



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 11:23 AM EDT

PDB ID : 4V0N
Title : Crystal structure of BBS1N in complex with ARL6DN, soaked with mercury
Authors : Mourao, A.; Lorentzen, E.
Deposited on : 2014-09-17
Resolution : 3.13 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

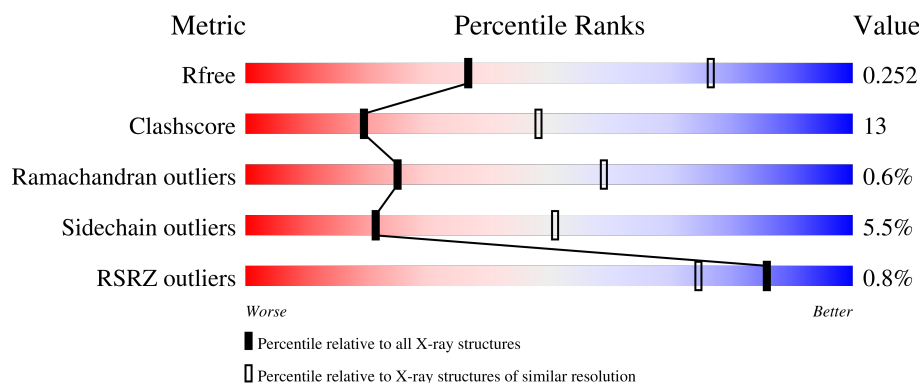
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	169	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	C	169	<div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	E	169	<div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	G	169	<div> <div>73%</div> <div>25%</div> <div>.</div> </div>
2	B	425	<div> <div>52%</div> <div>23%</div> <div>.</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	425	
2	F	425	
2	H	425	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HG	B	1426	-	-	-	X
5	HG	B	1432	-	-	-	X
5	HG	H	1434	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14532 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 ARF-LIKE SMALL GTPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1263	807	215	235	6			
1	C	166	Total	C	N	O	S	0	0	0
			1287	820	222	239	6			
1	E	166	Total	C	N	O	S	0	0	0
			1282	819	220	237	6			
1	G	166	Total	C	N	O	S	0	0	0
			1286	822	221	237	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A8JF99
A	13	ALA	-	expression tag	UNP A8JF99
A	14	ALA	-	expression tag	UNP A8JF99
A	15	SER	-	expression tag	UNP A8JF99
C	12	GLY	-	expression tag	UNP A8JF99
C	13	ALA	-	expression tag	UNP A8JF99
C	14	ALA	-	expression tag	UNP A8JF99
C	15	SER	-	expression tag	UNP A8JF99
E	12	GLY	-	expression tag	UNP A8JF99
E	13	ALA	-	expression tag	UNP A8JF99
E	14	ALA	-	expression tag	UNP A8JF99
E	15	SER	-	expression tag	UNP A8JF99
G	12	GLY	-	expression tag	UNP A8JF99
G	13	ALA	-	expression tag	UNP A8JF99
G	14	ALA	-	expression tag	UNP A8JF99
G	15	SER	-	expression tag	UNP A8JF99

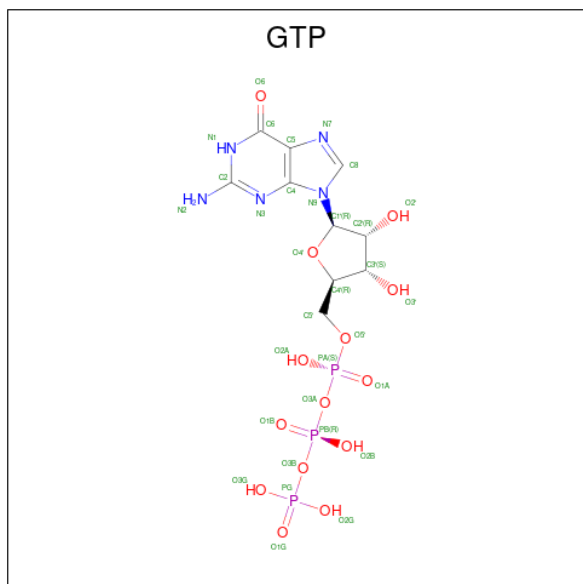
- Molecule 2 is a protein called BARDET-BIEDL SYNDROME 1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2442	1561	423	445	13			
2	D	304	Total	C	N	O	S	0	0	0
			2197	1399	383	403	12			
2	F	304	Total	C	N	O	S	0	0	0
			2200	1405	379	403	13			
2	H	325	Total	C	N	O	S	0	0	0
			2386	1526	410	437	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ARG	LYS	conflict	UNP A8JEA1
D	37	ARG	LYS	conflict	UNP A8JEA1
F	37	ARG	LYS	conflict	UNP A8JEA1
H	37	ARG	LYS	conflict	UNP A8JEA1

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		

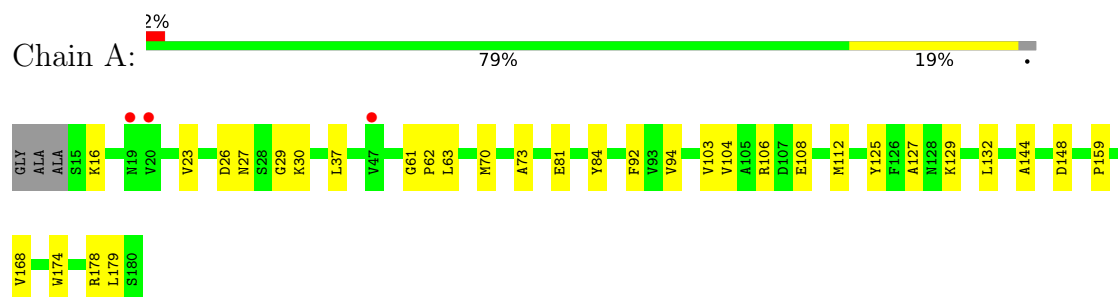
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Hg	0	0
			1	1		
5	B	13	Total	Hg	0	0
			13	13		
5	C	1	Total	Hg	0	0
			1	1		
5	D	12	Total	Hg	0	0
			12	12		
5	E	1	Total	Hg	0	0
			1	1		
5	F	14	Total	Hg	0	0
			14	14		
5	G	1	Total	Hg	0	0
			1	1		
5	H	14	Total	Hg	0	0
			14	14		

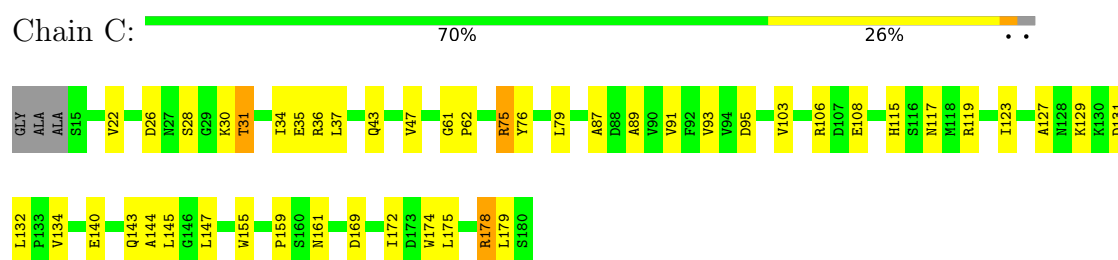
3 Residue-property plots [i](#)

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.

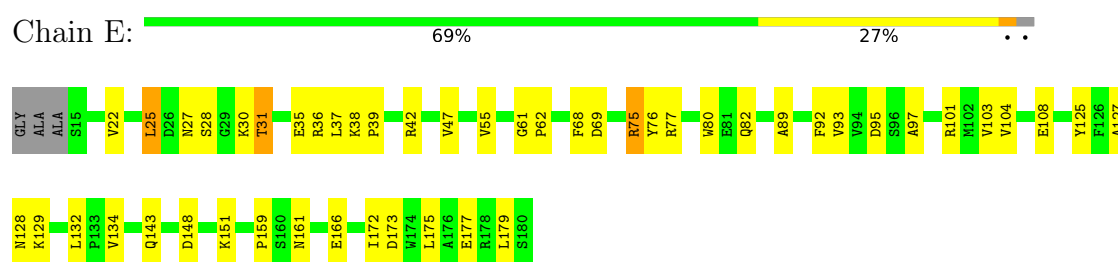
• Molecule 1: ARF-LIKE SMALL GTPASE



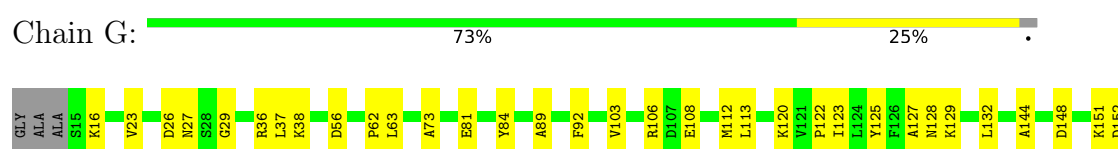
• Molecule 1: ARF-LIKE SMALL GTPASE

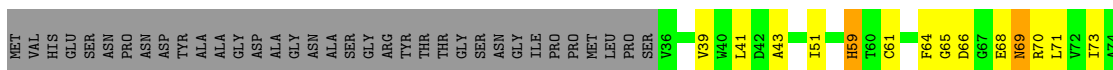


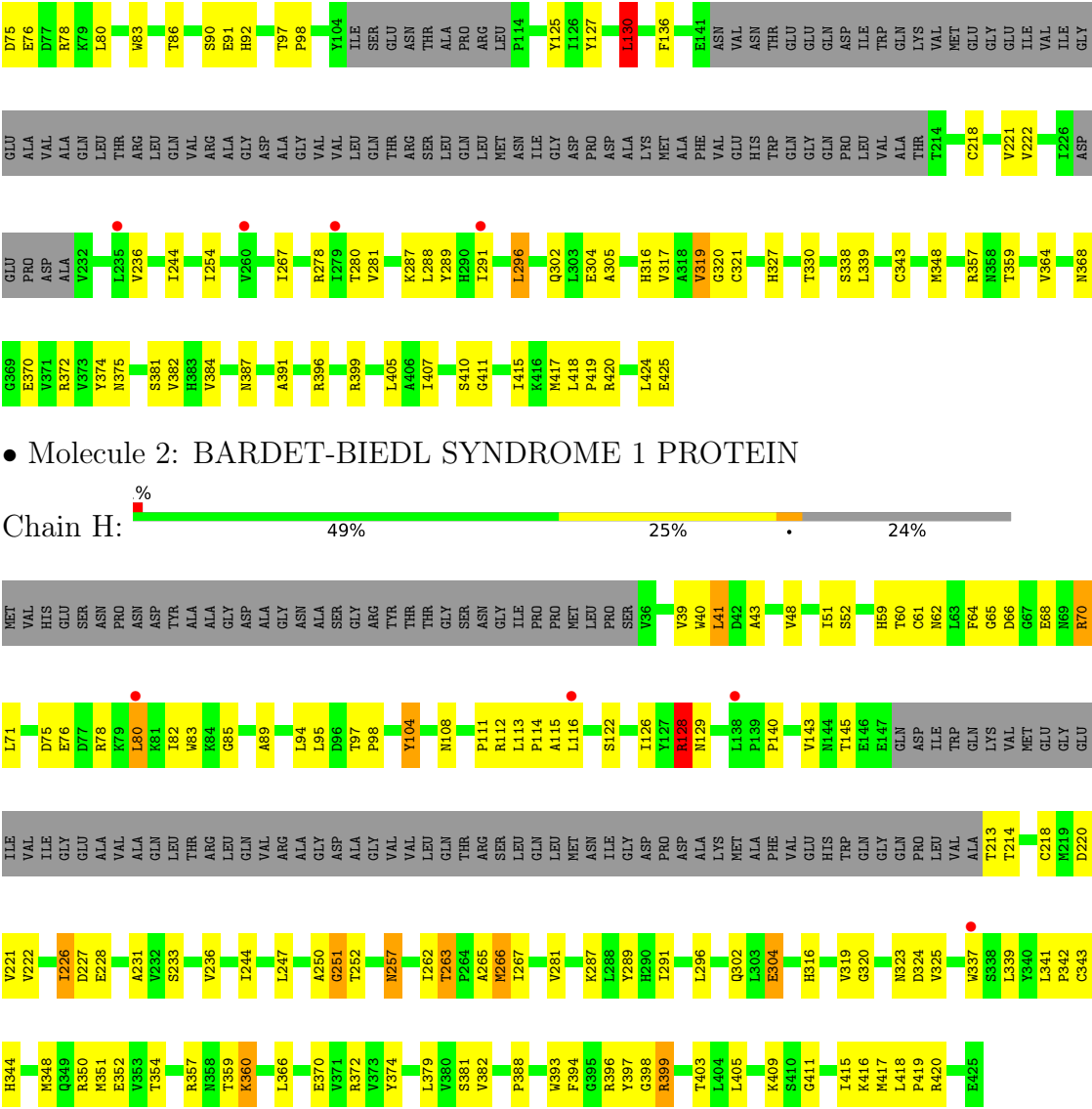
• Molecule 1: ARF-LIKE SMALL GTPASE



• Molecule 1: ARF-LIKE SMALL GTPASE







4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.75Å 123.75Å 443.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	96.50 – 3.13 96.50 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.0 (96.50-3.13) 99.2 (96.50-3.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.13Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.249 0.216 , 0.252	Depositor DCC
R_{free} test set	3506 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	104.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14532	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG, 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	0.44	0/1289	0.62	0/1755
1	C	0.59	0/1313	0.75	0/1784
1	E	0.62	0/1308	0.77	0/1777
1	G	0.46	0/1312	0.65	0/1781
2	B	0.54	0/2494	0.76	1/3412 (0.0%)
2	D	0.44	0/2240	0.66	0/3066
2	F	0.47	0/2244	0.68	0/3071
2	H	0.54	0/2437	0.79	3/3339 (0.1%)
All	All	0.51	0/14637	0.72	4/19985 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	H	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	LEU	CA-CB-CG	6.97	131.34	115.30
2	B	80	LEU	CA-CB-CG	6.23	129.62	115.30
2	H	41	LEU	CA-CB-CG	5.71	128.44	115.30
2	H	128	ARG	N-CA-C	-5.20	96.96	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	226	ILE	Peptide
2	H	145	THR	Peptide
2	H	226	ILE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1263	0	1241	22	0
1	C	1287	0	1285	31	0
1	E	1282	0	1283	37	0
1	G	1286	0	1294	31	0
2	B	2442	0	2400	70	0
2	D	2197	0	2087	60	0
2	F	2200	0	2111	57	0
2	H	2386	0	2324	83	0
3	A	32	0	12	2	0
3	C	32	0	12	3	0
3	E	32	0	12	2	0
3	G	32	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	B	13	0	0	0	0
5	C	1	0	0	0	0
5	D	12	0	0	0	0
5	E	1	0	0	0	0
5	F	14	0	0	0	0
5	G	1	0	0	0	0
5	H	14	0	0	0	0
All	All	14532	0	14073	365	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 13.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ARG:NH2	2:B:352:GLU:OE1	2.12	0.81
2:H:350:ARG:NH2	2:H:352:GLU:OE1	2.19	0.76
2:B:39:VAL:HG13	2:B:381:SER:HB2	1.67	0.76
1:E:101:ARG:NH1	2:F:399:ARG:HB2	2.01	0.75
2:D:247:LEU:HD22	2:D:254:ILE:HA	1.68	0.75
2:B:313:LEU:HD11	2:B:362:LEU:HD12	1.68	0.75
2:F:405:LEU:HD23	2:F:415:ILE:HG12	1.68	0.75
2:D:405:LEU:HD23	2:D:415:ILE:HG12	1.70	0.74
2:D:39:VAL:HG13	2:D:381:SER:HB2	1.71	0.72
2:H:341:LEU:HD23	2:H:366:LEU:HD21	1.71	0.72
2:B:405:LEU:HD23	2:B:415:ILE:HG12	1.72	0.72
2:H:43:ALA:HB2	2:H:417:MET:HE2	1.72	0.72
2:F:348:MET:HG2	2:F:364:VAL:HG12	1.72	0.71
1:C:30:LYS:N	3:C:600:GTP:O1B	2.20	0.70
1:E:25:LEU:HB3	1:E:101:ARG:HH21	1.57	0.70
2:F:267:ILE:HG22	2:F:281:VAL:HG22	1.74	0.70
2:F:375:ASN:ND2	2:F:424:LEU:O	2.21	0.69
2:F:372:ARG:HG2	2:F:382:VAL:HG22	1.72	0.69
2:D:348:MET:HG2	2:D:364:VAL:HG12	1.73	0.69
2:D:350:ARG:NH2	2:D:352:GLU:OE1	2.26	0.69
1:C:108:GLU:OE1	2:D:420:ARG:NH1	2.26	0.68
2:D:385:SER:OG	2:D:387:ASN:O	2.12	0.67
2:H:112:ARG:N	2:H:113:LEU:HA	2.10	0.67
2:B:71:LEU:HB3	2:B:83:TRP:HB2	1.77	0.67
1:E:31:THR:OG1	3:E:600:GTP:O2B	2.13	0.67
2:F:39:VAL:HG13	2:F:381:SER:HB2	1.75	0.66
1:E:129:LYS:HB3	1:E:132:LEU:HD12	1.76	0.66
2:F:222:VAL:HG13	2:F:236:VAL:HG21	1.77	0.66
1:G:89:ALA:HB1	1:G:175:LEU:HD11	1.78	0.66
1:C:129:LYS:HB3	1:C:132:LEU:HD12	1.77	0.66
2:F:68:GLU:HB2	2:F:399:ARG:NH1	2.11	0.66
1:G:103:VAL:HG22	2:H:41:LEU:HD13	1.78	0.65
2:D:140:PRO:HB3	2:D:214:THR:N	2.13	0.64
1:G:81:GLU:HA	1:G:84:TYR:CD2	2.33	0.63
2:B:64:PHE:O	2:B:66:ASP:N	2.31	0.63
1:C:31:THR:OG1	3:C:600:GTP:O2B	2.15	0.63
2:F:125:TYR:HB3	2:F:127:TYR:HE1	1.64	0.63
2:D:350:ARG:HH12	2:D:360:LYS:HD3	1.64	0.63
2:F:64:PHE:O	2:F:66:ASP:N	2.32	0.63
2:B:224:GLN:HA	2:B:273:LEU:HD12	1.80	0.62
1:G:108:GLU:OE1	2:H:420:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:SER:HB3	2:F:92:HIS:CE1	2.34	0.62
1:E:127:ALA:HB3	1:E:159:PRO:HA	1.82	0.62
2:D:305:ALA:HB3	2:D:321:CYS:HB3	1.82	0.61
2:B:222:VAL:HG23	2:B:236:VAL:HG21	1.81	0.61
2:F:92:HIS:CD2	2:F:130:LEU:HD11	2.35	0.61
1:C:174:TRP:CZ2	1:C:178:ARG:HD2	2.36	0.61
2:F:418:LEU:HD12	2:F:419:PRO:HD2	1.82	0.61
2:B:77:ASP:HB3	2:B:79:LYS:HG3	1.83	0.61
2:B:43:ALA:HB2	2:B:417:MET:HE2	1.82	0.61
2:F:75:ASP:OD1	2:F:76:GLU:N	2.34	0.60
2:B:339:LEU:HD21	2:B:374:TYR:CD2	2.36	0.60
1:E:108:GLU:OE1	2:F:420:ARG:NH1	2.35	0.60
2:H:111:PRO:C	2:H:113:LEU:HA	2.22	0.60
1:G:129:LYS:HB3	1:G:132:LEU:HD12	1.83	0.60
2:H:320:GLY:HA3	2:H:348:MET:CE	2.31	0.60
1:C:103:VAL:HG22	2:D:41:LEU:HD13	1.84	0.59
1:E:89:ALA:HB1	1:E:175:LEU:HD11	1.84	0.59
2:B:341:LEU:HD23	2:B:342:PRO:HD2	1.83	0.59
2:B:136:PHE:CE2	2:B:138:LEU:HD23	2.38	0.59
2:F:357:ARG:O	2:F:359:THR:HG23	2.02	0.59
2:D:368:ASN:OD1	2:D:370:GLU:HG2	2.03	0.59
2:H:262:ILE:HD12	2:H:263:THR:H	1.68	0.58
2:B:320:GLY:HA3	2:B:348:MET:CE	2.33	0.58
2:F:43:ALA:HB2	2:F:417:MET:HE2	1.85	0.58
2:D:423:ASN:OD1	2:D:423:ASN:N	2.32	0.58
1:E:25:LEU:HB3	1:E:101:ARG:NH2	2.19	0.58
2:F:305:ALA:HB3	2:F:321:CYS:HB3	1.85	0.58
1:A:30:LYS:NZ	1:A:70:MET:O	2.36	0.57
1:E:104:VAL:HG23	2:F:417:MET:HE3	1.84	0.57
2:B:70:ARG:NH1	2:B:84:LYS:HD2	2.19	0.57
2:B:129:ASN:N	2:B:129:ASN:OD1	2.36	0.57
2:D:136:PHE:CE2	2:D:253:ALA:HA	2.40	0.57
2:D:281:VAL:HB	2:D:289:TYR:HB2	1.87	0.56
2:D:82:ILE:HG22	2:D:89:ALA:HB3	1.88	0.56
2:F:288:LEU:HD11	2:F:319:VAL:HG21	1.88	0.56
2:B:40:TRP:HB3	2:B:416:LYS:HB3	1.87	0.56
2:D:320:GLY:HA3	2:D:348:MET:HE2	1.88	0.56
2:B:68:GLU:HB2	2:B:399:ARG:NH1	2.21	0.56
2:H:244:ILE:HD11	2:H:281:VAL:HG21	1.87	0.56
2:B:127:TYR:O	2:B:128:ARG:HG2	2.06	0.56
1:G:103:VAL:HG11	2:H:43:ALA:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:GLU:O	2:D:263:THR:HG22	2.06	0.55
2:H:126:ILE:HD11	2:H:251:GLY:HA3	1.88	0.55
1:C:75:ARG:HH11	1:C:76:TYR:HE2	1.51	0.55
2:F:368:ASN:OD1	2:F:370:GLU:HG2	2.06	0.55
1:G:127:ALA:HB3	1:G:159:PRO:HA	1.89	0.55
2:F:320:GLY:HA3	2:F:348:MET:CE	2.37	0.55
2:H:60:THR:HG1	2:H:393:TRP:HE1	1.54	0.55
2:H:228:GLU:HG3	2:H:231:ALA:HB2	1.89	0.55
2:D:370:GLU:HB3	2:D:384:VAL:HG22	1.89	0.54
2:H:76:GLU:C	2:H:78:ARG:H	2.09	0.54
2:H:39:VAL:HG13	2:H:381:SER:HB2	1.88	0.54
2:D:63:LEU:HA	2:D:114:PRO:HG2	1.88	0.54
2:F:61:CYS:O	2:F:69:ASN:ND2	2.40	0.54
2:D:327:HIS:ND1	2:D:338:SER:OG	2.40	0.54
1:G:37:LEU:HD21	1:G:172:ILE:HG13	1.90	0.54
1:G:16:LYS:HB3	1:G:63:LEU:HD23	1.90	0.54
2:F:291:ILE:HG12	2:F:296:LEU:HA	1.89	0.54
2:F:396:ARG:NH2	2:F:399:ARG:HA	2.23	0.54
2:H:140:PRO:HB3	2:H:213:THR:N	2.24	0.53
2:H:323:ASN:O	2:H:325:VAL:HG23	2.09	0.53
2:B:391:ALA:HB3	2:B:407:ILE:HB	1.90	0.53
2:D:71:LEU:HB3	2:D:83:TRP:HB2	1.89	0.53
2:H:75:ASP:OD1	2:H:76:GLU:N	2.42	0.53
2:B:129:ASN:C	2:B:131:ARG:H	2.12	0.53
2:B:378:LEU:HG	2:B:380:VAL:HG23	1.89	0.53
2:B:324:ASP:OD1	2:B:344:HIS:HA	2.08	0.53
2:B:379:LEU:HD21	2:B:382:VAL:HG23	1.90	0.53
2:D:357:ARG:O	2:D:359:THR:HG23	2.09	0.53
2:H:64:PHE:O	2:H:66:ASP:N	2.41	0.53
2:H:51:ILE:O	2:H:411:GLY:HA2	2.09	0.52
1:C:37:LEU:HD21	1:C:172:ILE:HG13	1.91	0.52
1:C:28:SER:HB2	1:C:93:VAL:HG12	1.91	0.52
1:A:92:PHE:HB3	1:A:125:TYR:CD2	2.45	0.52
2:B:339:LEU:HD21	2:B:374:TYR:CG	2.44	0.52
2:H:405:LEU:HD23	2:H:415:ILE:HG12	1.91	0.52
1:A:27:ASN:CG	2:B:399:ARG:HH21	2.13	0.52
1:A:106:ARG:HD2	1:A:144:ALA:O	2.09	0.52
2:H:68:GLU:HB2	2:H:399:ARG:NH1	2.24	0.51
1:C:127:ALA:HB3	1:C:159:PRO:HA	1.92	0.51
2:B:44:PHE:CZ	2:B:46:ASP:HB2	2.45	0.51
2:B:51:ILE:HD13	2:B:73:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:357:ARG:O	2:H:359:THR:HG23	2.10	0.51
2:D:289:TYR:CD2	2:D:300:ILE:HD12	2.45	0.51
1:G:103:VAL:CG2	2:H:41:LEU:HB3	2.41	0.51
2:H:71:LEU:HB3	2:H:83:TRP:HB2	1.91	0.51
2:H:341:LEU:CD2	2:H:366:LEU:HD21	2.40	0.51
2:H:291:ILE:HG12	2:H:296:LEU:HA	1.93	0.51
2:B:273:LEU:HD23	2:B:277:TYR:CE2	2.46	0.51
2:H:122:SER:HB3	2:H:214:THR:O	2.10	0.51
2:H:379:LEU:HD21	2:H:382:VAL:CG2	2.41	0.51
2:B:104:TYR:HD1	2:B:104:TYR:H	1.59	0.51
2:H:350:ARG:HH12	2:H:360:LYS:HZ2	1.59	0.51
1:E:161:ASN:HB3	1:E:166:GLU:HB3	1.93	0.50
2:H:222:VAL:HG23	2:H:236:VAL:HG21	1.92	0.50
1:E:25:LEU:HD23	1:E:101:ARG:HE	1.75	0.50
2:F:357:ARG:NH1	2:F:420:ARG:O	2.44	0.50
2:H:226:ILE:O	2:H:228:GLU:N	2.44	0.50
1:C:75:ARG:NH1	1:C:76:TYR:HE2	2.10	0.50
2:F:281:VAL:HB	2:F:289:TYR:HB2	1.94	0.50
2:H:379:LEU:HD21	2:H:382:VAL:HG23	1.93	0.50
2:F:244:ILE:HD11	2:F:281:VAL:HG21	1.94	0.50
2:H:396:ARG:NH2	2:H:399:ARG:HA	2.26	0.50
2:F:71:LEU:HB3	2:F:83:TRP:HB2	1.93	0.49
2:H:339:LEU:HD21	2:H:374:TYR:CD2	2.47	0.49
2:H:40:TRP:HB3	2:H:416:LYS:HB3	1.93	0.49
1:A:84:TYR:CZ	1:A:112:MET:HG3	2.48	0.49
1:G:29:GLY:HA3	1:G:128:ASN:ND2	2.27	0.49
1:C:36:ARG:NH1	1:C:43:GLN:OE1	2.46	0.49
1:E:30:LYS:N	3:E:600:GTP:O1B	2.32	0.49
2:F:327:HIS:ND1	2:F:338:SER:OG	2.44	0.49
2:H:257:ASN:O	2:H:257:ASN:ND2	2.45	0.49
2:B:370:GLU:OE1	2:B:372:ARG:NH2	2.37	0.49
2:H:339:LEU:HD21	2:H:374:TYR:CG	2.48	0.49
1:C:106:ARG:HD2	1:C:144:ALA:O	2.13	0.49
1:G:122:PRO:HA	1:G:154:PRO:HG2	1.95	0.49
2:D:287:LYS:HE2	2:D:302:GLN:OE1	2.12	0.49
2:D:320:GLY:HA3	2:D:348:MET:CE	2.42	0.48
2:H:41:LEU:CD2	2:H:419:PRO:HG3	2.43	0.48
2:H:370:GLU:OE2	2:H:372:ARG:NH2	2.41	0.48
1:A:16:LYS:HB3	1:A:63:LEU:HD23	1.95	0.48
1:C:129:LYS:HG2	3:C:600:GTP:C6	2.48	0.48
1:E:103:VAL:HG21	2:F:41:LEU:HB3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:LEU:HD22	2:B:366:LEU:HD11	1.95	0.48
2:D:85:GLY:O	2:D:397:TYR:OH	2.25	0.48
2:F:339:LEU:HD21	2:F:374:TYR:CG	2.49	0.48
1:A:127:ALA:HB3	1:A:159:PRO:HA	1.95	0.48
2:B:51:ILE:O	2:B:411:GLY:HA2	2.14	0.48
2:B:320:GLY:HA3	2:B:348:MET:HE1	1.96	0.48
1:E:173:ASP:O	1:E:177:GLU:HG3	2.13	0.48
2:H:82:ILE:HG22	2:H:89:ALA:HB3	1.94	0.48
1:G:84:TYR:CZ	1:G:112:MET:HG3	2.49	0.47
2:B:222:VAL:HG23	2:B:236:VAL:CG2	2.43	0.47
1:C:174:TRP:CE2	1:C:178:ARG:HD2	2.49	0.47
1:G:26:ASP:HB3	1:G:73:ALA:N	2.29	0.47
1:A:129:LYS:HB3	1:A:132:LEU:HD12	1.97	0.47
2:B:78:ARG:HG3	2:B:97:THR:HG22	1.96	0.47
2:H:388:PRO:HG2	2:H:409:LYS:CB	2.44	0.47
2:B:113:LEU:H	2:B:114:PRO:CD	2.27	0.47
2:B:222:VAL:HG11	2:B:273:LEU:HG	1.97	0.47
2:D:64:PHE:O	2:D:66:ASP:N	2.47	0.47
2:D:136:PHE:HE2	2:D:253:ALA:HA	1.80	0.47
1:E:103:VAL:CG2	2:F:41:LEU:HB3	2.44	0.47
2:B:262:ILE:HD12	2:B:263:THR:H	1.80	0.47
2:D:299:THR:O	2:D:300:ILE:HD13	2.14	0.47
2:D:396:ARG:NH2	2:D:399:ARG:HA	2.30	0.47
2:F:387:ASN:CG	2:F:410:SER:HB3	2.35	0.47
1:G:106:ARG:NH1	1:G:144:ALA:O	2.46	0.47
2:H:64:PHE:N	2:H:64:PHE:CD1	2.82	0.47
1:G:23:VAL:HG23	1:G:92:PHE:CD1	2.49	0.46
2:B:279:ILE:HB	2:B:291:ILE:HB	1.97	0.46
2:H:418:LEU:HD12	2:H:419:PRO:HD2	1.96	0.46
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.68	0.46
1:G:23:VAL:HG23	1:G:92:PHE:HD1	1.80	0.46
2:D:68:GLU:HB2	2:D:399:ARG:NH1	2.31	0.46
2:D:80:LEU:HB2	2:D:94:LEU:HD11	1.97	0.46
2:D:321:CYS:HB2	2:D:323:ASN:OD1	2.16	0.46
2:D:387:ASN:OD1	2:D:410:SER:HB3	2.15	0.46
1:E:103:VAL:HG11	2:F:43:ALA:HA	1.96	0.46
2:F:320:GLY:HA3	2:F:348:MET:HE2	1.96	0.46
1:G:16:LYS:N	1:G:62:PRO:O	2.48	0.46
2:H:113:LEU:H	2:H:114:PRO:HD3	1.79	0.46
2:H:250:ALA:O	2:H:252:THR:N	2.48	0.46
2:D:122:SER:HB3	2:D:214:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:91:GLU:O	2:F:92:HIS:ND1	2.48	0.46
1:A:104:VAL:HG23	2:B:417:MET:HE3	1.97	0.46
2:B:271:GLY:HA3	2:B:277:TYR:HA	1.96	0.46
2:B:396:ARG:NH2	2:B:399:ARG:HA	2.31	0.46
1:C:35:GLU:HB3	1:C:36:ARG:NH1	2.30	0.46
1:C:26:ASP:OD1	2:D:399:ARG:HD2	2.15	0.46
1:G:36:ARG:HG3	1:G:165:GLY:HA2	1.98	0.46
1:E:35:GLU:OE2	1:E:38:LYS:NZ	2.48	0.46
1:E:75:ARG:NH2	1:E:76:TYR:OH	2.48	0.46
2:F:69:ASN:HD22	2:F:69:ASN:HA	1.56	0.46
1:G:92:PHE:HB3	1:G:125:TYR:CD1	2.51	0.46
2:H:341:LEU:HA	2:H:342:PRO:HD3	1.82	0.46
2:H:372:ARG:NH1	2:H:374:TYR:OH	2.35	0.46
2:B:76:GLU:C	2:B:78:ARG:H	2.18	0.45
2:B:375:ASN:ND2	2:B:424:LEU:O	2.38	0.45
1:C:131:ASP:HB3	1:C:161:ASN:HD22	1.80	0.45
2:H:320:GLY:HA3	2:H:348:MET:HE1	1.98	0.45
1:C:103:VAL:HG21	2:D:41:LEU:HB3	1.96	0.45
2:D:59:HIS:CE1	2:D:103:SER:HB3	2.51	0.45
2:F:343:CYS:SG	2:F:368:ASN:HB3	2.56	0.45
1:G:108:GLU:OE2	2:H:420:ARG:HD3	2.16	0.45
2:D:288:LEU:HD23	2:D:288:LEU:HA	1.64	0.45
2:F:68:GLU:HB2	2:F:399:ARG:HH12	1.82	0.45
1:E:35:GLU:CD	1:E:38:LYS:HZ3	2.18	0.45
2:H:265:ALA:HB1	2:H:266:MET:HE3	1.97	0.45
1:C:89:ALA:HB1	1:C:175:LEU:HD11	1.99	0.45
2:D:267:ILE:HG22	2:D:281:VAL:HG22	1.97	0.45
1:E:37:LEU:HD21	1:E:172:ILE:HG13	1.98	0.45
2:F:391:ALA:HB3	2:F:407:ILE:HB	1.98	0.45
1:A:108:GLU:OE1	2:B:420:ARG:NH1	2.50	0.45
2:H:324:ASP:OD1	2:H:344:HIS:HA	2.17	0.45
1:C:115:HIS:CE1	1:C:117:ASN:HB2	2.52	0.45
2:D:222:VAL:HG13	2:D:236:VAL:HG21	1.97	0.45
2:B:79:LYS:HD2	2:B:91:GLU:OE1	2.16	0.45
1:E:35:GLU:HA	1:E:38:LYS:HD3	1.99	0.45
2:H:320:GLY:HA3	2:H:348:MET:HE2	1.99	0.45
1:G:103:VAL:HG21	2:H:41:LEU:HB3	1.98	0.45
2:B:112:ARG:N	2:B:113:LEU:HA	2.31	0.44
2:H:228:GLU:CG	2:H:231:ALA:HB2	2.47	0.44
1:C:61:GLY:HA3	1:C:62:PRO:HD2	1.86	0.44
1:E:104:VAL:CG2	2:F:417:MET:HE3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:ASN:CG	2:H:399:ARG:HH21	2.20	0.44
1:A:81:GLU:HA	1:A:84:TYR:CD2	2.52	0.44
2:F:97:THR:HA	2:F:98:PRO:HD3	1.76	0.44
2:F:280:THR:HG21	2:F:317:VAL:HG21	1.99	0.44
2:H:97:THR:HA	2:H:98:PRO:HD3	1.67	0.44
2:D:417:MET:HB3	2:D:417:MET:HE2	1.63	0.44
2:F:51:ILE:O	2:F:411:GLY:HA2	2.17	0.44
2:H:43:ALA:HB2	2:H:417:MET:CE	2.43	0.44
2:H:78:ARG:HG3	2:H:97:THR:HG22	1.99	0.44
1:A:174:TRP:O	1:A:178:ARG:HG2	2.18	0.44
1:E:22:VAL:HG12	1:E:30:LYS:HG2	1.99	0.44
1:G:148:ASP:O	1:G:151:LYS:HE3	2.17	0.44
2:H:262:ILE:CD1	2:H:263:THR:H	2.30	0.44
1:C:145:LEU:HB2	1:C:147:LEU:HG	2.00	0.44
1:E:27:ASN:CG	2:F:399:ARG:HH21	2.21	0.44
2:H:61:CYS:SG	2:H:62:ASN:N	2.90	0.44
1:A:29:GLY:N	3:A:600:GTP:O1B	2.44	0.44
1:E:95:ASP:OD1	1:E:97:ALA:N	2.48	0.44
2:B:310:LEU:HD13	2:B:319:VAL:HG13	1.98	0.44
2:D:244:ILE:HD11	2:D:281:VAL:HG21	2.00	0.44
2:H:76:GLU:C	2:H:78:ARG:N	2.70	0.44
1:E:28:SER:HB2	1:E:93:VAL:HG12	2.00	0.43
1:A:23:VAL:HG23	1:A:92:PHE:CD1	2.53	0.43
2:B:92:HIS:NE2	2:B:130:LEU:HD13	2.33	0.43
2:B:122:SER:HB3	2:B:214:THR:O	2.19	0.43
2:D:61:CYS:SG	2:D:62:ASN:N	2.91	0.43
2:H:337:TRP:CZ3	2:H:339:LEU:HD13	2.52	0.43
2:B:129:ASN:O	2:B:131:ARG:N	2.51	0.43
1:C:140:GLU:O	1:C:143:GLN:HB3	2.18	0.43
1:E:39:PRO:O	1:E:42:ARG:N	2.49	0.43
2:H:60:THR:OG1	2:H:393:TRP:NE1	2.49	0.43
2:B:90:SER:HG	2:B:92:HIS:CE1	2.36	0.43
1:C:22:VAL:HG22	1:C:91:VAL:HB	2.00	0.43
2:D:273:LEU:HA	2:D:277:TYR:CD1	2.53	0.43
2:H:41:LEU:HD21	2:H:419:PRO:HG3	2.00	0.43
2:H:351:MET:HG3	2:H:394:PHE:CE2	2.54	0.43
2:B:97:THR:HA	2:B:98:PRO:HD3	1.74	0.43
2:B:127:TYR:C	2:B:128:ARG:HG2	2.39	0.43
2:B:351:MET:HB3	2:B:361:ALA:HB3	2.00	0.43
2:D:95:LEU:HD22	2:D:95:LEU:H	1.83	0.43
2:F:59:HIS:O	2:F:71:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:ASN:HB3	1:G:166:GLU:HB3	2.01	0.43
1:A:26:ASP:HB3	1:A:73:ALA:N	2.34	0.43
1:A:103:VAL:HG11	2:B:43:ALA:HA	2.01	0.43
2:B:64:PHE:N	2:B:64:PHE:CD1	2.86	0.43
2:H:94:LEU:HD13	2:H:98:PRO:HG3	2.00	0.43
2:H:104:TYR:CE1	2:H:115:ALA:HB3	2.54	0.43
2:F:73:ILE:O	2:F:80:LEU:HD22	2.19	0.43
2:H:250:ALA:C	2:H:252:THR:H	2.21	0.42
2:H:351:MET:HG3	2:H:394:PHE:CD2	2.54	0.42
2:B:357:ARG:O	2:B:359:THR:HG23	2.19	0.42
1:E:55:VAL:HG22	1:E:68:PHE:CD2	2.54	0.42
2:H:80:LEU:HD21	2:H:116:LEU:HD21	2.01	0.42
2:B:351:MET:HG3	2:B:394:PHE:CD2	2.55	0.42
1:C:28:SER:HA	1:C:95:ASP:HB2	2.00	0.42
2:H:113:LEU:N	2:H:114:PRO:HD3	2.34	0.42
1:A:37:LEU:HD21	1:A:168:VAL:HG12	2.00	0.42
2:B:257:ASN:O	2:B:257:ASN:ND2	2.52	0.42
2:D:291:ILE:HG12	2:D:296:LEU:HA	2.00	0.42
1:G:38:LYS:HE2	1:G:56:ASP:OD2	2.19	0.42
1:G:120:LYS:HE3	1:G:152:ASP:HB2	2.02	0.42
2:H:85:GLY:O	2:H:397:TYR:OH	2.29	0.42
2:B:43:ALA:HB2	2:B:417:MET:CE	2.48	0.42
2:D:41:LEU:HB2	2:D:417:MET:O	2.19	0.42
2:F:370:GLU:HB3	2:F:384:VAL:HG22	2.02	0.42
2:H:68:GLU:HG3	2:H:398:GLY:HA2	2.01	0.42
1:A:61:GLY:HA3	1:A:62:PRO:HD2	1.89	0.42
2:B:70:ARG:CZ	2:B:84:LYS:HD2	2.48	0.42
2:B:320:GLY:HA3	2:B:348:MET:HE2	2.00	0.42
2:D:387:ASN:CG	2:D:410:SER:HB3	2.40	0.42
1:E:148:ASP:O	1:E:151:LYS:HE3	2.20	0.42
2:H:267:ILE:HG22	2:H:281:VAL:HG22	2.00	0.42
1:A:129:LYS:HG2	3:A:600:GTP:C6	2.54	0.42
2:F:64:PHE:C	2:F:66:ASP:H	2.22	0.42
2:B:316:HIS:CD2	2:B:316:HIS:N	2.88	0.42
1:C:22:VAL:HG21	1:C:34:ILE:HD11	2.01	0.42
2:F:287:LYS:HE2	2:F:302:GLN:NE2	2.35	0.42
2:F:288:LEU:HD23	2:F:288:LEU:HA	1.90	0.42
2:B:220:ASP:O	2:B:236:VAL:N	2.28	0.42
2:D:337:TRP:CE3	2:D:339:LEU:HD13	2.55	0.41
1:E:77:ARG:HG2	1:E:80:TRP:CZ2	2.55	0.41
2:H:287:LYS:HB2	2:H:289:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:CYS:HB2	2:B:323:ASN:OD1	2.20	0.41
2:H:104:TYR:HB2	2:H:233:SER:HB2	2.02	0.41
1:C:87:ALA:O	1:C:119:ARG:NH2	2.48	0.41
1:C:179:LEU:HD23	1:C:179:LEU:HA	1.68	0.41
1:G:179:LEU:HA	1:G:179:LEU:HD23	1.81	0.41
2:D:76:GLU:C	2:D:78:ARG:H	2.24	0.41
2:F:278:ARG:HA	2:F:291:ILE:O	2.20	0.41
2:D:75:ASP:OD1	2:D:76:GLU:N	2.54	0.41
2:D:418:LEU:HD12	2:D:419:PRO:HD2	2.03	0.41
1:E:103:VAL:HG22	2:F:41:LEU:HD13	2.02	0.41
2:B:245:LEU:HD13	2:B:254:ILE:CD1	2.50	0.41
1:C:79:LEU:HD21	1:E:82:GLN:HE21	1.86	0.41
2:D:81:LYS:C	2:D:82:ILE:HD12	2.41	0.41
2:D:287:LYS:HB2	2:D:289:TYR:CE1	2.55	0.41
1:E:36:ARG:HA	1:E:36:ARG:HD3	1.99	0.41
1:G:84:TYR:CE1	1:G:112:MET:HG3	2.56	0.41
1:G:113:LEU:HD21	1:G:123:ILE:HD11	2.03	0.41
1:A:178:ARG:CZ	1:A:178:ARG:HA	2.51	0.41
2:F:136:PHE:HZ	2:F:254:ILE:HG13	1.85	0.41
1:G:156:GLN:HB2	1:G:174:TRP:CZ2	2.56	0.41
1:A:103:VAL:HG22	2:B:41:LEU:HD13	2.03	0.40
1:E:128:ASN:CG	1:E:129:LYS:H	2.23	0.40
2:H:287:LYS:HE2	2:H:302:GLN:OE1	2.21	0.40
2:D:341:LEU:HA	2:D:342:PRO:HD3	1.88	0.40
2:F:76:GLU:C	2:F:78:ARG:H	2.24	0.40
2:H:70:ARG:HH11	2:H:70:ARG:HD3	1.74	0.40
2:H:388:PRO:HG2	2:H:409:LYS:HB2	2.02	0.40
2:B:316:HIS:HB3	2:B:330:THR:HA	2.04	0.40
1:C:123:ILE:O	1:C:155:TRP:HA	2.21	0.40
2:D:46:ASP:HA	2:D:47:PRO:HD2	1.93	0.40
1:E:31:THR:HG23	1:E:69:ASP:OD2	2.21	0.40
1:E:61:GLY:HA3	1:E:62:PRO:HD2	1.92	0.40
2:H:220:ASP:O	2:H:236:VAL:N	2.30	0.40
2:H:394:PHE:HA	2:H:403:THR:O	2.21	0.40
2:D:306:GLN:HG2	2:D:307:PRO:HD2	2.04	0.40
2:D:312:ARG:HH12	2:D:360:LYS:NZ	2.20	0.40
1:E:92:PHE:HB3	1:E:125:TYR:CD2	2.57	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	164/169 (97%)	155 (94%)	9 (6%)	0	100	100
1	C	164/169 (97%)	158 (96%)	6 (4%)	0	100	100
1	E	164/169 (97%)	155 (94%)	9 (6%)	0	100	100
1	G	164/169 (97%)	154 (94%)	10 (6%)	0	100	100
2	B	326/425 (77%)	290 (89%)	32 (10%)	4 (1%)	13	42
2	D	294/425 (69%)	269 (92%)	24 (8%)	1 (0%)	41	72
2	F	296/425 (70%)	271 (92%)	23 (8%)	2 (1%)	22	56
2	H	321/425 (76%)	288 (90%)	28 (9%)	5 (2%)	9	35
All	All	1893/2376 (80%)	1740 (92%)	141 (7%)	12 (1%)	25	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	65	GLY
2	B	113	LEU
2	B	130	LEU
2	F	65	GLY
2	D	65	GLY
2	H	65	GLY
2	B	140	PRO
2	H	227	ASP
2	H	128	ARG
2	F	130	LEU
2	H	251	GLY
2	H	304	GLU

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	131/142 (92%)	129 (98%)	2 (2%)	65	84
1	C	137/142 (96%)	131 (96%)	6 (4%)	28	59
1	E	136/142 (96%)	129 (95%)	7 (5%)	24	54
1	G	137/142 (96%)	137 (100%)	0	100	100
2	B	250/352 (71%)	232 (93%)	18 (7%)	14	41
2	D	214/352 (61%)	202 (94%)	12 (6%)	21	50
2	F	218/352 (62%)	205 (94%)	13 (6%)	19	48
2	H	242/352 (69%)	219 (90%)	23 (10%)	8	29
All	All	1465/1976 (74%)	1384 (94%)	81 (6%)	21	51

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	148	ASP
2	B	52	SER
2	B	70	ARG
2	B	94	LEU
2	B	104	TYR
2	B	128	ARG
2	B	129	ASN
2	B	218	CYS
2	B	233	SER
2	B	257	ASN
2	B	263	THR
2	B	266	MET
2	B	270	GLN
2	B	306	GLN
2	B	316	HIS
2	B	317	VAL
2	B	319	VAL
2	B	343	CYS
2	B	350	ARG
1	C	31	THR
1	C	47	VAL
1	C	75	ARG

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Mol	Chain	Res	Type
1	C	134	VAL
1	C	169	ASP
1	C	178	ARG
2	D	70	ARG
2	D	266	MET
2	D	299	THR
2	D	304	GLU
2	D	306	GLN
2	D	316	HIS
2	D	319	VAL
2	D	332	THR
2	D	338	SER
2	D	343	CYS
2	D	356	GLN
2	D	421	THR
1	E	25	LEU
1	E	31	THR
1	E	47	VAL
1	E	75	ARG
1	E	134	VAL
1	E	143	GLN
1	E	179	LEU
2	F	59	HIS
2	F	69	ASN
2	F	70	ARG
2	F	86	THR
2	F	130	LEU
2	F	218	CYS
2	F	221	VAL
2	F	296	LEU
2	F	304	GLU
2	F	316	HIS
2	F	319	VAL
2	F	330	THR
2	F	425	GLU
2	H	48	VAL
2	H	52	SER
2	H	59	HIS
2	H	70	ARG
2	H	95	LEU
2	H	104	TYR
2	H	108	ASN

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Mol	Chain	Res	Type
2	H	128	ARG
2	H	129	ASN
2	H	143	VAL
2	H	218	CYS
2	H	221	VAL
2	H	247	LEU
2	H	257	ASN
2	H	263	THR
2	H	266	MET
2	H	304	GLU
2	H	316	HIS
2	H	319	VAL
2	H	343	CYS
2	H	354	THR
2	H	360	LYS
2	H	399	ARG

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

Mol	Chain	Res	Type
2	B	356	GLN
2	F	69	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 61 are monoatomic - leaving 4 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$
3	GTP	A	600	4	26,34,34	1.11	2 (7%)	32,54,54	1.61	7 (21%)
3	GTP	G	600	4	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
3	GTP	C	600	4	26,34,34	1.25	2 (7%)	32,54,54	1.86	11 (34%)
3	GTP	E	600	4	26,34,34	1.01	2 (7%)	32,54,54	1.66	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	600	4	-	4/18/38/38	0/3/3/3
3	GTP	G	600	4	-	2/18/38/38	0/3/3/3
3	GTP	C	600	4	-	8/18/38/38	0/3/3/3
3	GTP	E	600	4	-	4/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	GTP	C5-C6	-4.69	1.37	1.47
3	G	600	GTP	C5-C6	-3.85	1.39	1.47
3	A	600	GTP	C5-C6	-3.71	1.39	1.47
3	E	600	GTP	C5-C6	-3.08	1.41	1.47
3	E	600	GTP	C2-N3	2.33	1.38	1.33
3	A	600	GTP	C2-N3	2.30	1.38	1.33
3	G	600	GTP	C2-N3	2.21	1.38	1.33
3	C	600	GTP	C2-N3	2.07	1.38	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	600	GTP	PA-O3A-PB	-4.59	117.08	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	GTP	PA-O3A-PB	-4.16	118.54	132.83
3	E	600	GTP	PA-O3A-PB	-3.64	120.35	132.83
3	C	600	GTP	C5-C6-N1	3.58	120.28	113.95
3	G	600	GTP	PB-O3B-PG	-3.56	120.61	132.83
3	A	600	GTP	PB-O3B-PG	-3.44	121.02	132.83
3	C	600	GTP	O6-C6-C5	-3.40	117.74	124.37
3	E	600	GTP	C8-N7-C5	3.30	109.27	102.99
3	G	600	GTP	PA-O3A-PB	-3.18	121.93	132.83
3	E	600	GTP	O4'-C1'-C2'	-3.11	102.38	106.93
3	G	600	GTP	O2G-PG-O3B	3.08	114.98	104.64
3	A	600	GTP	C8-N7-C5	3.03	108.75	102.99
3	C	600	GTP	C2-N1-C6	-2.97	119.63	125.10
3	C	600	GTP	C8-N7-C5	2.91	108.54	102.99
3	E	600	GTP	C2-N1-C6	-2.89	119.78	125.10
3	G	600	GTP	C8-N7-C5	2.88	108.47	102.99
3	A	600	GTP	C5-C6-N1	2.86	118.99	113.95
3	E	600	GTP	C5-C6-N1	2.81	118.91	113.95
3	G	600	GTP	C5-C6-N1	2.72	118.76	113.95
3	C	600	GTP	PB-O3B-PG	-2.70	123.56	132.83
3	A	600	GTP	C2-N1-C6	-2.69	120.14	125.10
3	E	600	GTP	PB-O3B-PG	-2.46	124.38	132.83
3	C	600	GTP	N2-C2-N1	2.44	121.90	116.71
3	G	600	GTP	C2-N1-C6	-2.38	120.72	125.10
3	G	600	GTP	C3'-C2'-C1'	2.37	104.55	100.98
3	C	600	GTP	C2'-C3'-C4'	-2.30	98.18	102.64
3	A	600	GTP	C5'-C4'-C3'	-2.28	106.62	115.18
3	E	600	GTP	O5'-C5'-C4'	2.23	116.67	108.99
3	C	600	GTP	N1-C2-N3	-2.17	119.27	123.32
3	C	600	GTP	O4'-C1'-C2'	-2.13	103.81	106.93
3	A	600	GTP	O6-C6-C5	-2.09	120.29	124.37
3	C	600	GTP	C3'-C2'-C1'	-2.05	97.89	100.98

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	600	GTP	C5'-O5'-PA-O1A
3	C	600	GTP	O4'-C4'-C5'-O5'
3	G	600	GTP	PB-O3B-PG-O2G
3	C	600	GTP	PG-O3B-PB-O1B
3	A	600	GTP	PB-O3B-PG-O1G
3	C	600	GTP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	C	600	GTP	C3'-C4'-C5'-O5'
3	E	600	GTP	PB-O3B-PG-O1G
3	A	600	GTP	PB-O3B-PG-O2G
3	A	600	GTP	PB-O3B-PG-O3G
3	C	600	GTP	PB-O3B-PG-O2G
3	E	600	GTP	PB-O3B-PG-O2G
3	E	600	GTP	PB-O3B-PG-O3G
3	C	600	GTP	C5'-O5'-PA-O3A
3	A	600	GTP	O4'-C4'-C5'-O5'
3	C	600	GTP	PA-O3A-PB-O1B
3	E	600	GTP	PA-O3A-PB-O2B
3	G	600	GTP	O4'-C4'-C5'-O5'

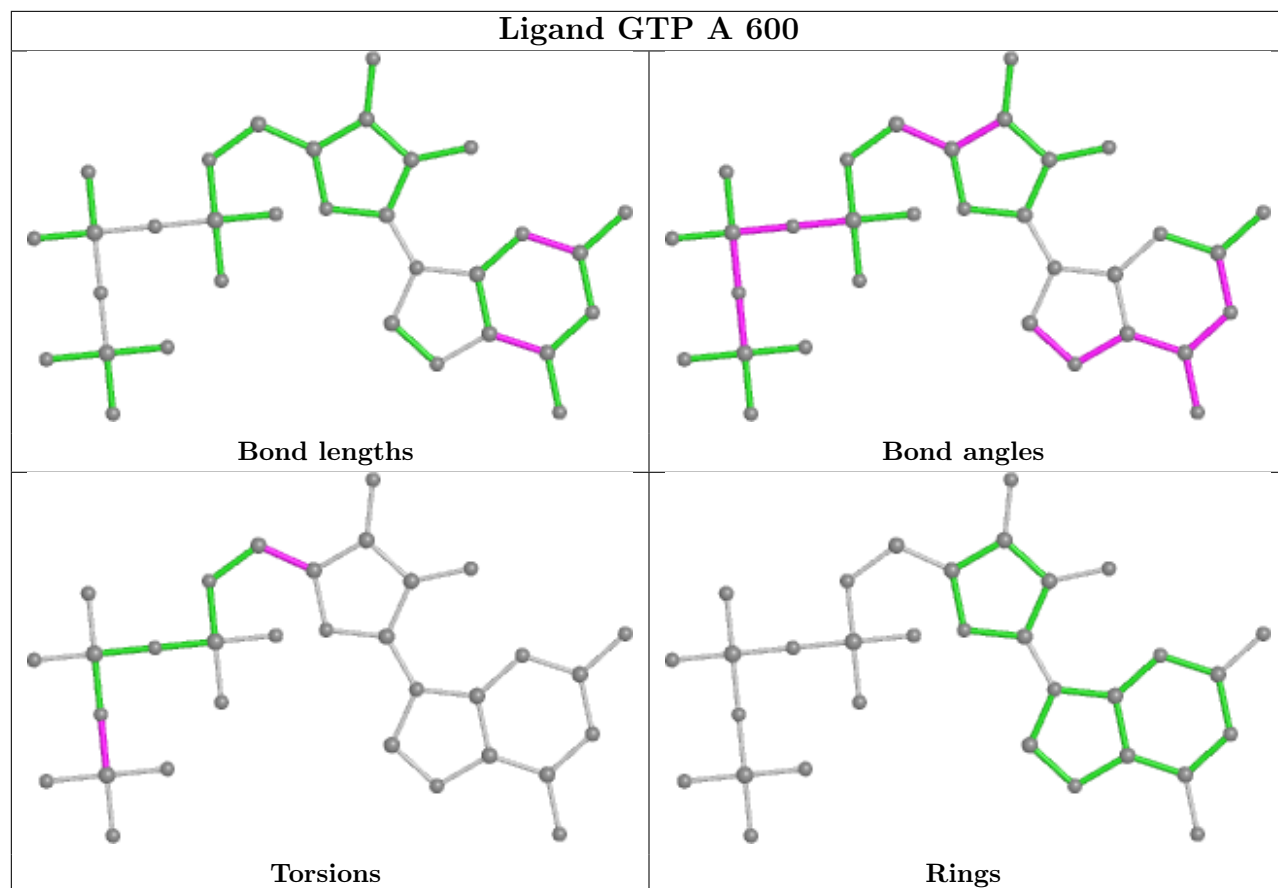
There are no ring outliers.

3 monomers are involved in 7 short contacts:

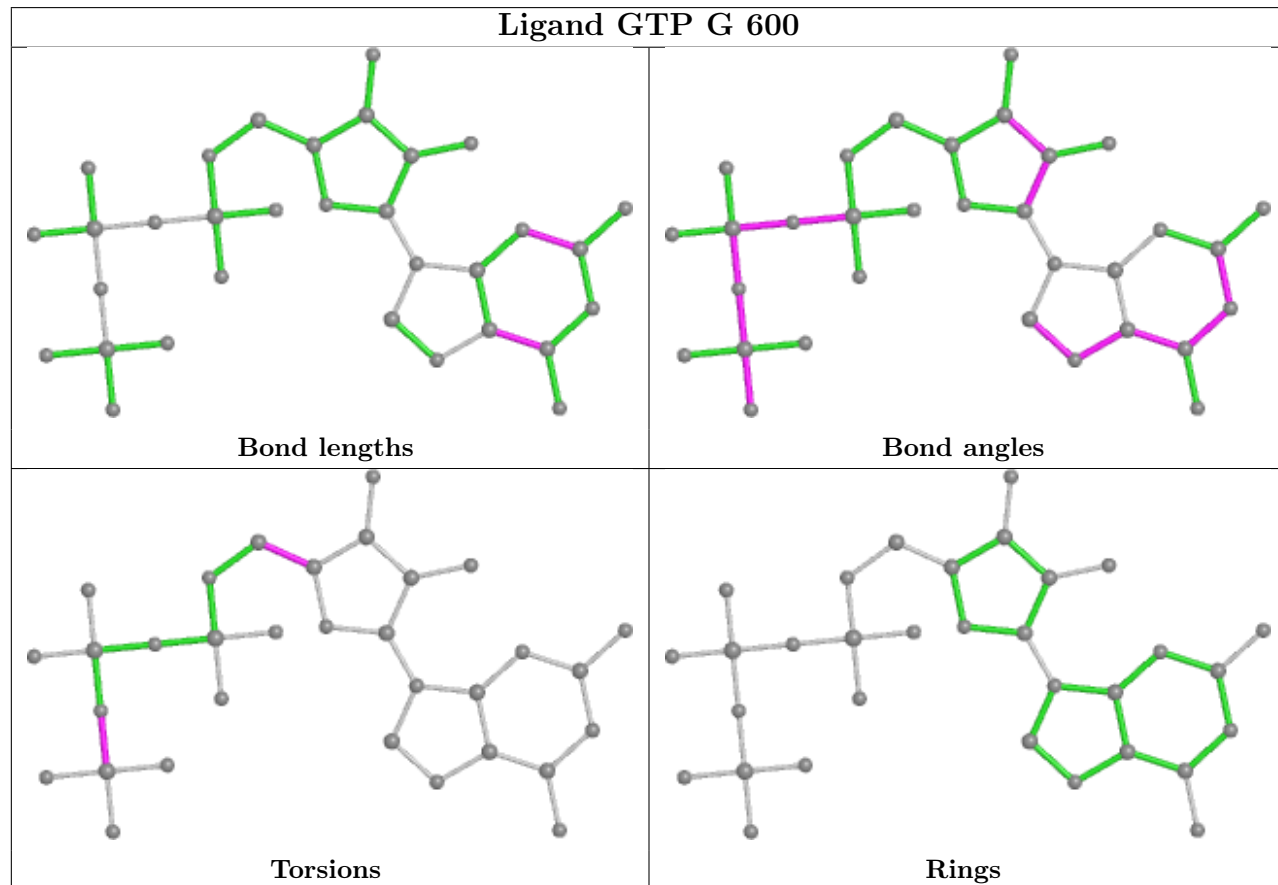
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	GTP	2	0
3	C	600	GTP	3	0
3	E	600	GTP	2	0

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.

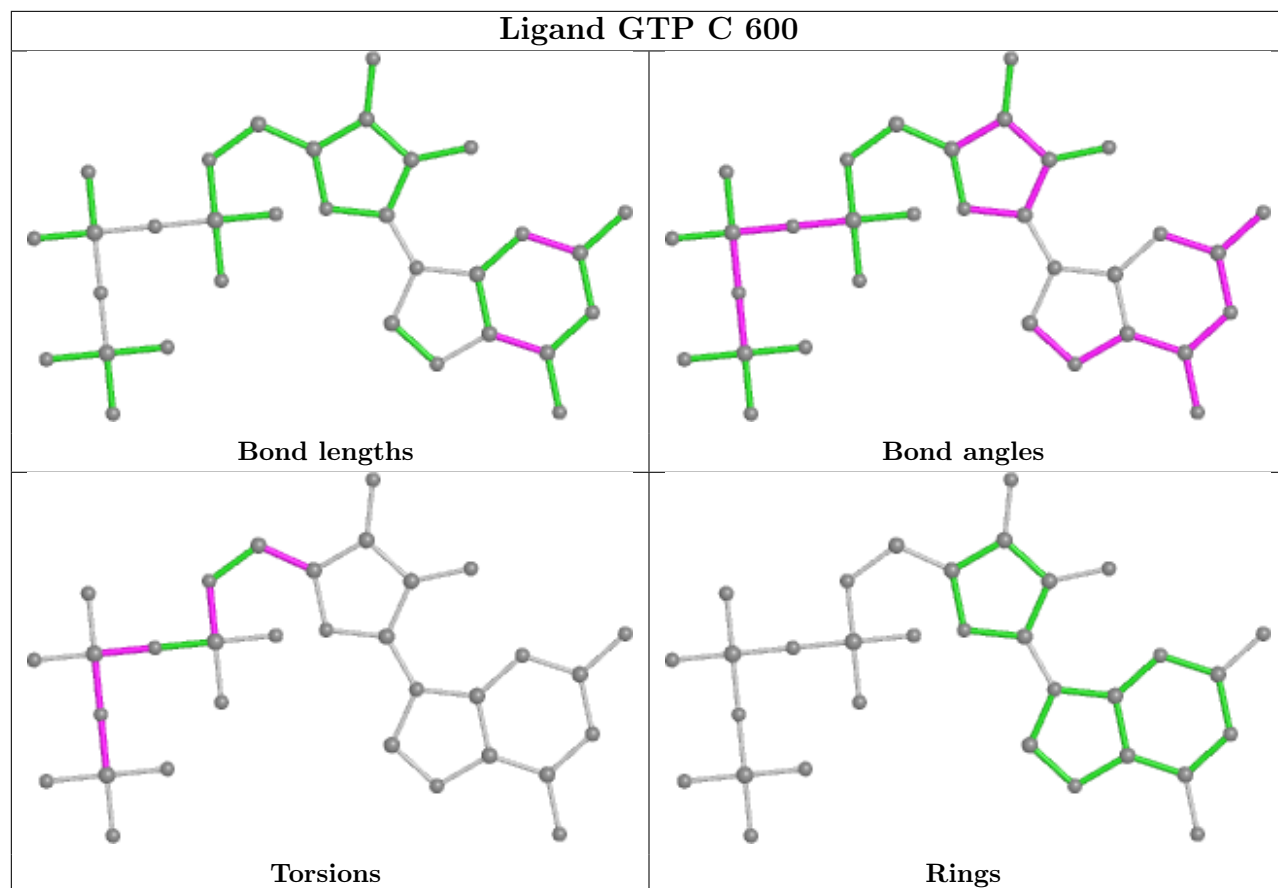
Ligand GTP A 600



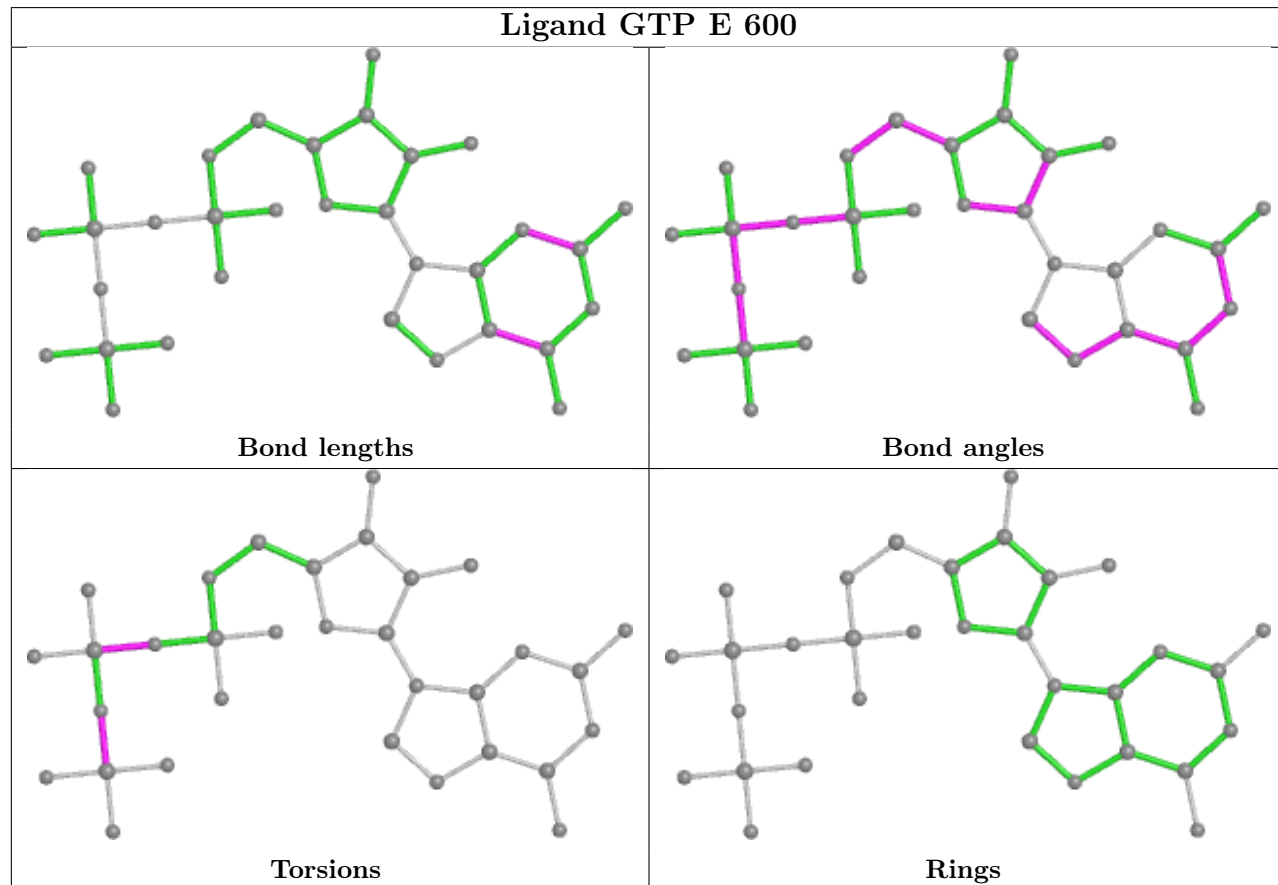
Ligand GTP G 600



Ligand GTP C 600



Ligand GTP E 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	166/169 (98%)	0.05	3 (1%) 68 49	37, 62, 88, 105	0
1	C	166/169 (98%)	0.03	0 100 100	19, 31, 56, 74	0
1	E	166/169 (98%)	-0.02	0 100 100	20, 35, 68, 83	0
1	G	166/169 (98%)	0.09	0 100 100	32, 51, 70, 80	0
2	B	330/425 (77%)	0.11	1 (0%) 94 89	21, 43, 77, 101	0
2	D	304/425 (71%)	-0.16	3 (0%) 82 70	23, 67, 106, 118	0
2	F	304/425 (71%)	-0.09	4 (1%) 77 61	23, 66, 110, 120	0
2	H	325/425 (76%)	0.14	4 (1%) 79 64	24, 44, 79, 106	0
All	All	1927/2376 (81%)	0.02	15 (0%) 86 74	19, 48, 101, 120	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	235	LEU	3.2
2	B	251	GLY	3.1
1	A	20	VAL	3.1
2	D	235	LEU	2.7
2	D	260	VAL	2.7
2	F	279	ILE	2.7
2	D	133	TYR	2.6
2	F	260	VAL	2.6
1	A	47	VAL	2.6
1	A	19	ASN	2.5
2	H	138	LEU	2.3
2	H	337	TRP	2.1
2	F	291	ILE	2.1
2	H	80	LEU	2.1
2	H	116	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(\AA^2)	Q<0.9
5	HG	H	1434	1/1	0.45	0.41	79,79,79,79	1
5	HG	B	1432	1/1	0.62	0.56	69,69,69,69	1
5	HG	F	1434	1/1	0.68	0.17	113,113,113,113	1
5	HG	B	1426	1/1	0.76	1.01	38,38,38,38	1
5	HG	G	1181	1/1	0.89	0.13	50,50,50,50	1
5	HG	H	1435	1/1	0.89	0.25	42,42,42,42	1
5	HG	C	1181	1/1	0.92	0.24	53,53,53,53	1
5	HG	B	1435	1/1	0.94	1.36	40,40,40,40	1
5	HG	E	1181	1/1	0.94	0.24	51,51,51,51	1
5	HG	B	1437	1/1	0.94	0.67	39,39,39,39	1
3	GTP	E	600	32/32	0.95	0.21	26,32,40,41	0
5	HG	A	1181	1/1	0.95	0.14	54,54,54,54	1
5	HG	F	1428	1/1	0.96	0.26	102,102,102,102	1
5	HG	F	1433	1/1	0.96	0.14	118,118,118,118	1
3	GTP	A	600	32/32	0.96	0.18	55,60,67,72	0
5	HG	F	1436	1/1	0.96	0.22	73,73,73,73	1
5	HG	D	1430	1/1	0.96	0.23	98,98,98,98	1
5	HG	D	1436	1/1	0.96	0.10	100,100,100,100	1
3	GTP	C	600	32/32	0.96	0.24	27,31,37,39	0
4	MG	G	601	1/1	0.97	0.29	45,45,45,45	0
5	HG	D	1427	1/1	0.97	0.25	85,85,85,85	1
5	HG	D	1428	1/1	0.97	0.23	96,96,96,96	1
3	GTP	G	600	32/32	0.97	0.20	40,44,47,50	0
5	HG	D	1433	1/1	0.97	0.12	82,82,82,82	1
5	HG	D	1434	1/1	0.97	0.18	80,80,80,80	1
5	HG	H	1433	1/1	0.97	0.19	43,43,43,43	1
5	HG	D	1435	1/1	0.97	0.16	109,109,109,109	1

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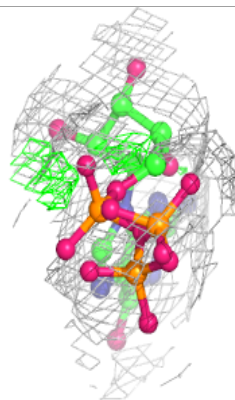
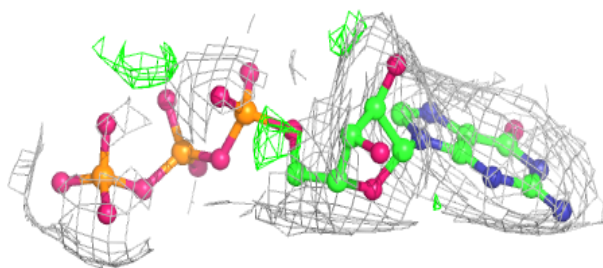
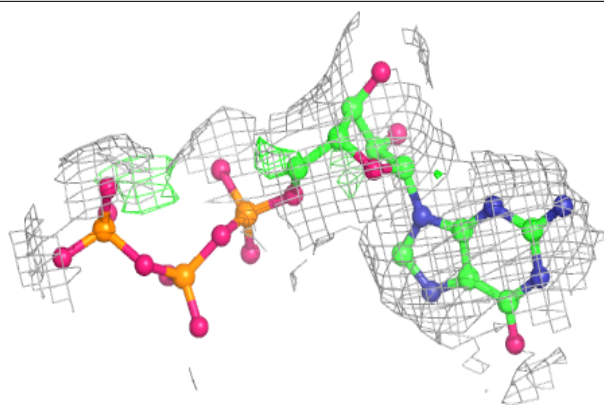
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	C	601	1/1	0.97	0.30	27,27,27,27	0
5	HG	B	1431	1/1	0.98	0.27	43,43,43,43	1
5	HG	D	1437	1/1	0.98	0.19	87,87,87,87	1
5	HG	B	1436	1/1	0.98	0.25	51,51,51,51	1
5	HG	H	1430	1/1	0.98	0.27	62,62,62,62	1
5	HG	B	1429	1/1	0.98	0.27	64,64,64,64	1
5	HG	F	1429	1/1	0.98	0.22	78,78,78,78	1
5	HG	D	1429	1/1	0.98	0.24	82,82,82,82	1
5	HG	H	1439	1/1	0.98	0.19	41,41,41,41	1
5	HG	F	1427	1/1	0.99	0.24	66,66,66,66	1
5	HG	B	1428	1/1	0.99	0.27	61,61,61,61	1
4	MG	E	601	1/1	0.99	0.21	31,31,31,31	0
5	HG	F	1430	1/1	0.99	0.23	82,82,82,82	1
5	HG	F	1431	1/1	0.99	0.21	108,108,108,108	1
5	HG	F	1432	1/1	0.99	0.14	73,73,73,73	1
5	HG	D	1431	1/1	0.99	0.16	109,109,109,109	1
5	HG	D	1432	1/1	0.99	0.19	62,62,62,62	1
5	HG	F	1435	1/1	0.99	0.17	80,80,80,80	1
4	MG	A	601	1/1	0.99	0.25	58,58,58,58	0
5	HG	F	1437	1/1	0.99	0.18	122,122,122,122	1
5	HG	F	1438	1/1	0.99	0.16	76,76,76,76	1
5	HG	F	1439	1/1	0.99	0.20	68,68,68,68	1
5	HG	B	1438	1/1	0.99	0.25	23,23,23,23	1
5	HG	H	1426	1/1	0.99	0.26	41,41,41,41	1
5	HG	H	1427	1/1	0.99	0.22	41,41,41,41	1
5	HG	H	1429	1/1	0.99	0.24	68,68,68,68	1
5	HG	B	1427	1/1	0.99	0.24	42,42,42,42	1
5	HG	H	1431	1/1	0.99	0.23	43,43,43,43	1
5	HG	H	1432	1/1	0.99	0.24	41,41,41,41	1
5	HG	D	1426	1/1	0.99	0.23	63,63,63,63	1
5	HG	B	1433	1/1	0.99	0.23	48,48,48,48	1
5	HG	B	1434	1/1	0.99	0.23	45,45,45,45	1
5	HG	H	1436	1/1	0.99	0.20	46,46,46,46	1
5	HG	H	1437	1/1	0.99	0.22	30,30,30,30	1
5	HG	H	1438	1/1	0.99	0.24	60,60,60,60	1
5	HG	F	1426	1/1	0.99	0.23	57,57,57,57	1
5	HG	H	1428	1/1	1.00	0.26	49,49,49,49	1
5	HG	B	1430	1/1	1.00	0.26	45,45,45,45	1

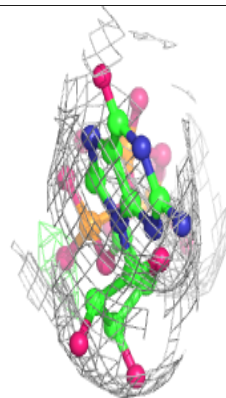
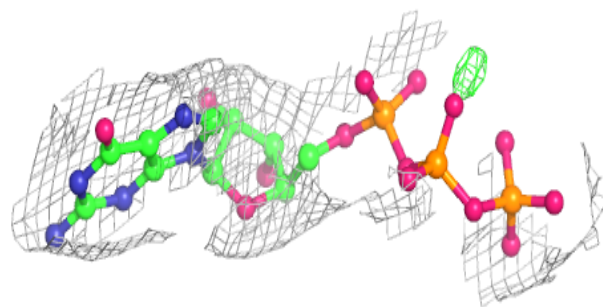
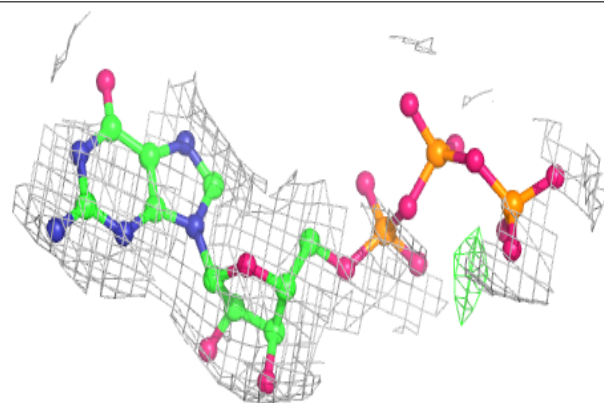
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP E 600:

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

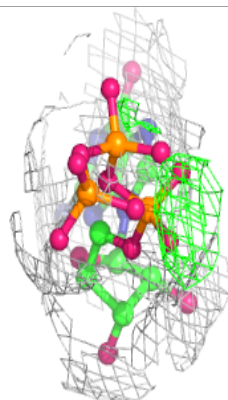
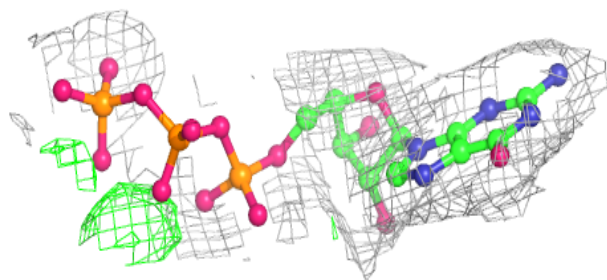
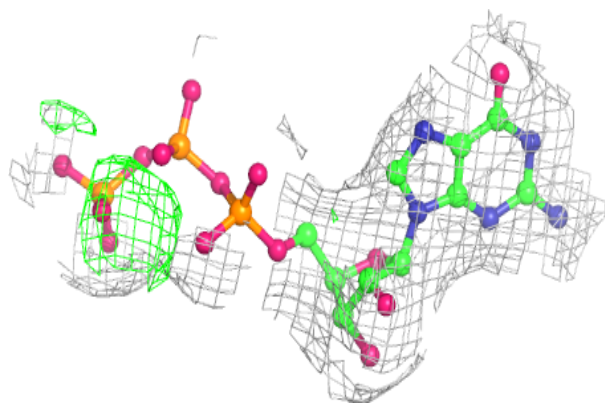
**Electron density around GTP A 600:**

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

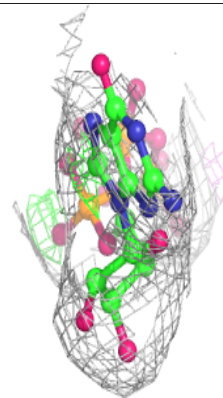
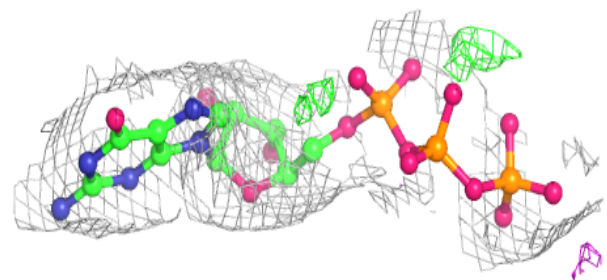
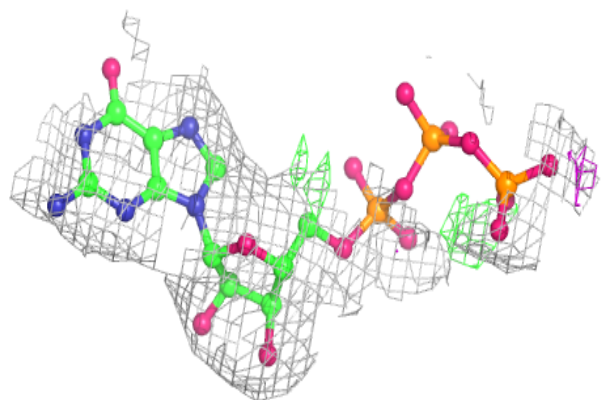


Electron density around GTP C 600:

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

**Electron density around GTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.