GTP	C5-C6-N1	2.51	119.63	113.25
5	A	600	GTP	C5-C6-N1	2.47	119.53	113.25
7	D	600	GDP	C4-C5-N7	-2.46	106.77	110.67
5	A	600	GTP	C8-N7-C5	2.44	108.60	104.26
5	A	600	GTP	O6-C6-C5	-2.34	120.34	126.53
5	C	600	GTP	O6-C6-C5	-2.28	120.50	126.53
5	G	600	GTP	O6-C6-C5	-2.27	120.54	126.53
5	I	600	GTP	O6-C6-C5	-2.23	120.65	126.53
7	J	600	GDP	O6-C6-C5	-2.18	120.78	126.53
7	D	600	GDP	O6-C6-C5	-2.18	120.78	126.53
7	B	600	GDP	O6-C6-C5	-2.13	120.92	126.53
7	H	600	GDP	O6-C6-C5	-2.02	121.21	126.53
5	I	600	GTP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	GTP	PB-O3B-PG-O2G
5	A	600	GTP	C5'-O5'-PA-O3A
5	A	600	GTP	C5'-O5'-PA-O1A
5	A	600	GTP	C5'-O5'-PA-O2A
5	C	600	GTP	C5'-O5'-PA-O3A
5	C	600	GTP	C5'-O5'-PA-O1A
5	G	600	GTP	C5'-O5'-PA-O3A
5	G	600	GTP	C5'-O5'-PA-O1A
5	G	600	GTP	C5'-O5'-PA-O2A
5	I	600	GTP	PB-O3B-PG-O3G
5	I	600	GTP	C5'-O5'-PA-O3A
5	I	600	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	I	600	GTP	C5'-O5'-PA-O2A
7	B	600	GDP	C5'-O5'-PA-O3A
7	B	600	GDP	C5'-O5'-PA-O1A
7	B	600	GDP	C5'-O5'-PA-O2A
7	D	600	GDP	C5'-O5'-PA-O3A
7	D	600	GDP	C5'-O5'-PA-O1A
7	D	600	GDP	C5'-O5'-PA-O2A
7	H	600	GDP	C5'-O5'-PA-O3A
7	H	600	GDP	C5'-O5'-PA-O1A
7	H	600	GDP	C5'-O5'-PA-O2A
7	J	600	GDP	C5'-O5'-PA-O3A
7	J	600	GDP	C5'-O5'-PA-O1A
7	J	600	GDP	C5'-O5'-PA-O2A
5	C	600	GTP	PB-O3B-PG-O3G
5	C	600	GTP	PB-O3A-PA-O2A
7	B	600	GDP	PB-O3A-PA-O2A
7	D	600	GDP	PB-O3A-PA-O2A
7	H	600	GDP	PB-O3A-PA-O1A
7	J	600	GDP	PB-O3A-PA-O1A
5	C	600	GTP	C5'-O5'-PA-O2A
5	A	600	GTP	PB-O3A-PA-O2A
5	C	600	GTP	C4'-C5'-O5'-PA
5	I	600	GTP	C4'-C5'-O5'-PA
5	G	600	GTP	PB-O3A-PA-O1A
5	I	600	GTP	PB-O3A-PA-O1A
5	A	600	GTP	C4'-C5'-O5'-PA
5	G	600	GTP	C4'-C5'-O5'-PA
5	C	600	GTP	C3'-C4'-C5'-O5'
5	I	600	GTP	PB-O3B-PG-O2G
5	I	600	GTP	PB-O3A-PA-O2A
7	B	600	GDP	PB-O3A-PA-O1A
5	C	600	GTP	O4'-C4'-C5'-O5'
5	G	600	GTP	PB-O3A-PA-O2A
7	H	600	GDP	PB-O3A-PA-O2A
7	J	600	GDP	PB-O3A-PA-O2A

There are no ring outliers.

7 monomers are involved in 8 short contacts:

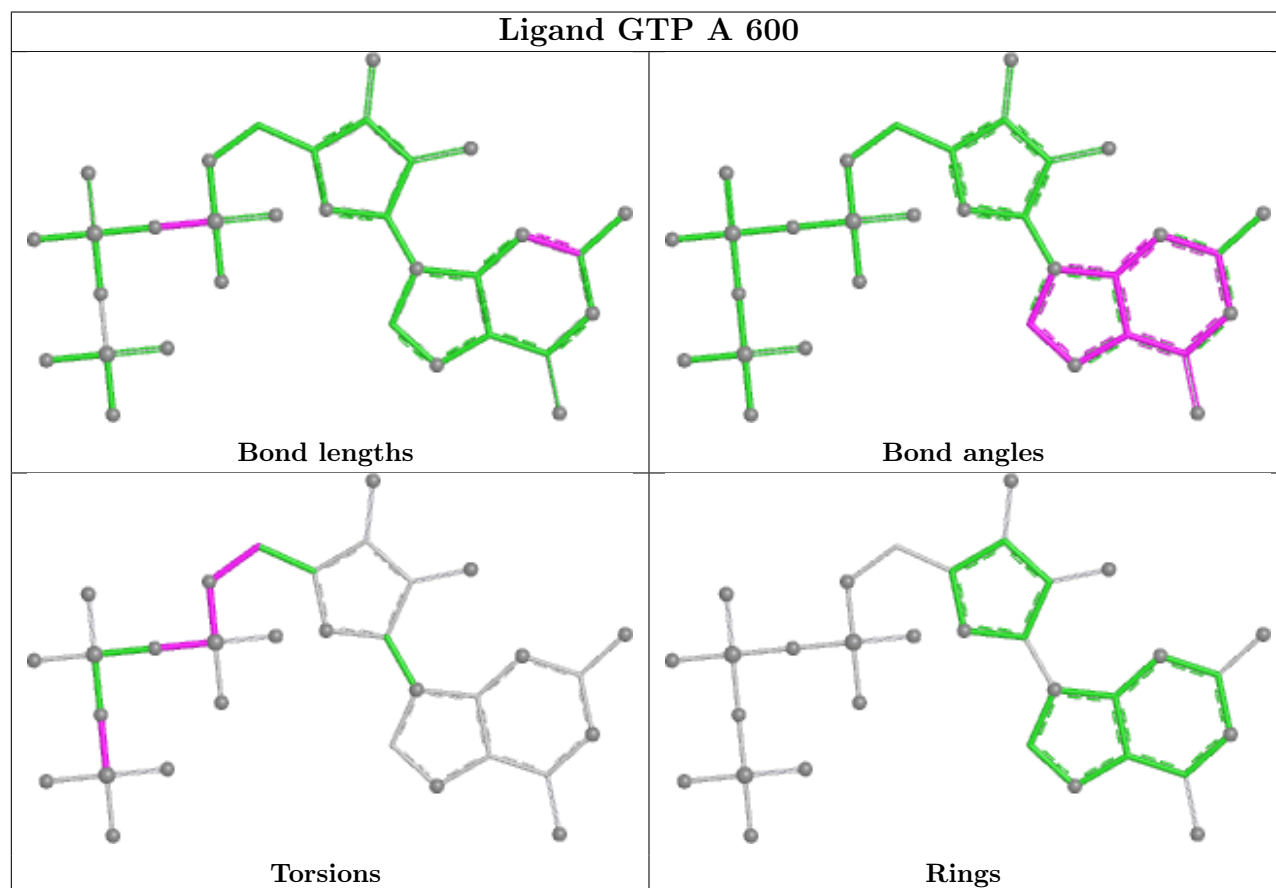
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	GTP	1	0
7	B	600	GDP	1	0

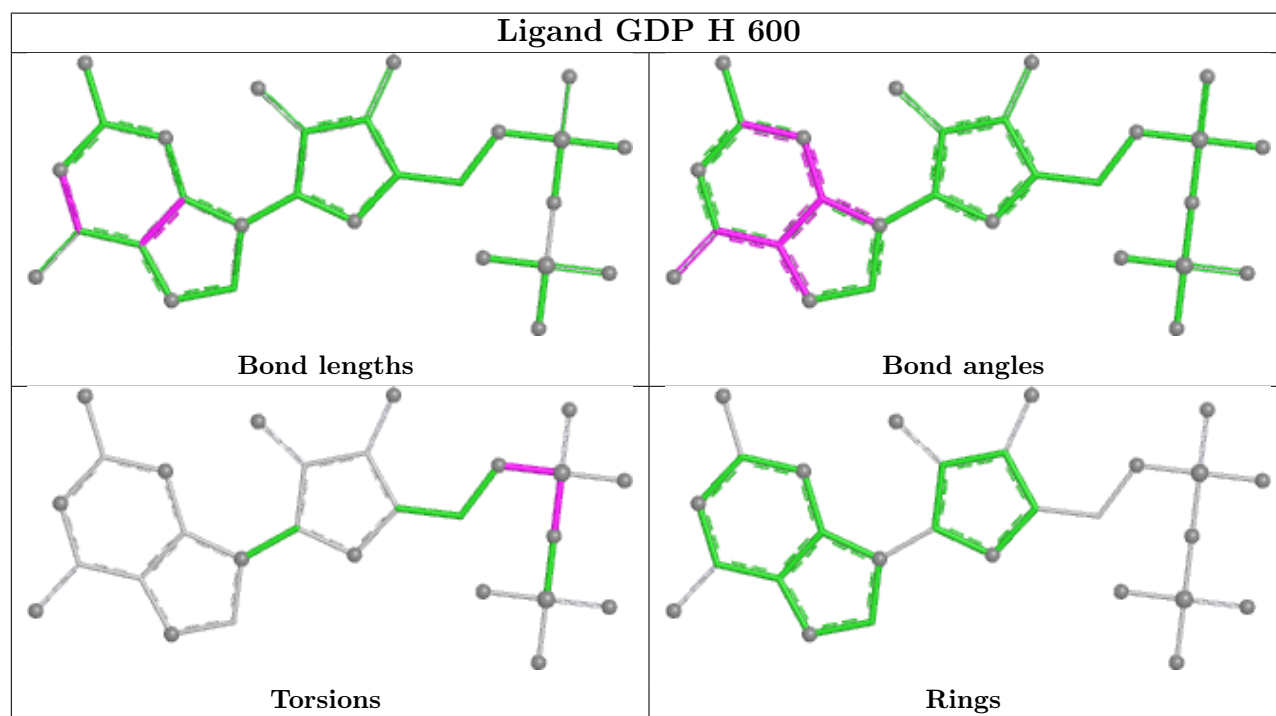
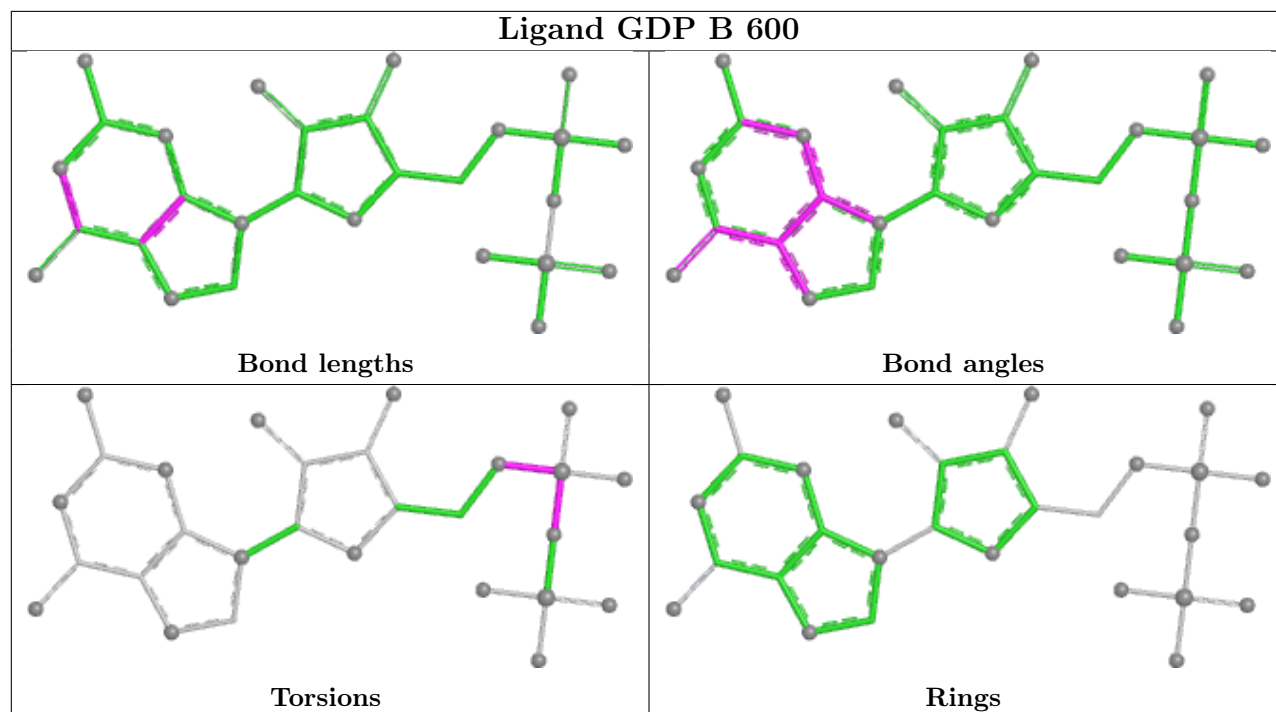
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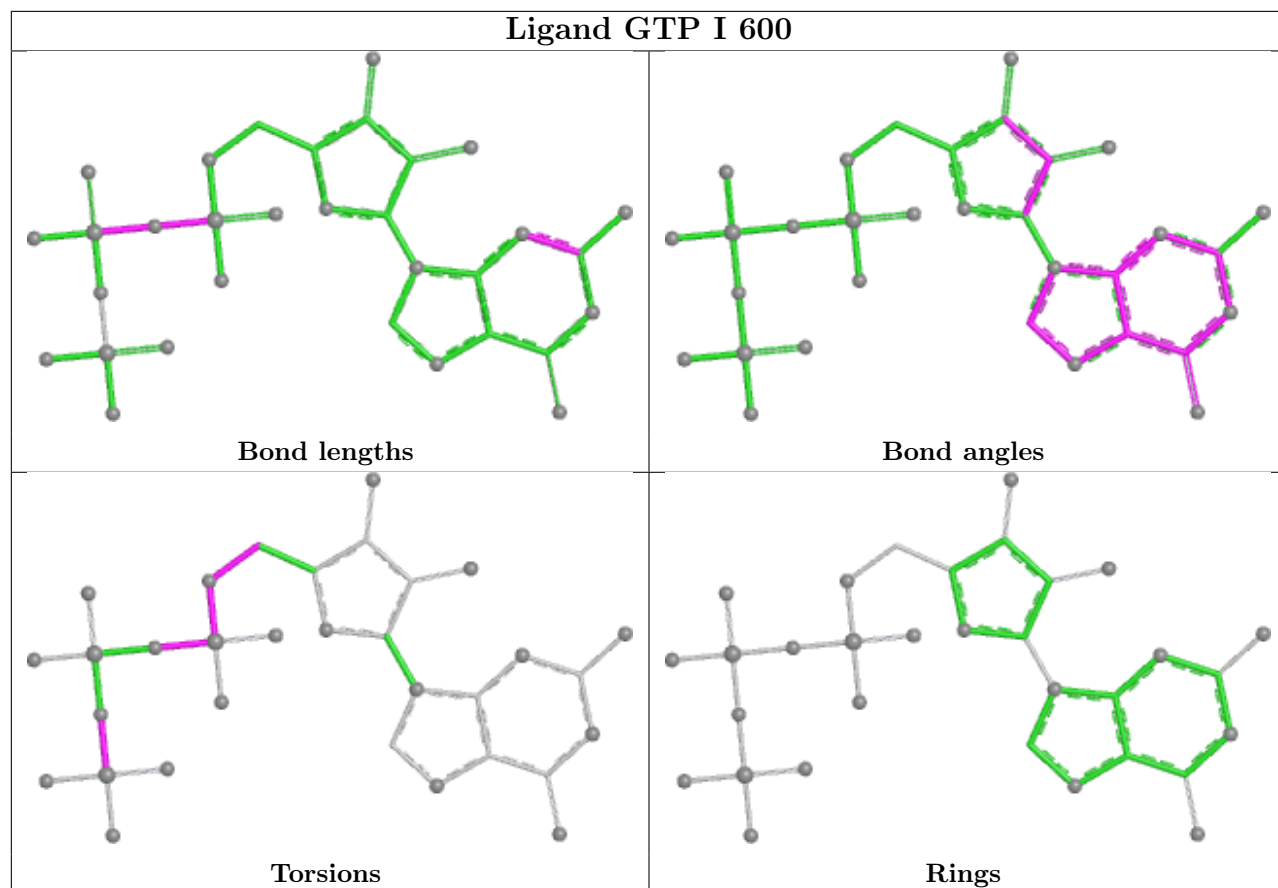
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	600	GDP	1	0
5	I	600	GTP	1	0
5	C	600	GTP	1	0
7	J	600	GDP	1	0
7	D	600	GDP	2	0

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.

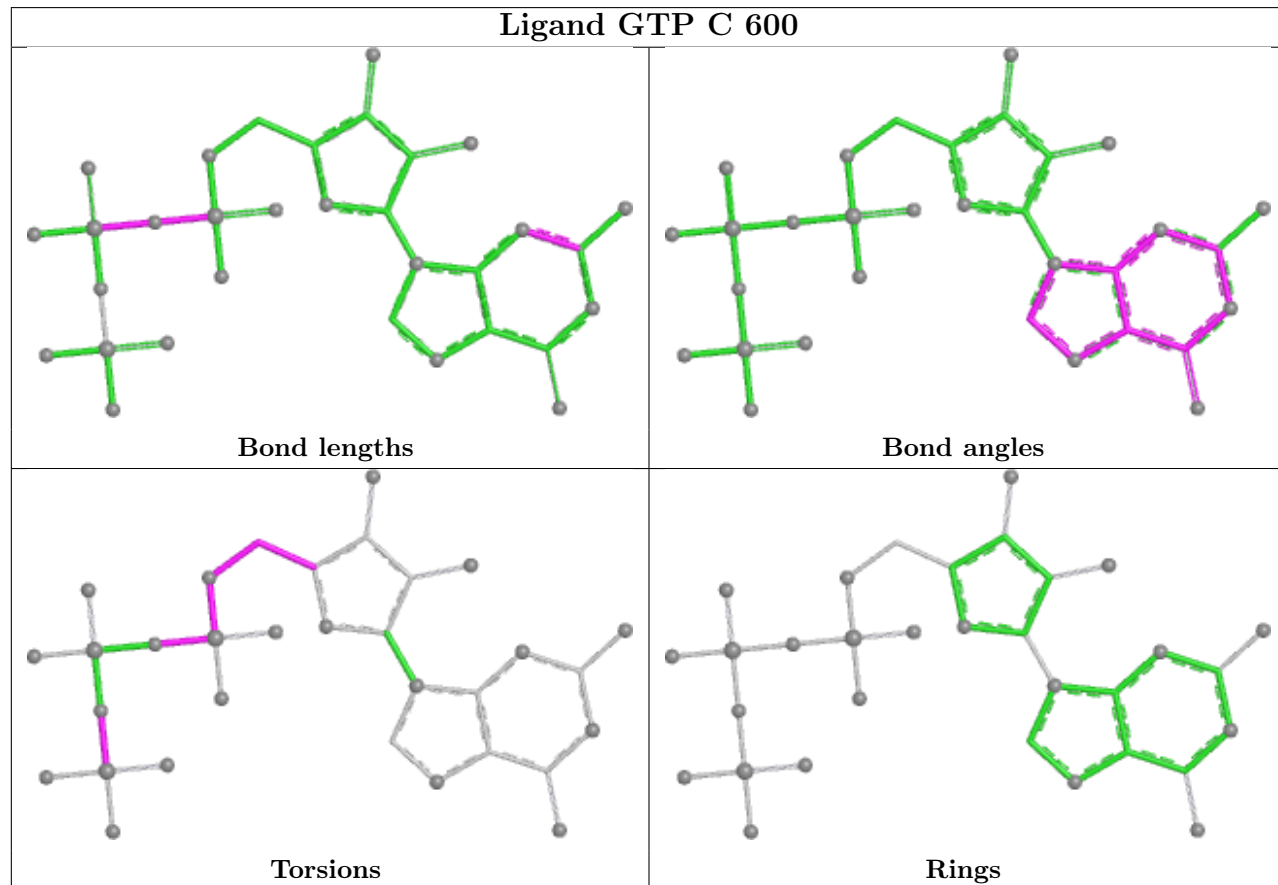


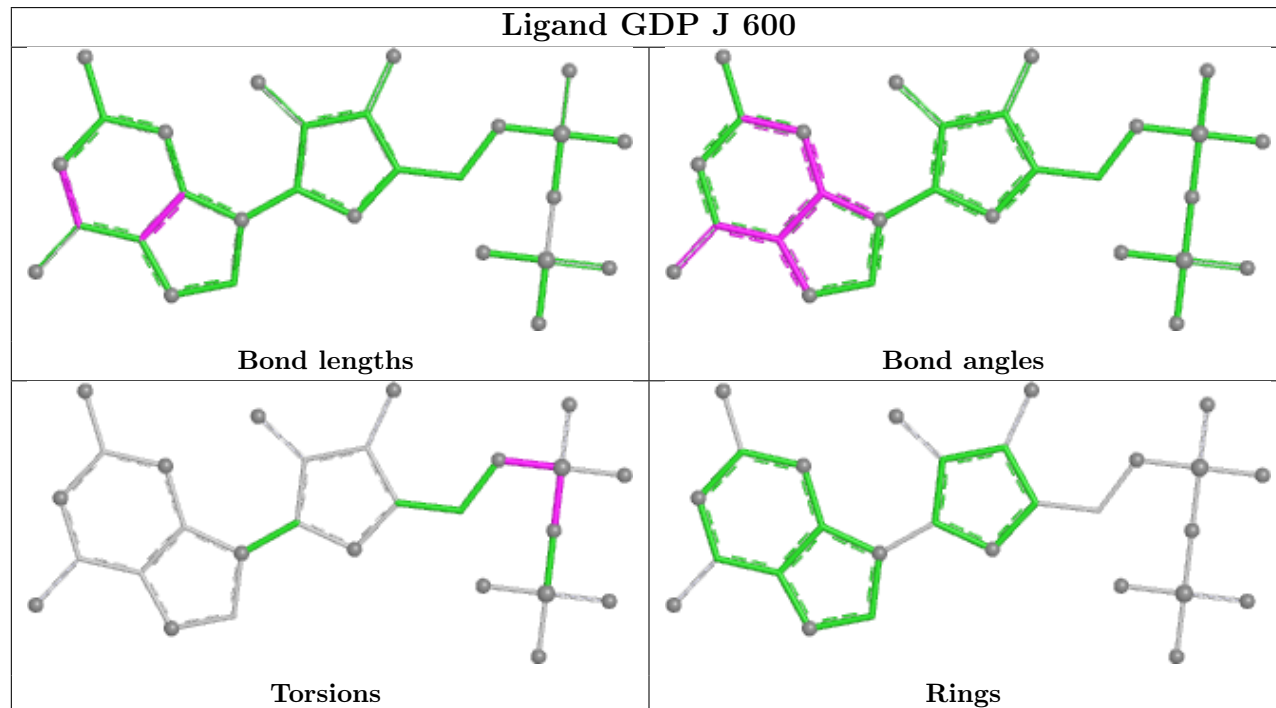
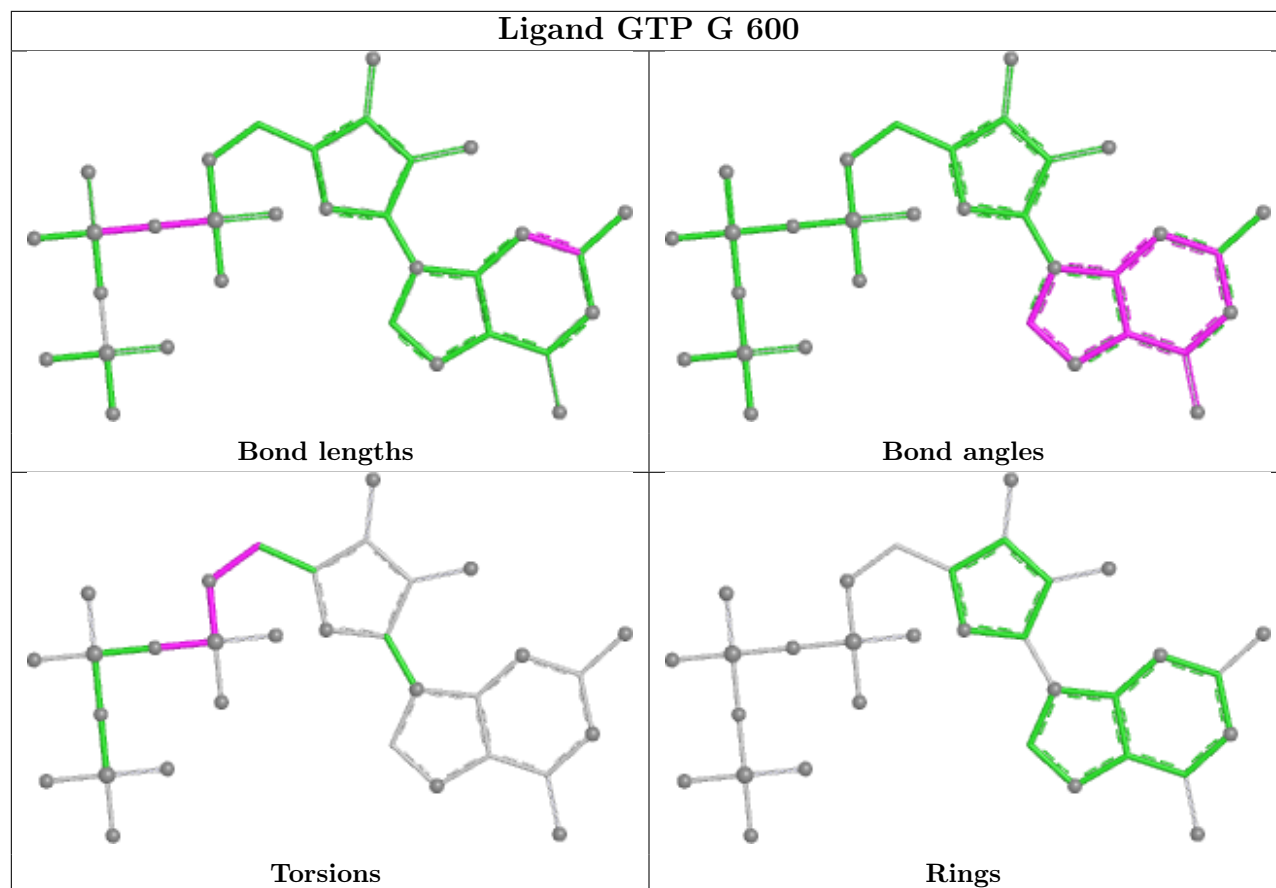


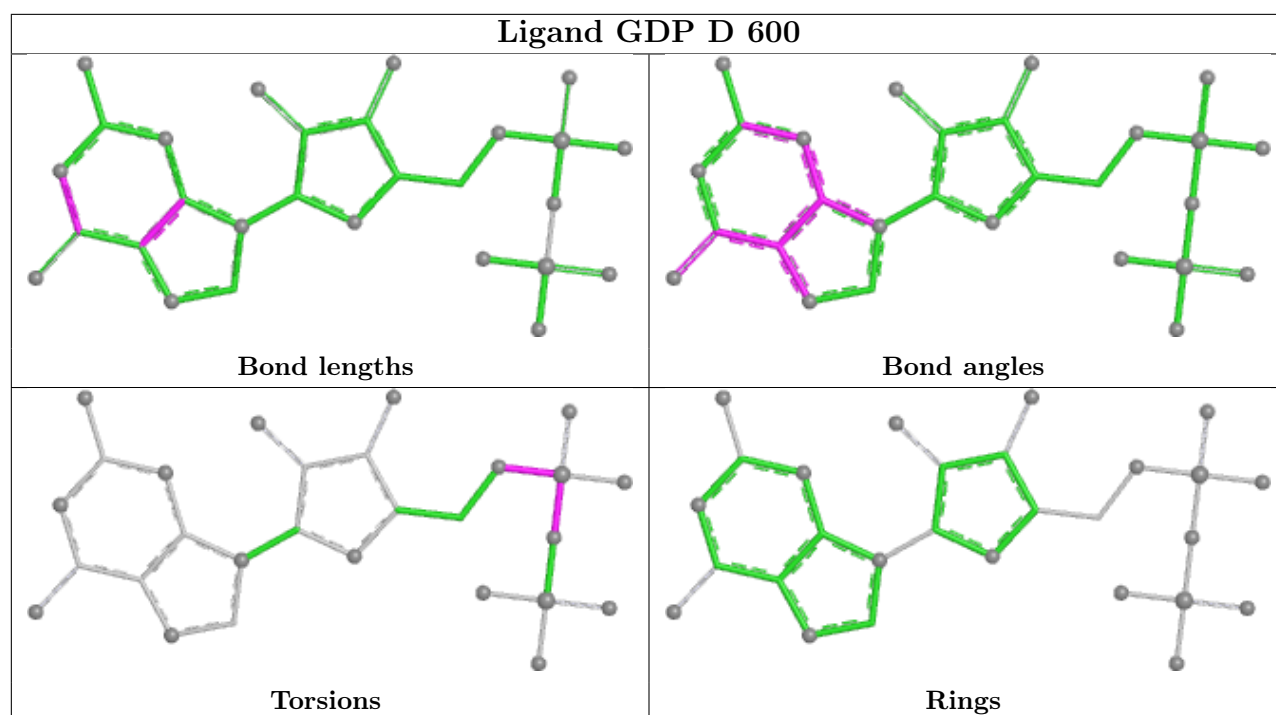
Ligand GTP I 600



Ligand GTP C 600







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	427/451 (94%)	-1.63	0 100 100	13, 44, 82, 123	0
1	C	434/451 (96%)	-1.69	0 100 100	12, 32, 61, 80	0
1	G	425/451 (94%)	-1.65	0 100 100	15, 40, 76, 97	0
1	I	436/451 (96%)	-1.66	0 100 100	13, 35, 73, 122	0
2	B	430/445 (96%)	-1.66	0 100 100	15, 43, 86, 124	0
2	D	428/445 (96%)	-1.59	0 100 100	20, 50, 92, 124	0
2	H	429/445 (96%)	-1.66	0 100 100	17, 38, 78, 116	0
2	J	428/445 (96%)	-1.55	0 100 100	22, 56, 95, 131	0
3	E	487/554 (87%)	-1.62	0 100 100	13, 45, 95, 133	0
3	K	487/554 (87%)	-1.56	0 100 100	22, 52, 102, 127	0
4	F	125/140 (89%)	-1.58	0 100 100	17, 53, 95, 105	0
4	L	125/140 (89%)	-1.54	0 100 100	31, 53, 111, 147	0
All	All	4661/4972 (93%)	-1.62	0 100 100	12, 44, 90, 147	0

There are no RSRZ outliers to report.

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 ⓘ

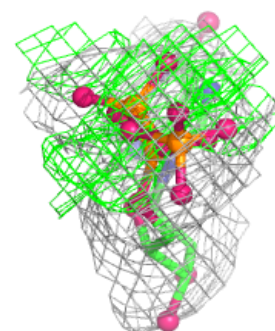
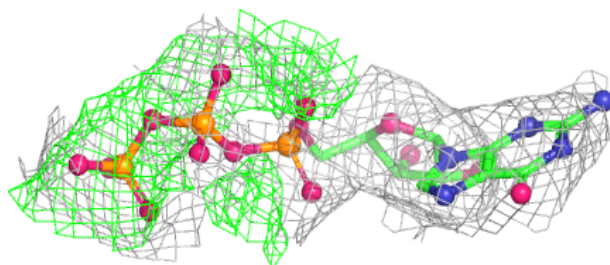
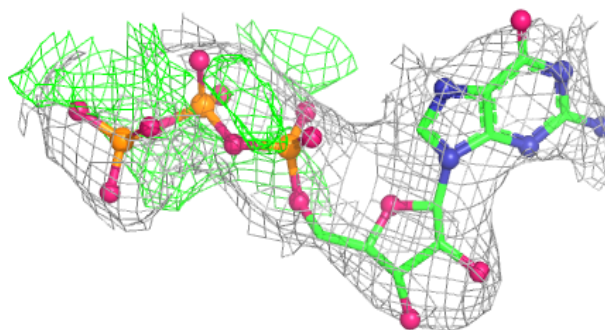
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	B	601	1/1	0.99	0.07	52,52,52,52	0
6	MG	H	601	1/1	0.99	0.02	13,13,13,13	0
6	MG	J	601	1/1	0.99	0.02	10,10,10,10	0
5	GTP	I	600	32/32	1.00	0.04	0,41,57,66	0
6	MG	A	601	1/1	1.00	0.04	20,20,20,20	0
5	GTP	A	600	32/32	1.00	0.03	3,30,46,61	0
6	MG	C	601	1/1	1.00	0.06	11,11,11,11	0
6	MG	D	601	1/1	1.00	0.05	18,18,18,18	0
6	MG	G	601	1/1	1.00	0.04	15,15,15,15	0
5	GTP	C	600	32/32	1.00	0.03	0,30,44,51	0
6	MG	I	601	1/1	1.00	0.05	1,1,1,1	0
5	GTP	G	600	32/32	1.00	0.03	8,33,57,60	0
7	GDP	B	600	28/28	1.00	0.03	25,47,59,62	0
7	GDP	D	600	28/28	1.00	0.03	20,46,63,68	0
7	GDP	H	600	28/28	1.00	0.03	11,29,51,71	0
7	GDP	J	600	28/28	1.00	0.03	25,42,53,61	0

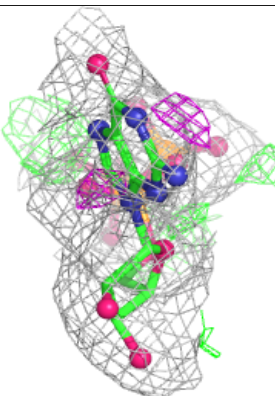
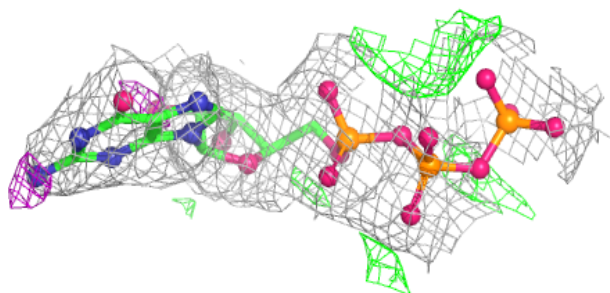
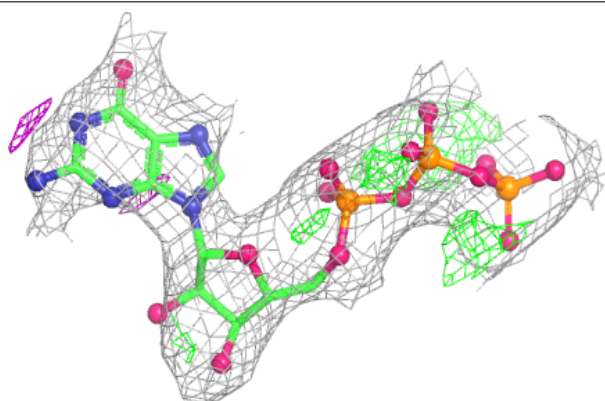
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP I 600:

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

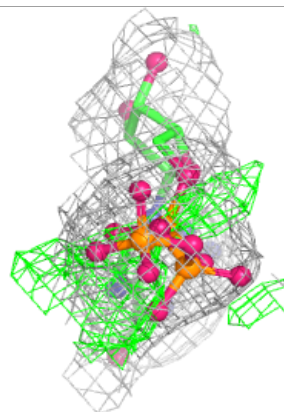
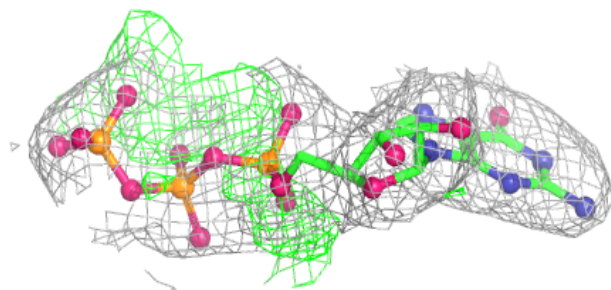
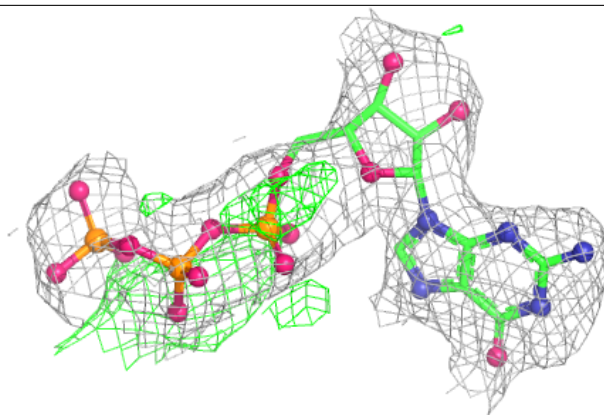
**Electron density around GTP A 600:**

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

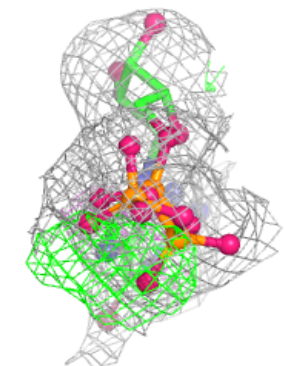
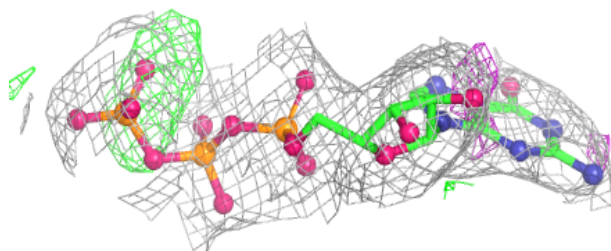
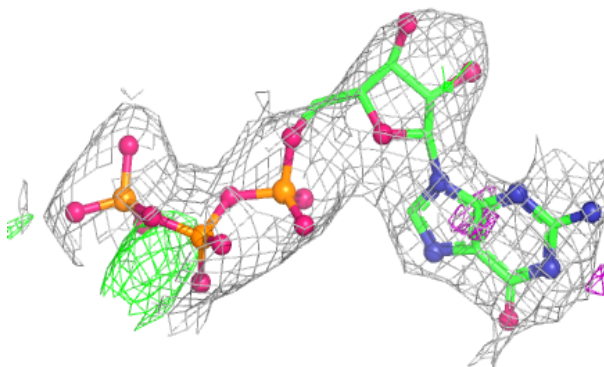


Electron density around GTP C 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

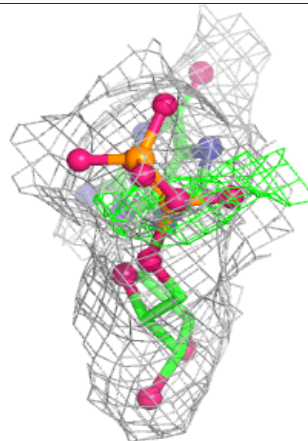
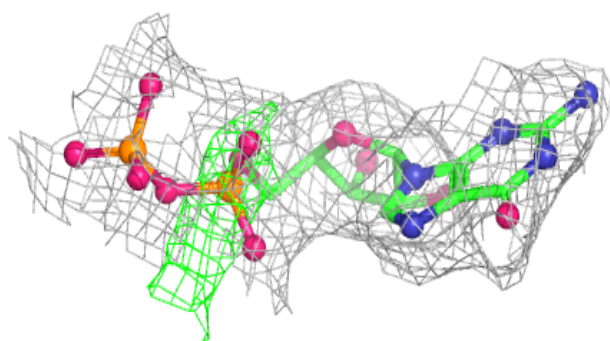
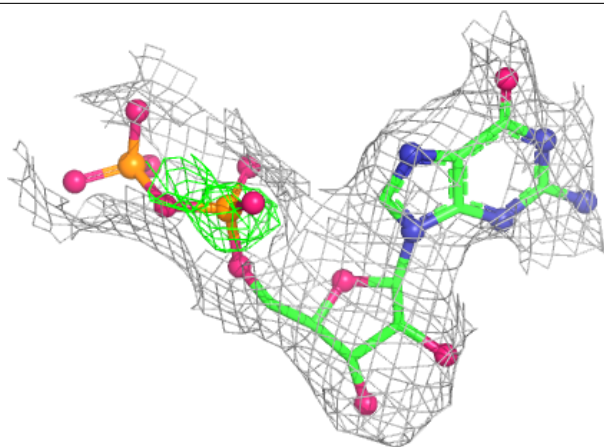
**Electron density around GTP G 600:**

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



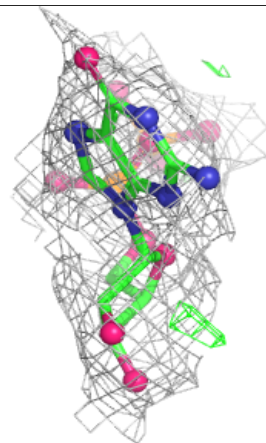
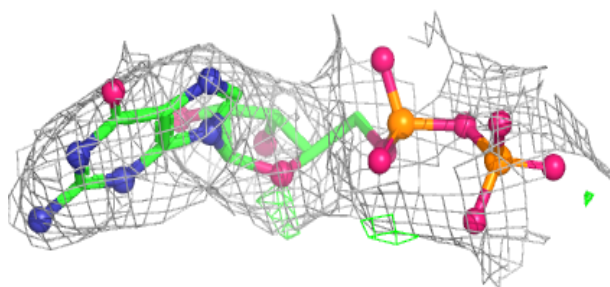
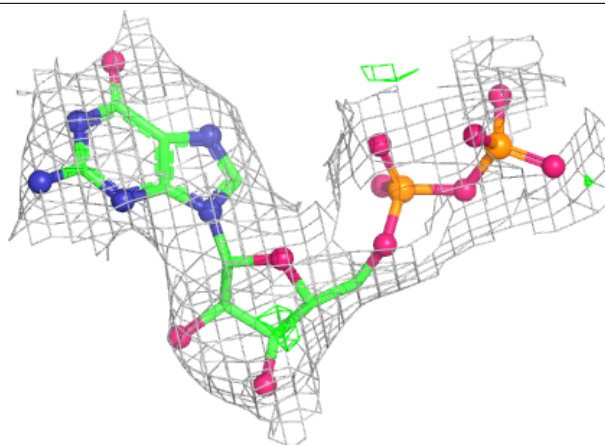
Electron density around GDP B 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



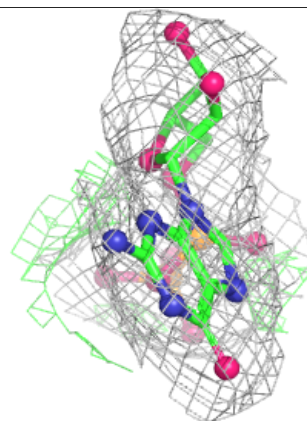
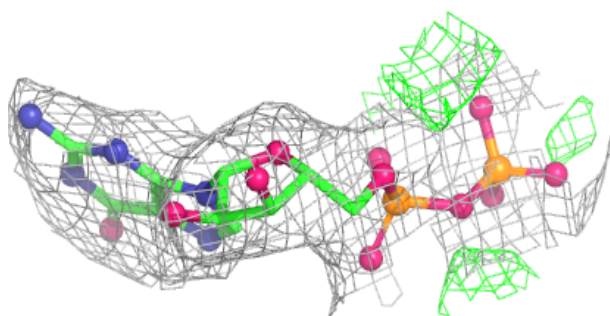
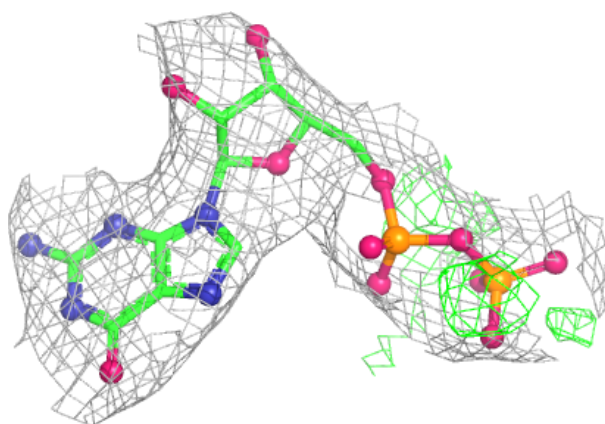
Electron density around GDP D 600:

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and green (positive)

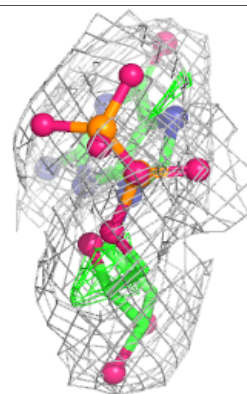
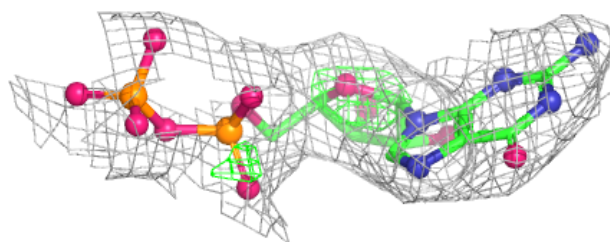
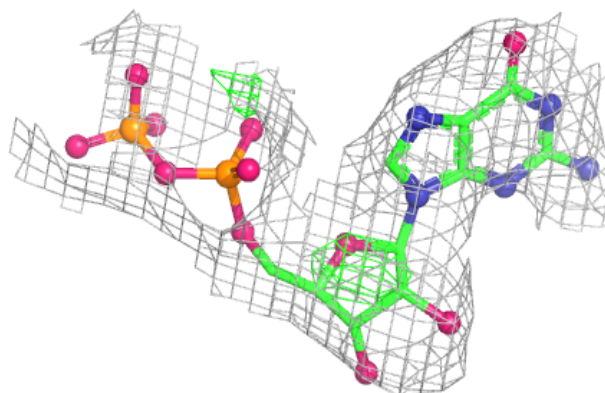


Electron density around GDP H 600:

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

**Electron density around GDP J 600:**

$2mF_o-DF_c$ (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.