Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 02:37 AM EDT

PDB ID	:	4F61
Title	:	Tubulin:Stathmin-like domain complex
Authors	:	Gigant, B.; Mignot, I.; Knossow, M.
Deposited on	:	2012-05-14
Resolution	:	4.17 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 (i) 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 (i)) were used in the production of this report:

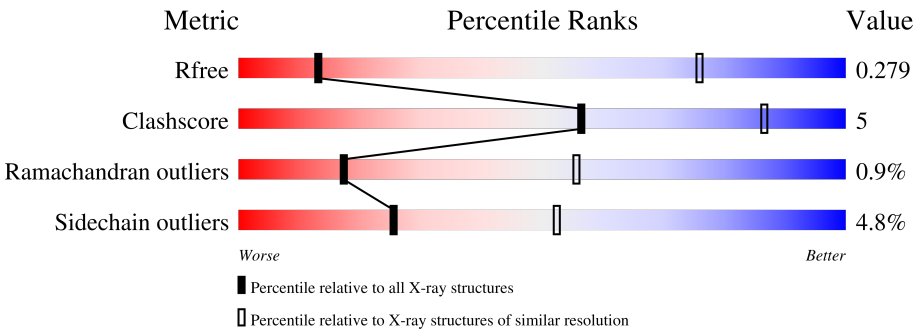
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.17 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	1034 (4.60-3.76)
Clashscore	141614	1030 (4.54-3.80)
Ramachandran outliers	138981	1006 (4.58-3.78)
Sidechain outliers	138945	1037 (4.60-3.76)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	451	82% 13% •
1	C	451	81% 14% • •
1	E	451	84% 11% • •
1	G	451	82% 13% • •
2	B	445	83% 13% • •
2	D	445	82% 14% • •
2	F	445	82% 15% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	445	80% 16%
3	I	240	63% 30%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 29129 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3380	2141	574	643	22	0	0	0
1	C	431	3352	2123	570	637	22	0	0	0
1	E	431	3352	2123	570	637	22	0	0	0
1	G	431	3352	2123	570	637	22	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
E	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
E	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
G	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
G	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	432	3383	2124	576	657	26	0	0	0
2	D	432	3383	2124	576	657	26	0	0	0
2	F	432	3383	2124	576	657	26	0	0	0
2	H	431	3375	2116	579	655	25	0	0	0

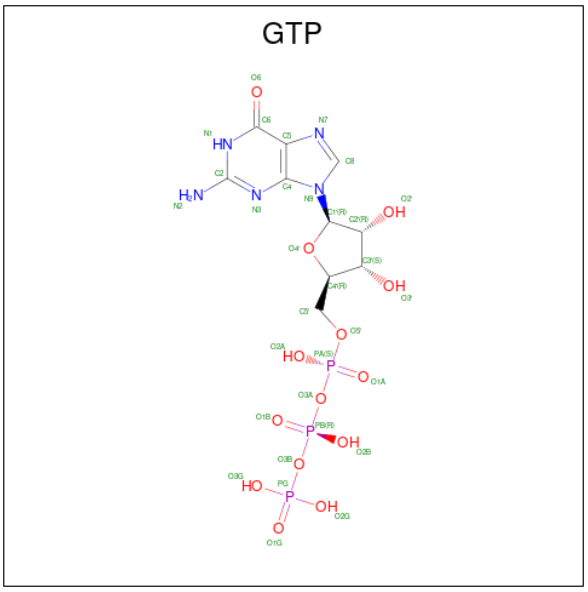
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
F	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
H	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9

- Molecule 3 is a protein called Stathmin-like domain R4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	234	1925	1185	362	369	9	0	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

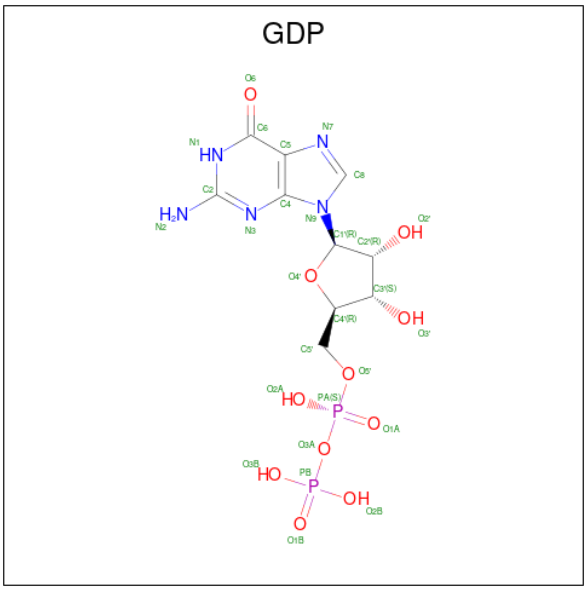


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
4	C	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
4	E	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
4	G	1	32	10	5	14	3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



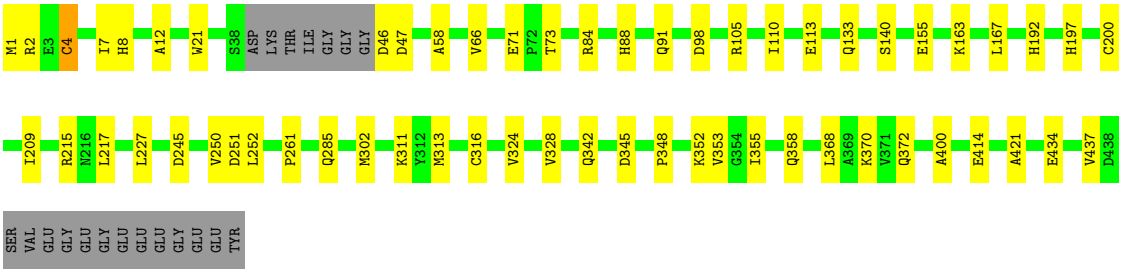
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
6	D	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
6	F	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
6	H	1	28	10	5	11	2	0	0

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. 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. 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 chain

Chain A:

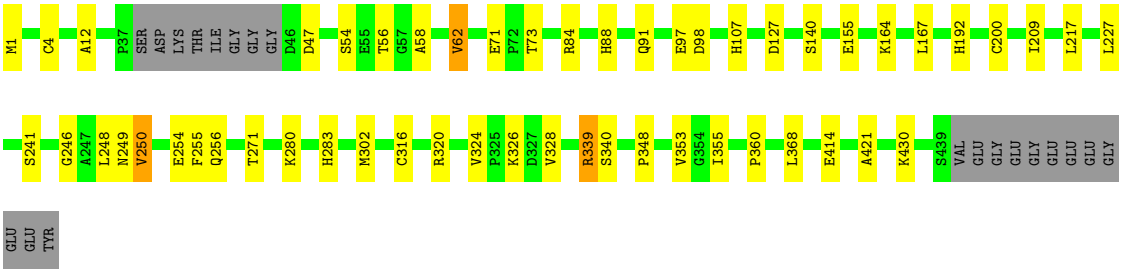


- Molecule 1: Tubulin alpha chain

Chain C:

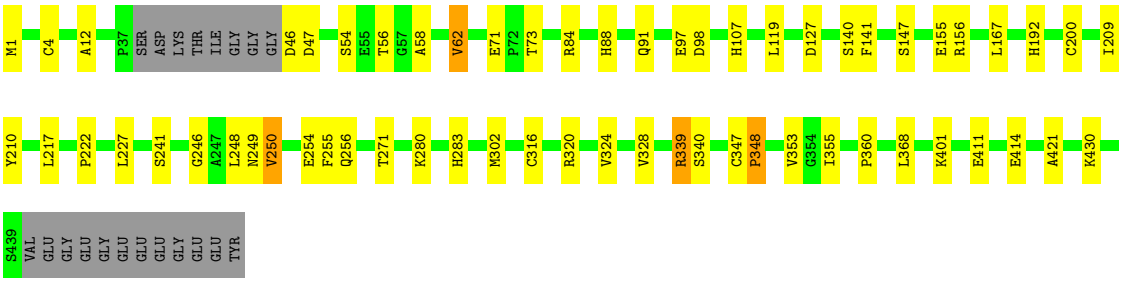
- Molecule 1: Tubulin alpha chain

Chain E:



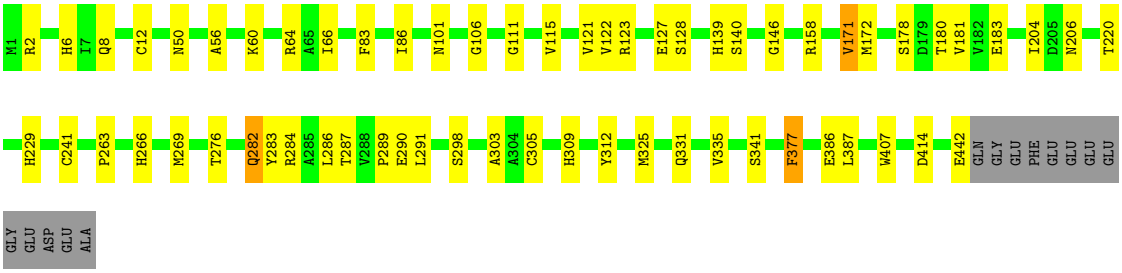
- Molecule 1: Tubulin alpha chain

Chain G:



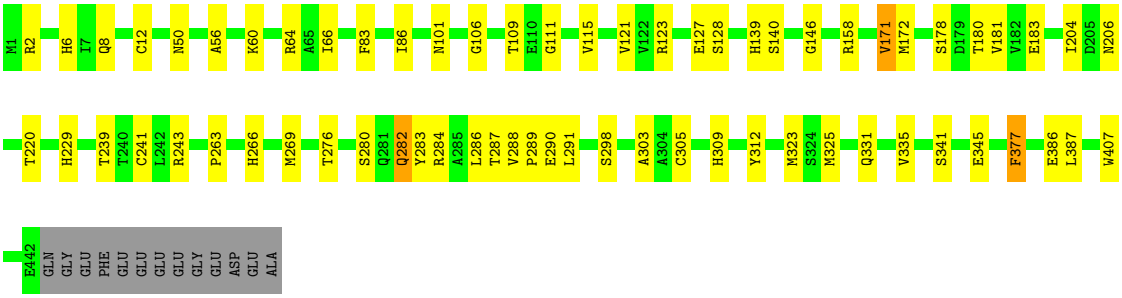
- Molecule 2: Tubulin beta chain

Chain B:



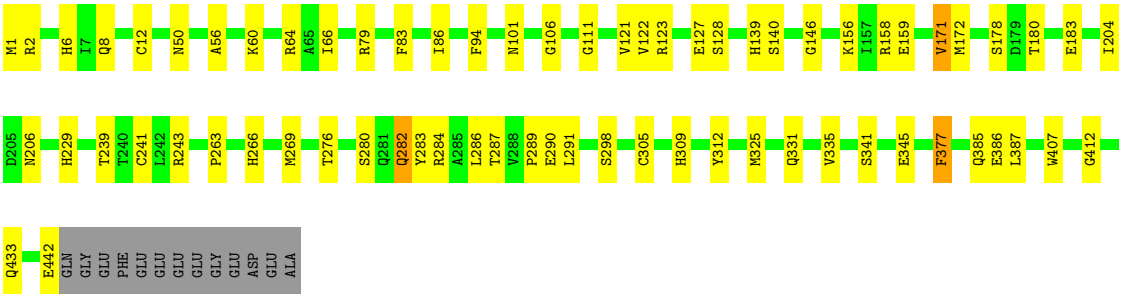
- Molecule 2: Tubulin beta chain

Chain D:



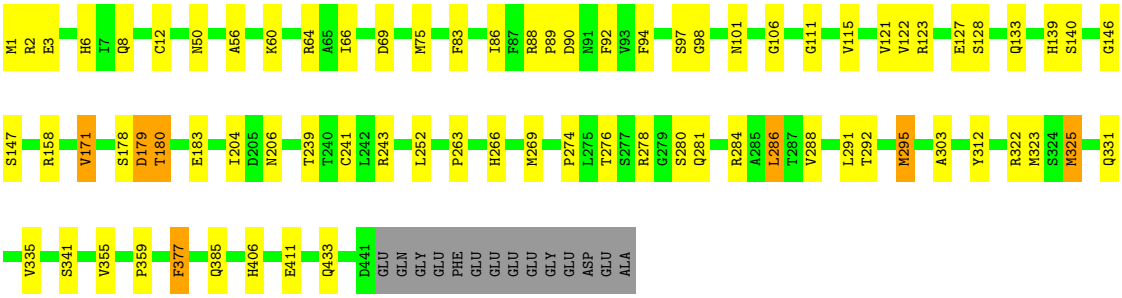
- Molecule 2: Tubulin beta chain

Chain F:



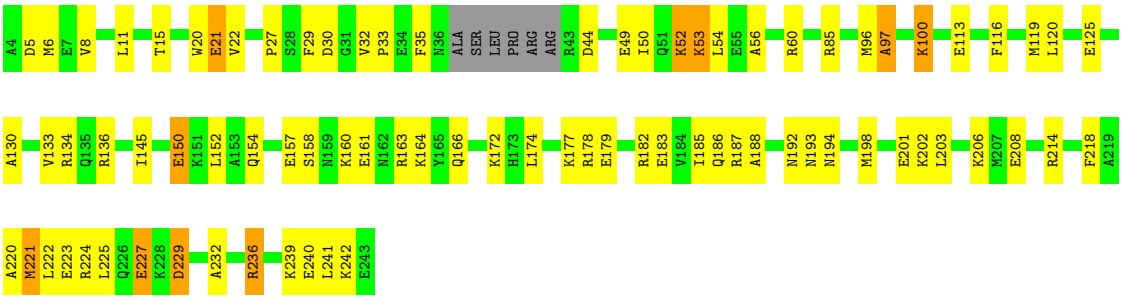
• Molecule 2: Tubulin beta chain

Chain H:



• Molecule 3: Stathmin-like domain R4

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	639.74Å 66.10Å 128.13Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	49.04 – 4.17 49.04 – 4.17	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.04-4.17) 98.7 (49.04-4.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.241 , 0.261 0.258 , 0.279	Depositor DCC
R_{free} test set	2024 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	150.8	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 182.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	29129	wwPDB-VP
Average B, all atoms (Å^2)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP, 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	0.51	0/3457	0.72	0/4693
1	C	0.45	0/3427	0.70	0/4655
1	E	0.47	0/3427	0.70	0/4655
1	G	0.52	0/3427	0.73	0/4655
2	B	0.48	0/3458	0.70	0/4686
2	D	0.44	0/3458	0.69	0/4686
2	F	0.47	0/3458	0.70	0/4686
2	H	0.63	0/3449	0.81	4/4673 (0.1%)
3	I	0.59	0/1947	0.91	0/2592
All	All	0.50	0/29508	0.73	4/39981 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	179	ASP	C-N-CA	-6.06	106.56	121.70
2	H	281	GLN	C-N-CA	5.82	136.25	121.70
2	H	180	THR	N-CA-CB	5.78	121.28	110.30
2	H	97	SER	N-CA-C	5.58	126.06	111.00

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	3380	0	3290	25	1
1	C	3352	0	3253	32	0
1	E	3352	0	3253	24	0
1	G	3352	0	3253	27	0
2	B	3383	0	3246	38	0
2	D	3383	0	3246	38	0
2	F	3383	0	3246	38	0
2	H	3375	0	3246	49	1
3	I	1925	0	1912	40	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	E	32	0	12	0	0
4	G	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	1	0
6	F	28	0	12	1	0
6	H	28	0	12	1	0
All	All	29129	0	28041	287	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (287) 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:H:1:MET:SD	2:H:1:MET:CE	2.01	1.48
1:G:250:VAL:HG23	1:G:254:GLU:HB3	1.36	1.07
1:E:250:VAL:HG23	1:E:254:GLU:HB3	1.40	1.03
1:C:250:VAL:HG23	1:C:254:GLU:HB3	1.39	1.01
2:H:286:LEU:HD12	2:H:291:LEU:HD23	1.44	0.97
2:H:295:MET:SD	2:H:377:PHE:HB2	2.09	0.92
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.66	0.78
2:H:292:THR:HG22	2:H:335:VAL:HG21	1.62	0.78
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.67	0.76
1:G:71:GLU:HB3	1:G:98:ASP:HB3	1.67	0.75
2:H:206:ASN:HD21	6:H:600:GDP:HN22	1.34	0.75
1:E:250:VAL:HG22	1:E:255:PHE:CD1	2.22	0.74
2:F:206:ASN:HD21	6:F:600:GDP:HN22	1.34	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:GLU:HB3	1:E:98:ASP:HB3	1.70	0.73
2:B:206:ASN:HD21	6:B:600:GDP:HN22	1.33	0.72
1:C:250:VAL:HG22	1:C:255:PHE:CD1	2.24	0.72
1:G:250:VAL:HG22	1:G:255:PHE:CD1	2.25	0.71
2:D:206:ASN:HD21	6:D:600:GDP:HN22	1.40	0.69
1:A:245:ASP:HB3	3:I:15:THR:HB	1.77	0.66
2:D:263:PRO:O	2:D:266:HIS:HD2	1.80	0.65
3:I:198:MET:SD	3:I:202:LYS:HD2	2.36	0.65
3:I:11:LEU:HG	3:I:20:TRP:HA	1.79	0.65
1:E:328:VAL:HG11	1:E:353:VAL:HG11	1.80	0.64
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.32	0.64
3:I:192:ASN:C	3:I:194:ASN:H	2.01	0.64
2:H:133:GLN:HE22	2:H:252:LEU:H	1.43	0.64
2:B:263:PRO:O	2:B:266:HIS:HD2	1.81	0.63
2:F:263:PRO:O	2:F:266:HIS:HD2	1.81	0.63
2:H:263:PRO:O	2:H:266:HIS:HD2	1.82	0.63
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.80	0.62
2:H:92:PHE:HD2	2:H:94:PHE:HE2	1.47	0.62
2:D:50:ASN:O	2:D:64:ARG:NH2	2.34	0.60
1:G:328:VAL:HG11	1:G:353:VAL:HG11	1.82	0.60
2:H:322:ARG:HH22	2:H:359:PRO:HD3	1.67	0.60
2:D:229:HIS:HE1	2:D:276:THR:HG23	1.66	0.60
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.67	0.59
2:H:6:HIS:HE1	2:H:8:GLN:HG3	1.67	0.59
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.83	0.59
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.68	0.58
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.68	0.58
2:F:309:HIS:HD2	2:F:386:GLU:OE1	1.86	0.58
2:F:172:MET:HG3	2:F:387:LEU:HD11	1.86	0.58
2:F:180:THR:HG23	2:F:183:GLU:HG3	1.86	0.57
1:G:248:LEU:HB2	1:G:355:ILE:H	1.69	0.57
2:F:6:HIS:HE1	2:F:8:GLN:HG3	1.70	0.57
2:B:229:HIS:HE1	2:B:276:THR:HG23	1.70	0.57
2:F:229:HIS:HE1	2:F:276:THR:HG23	1.69	0.57
1:G:88:HIS:HB2	1:G:91:GLN:HE21	1.70	0.56
2:B:180:THR:HG23	2:B:183:GLU:HG3	1.87	0.56
1:C:56:THR:HG23	1:C:58:ALA:H	1.71	0.56
2:D:180:THR:HG23	2:D:183:GLU:HG3	1.87	0.56
2:F:159:GLU:HA	3:I:174:LEU:HD13	1.88	0.56
3:I:52:LYS:O	3:I:56:ALA:HB2	2.04	0.56
1:G:56:THR:HG23	1:G:58:ALA:H	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:VAL:HG22	3:I:22:VAL:HG22	1.86	0.56
2:H:56:ALA:HB3	2:H:60:LYS:HG3	1.87	0.56
2:F:56:ALA:HB3	2:F:60:LYS:HG3	1.88	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.87	0.55
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.55
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.89	0.55
1:E:88:HIS:HB2	1:E:91:GLN:HE21	1.71	0.55
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.55	0.55
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.89	0.55
1:A:105:ARG:HB3	1:A:110:ILE:CD1	2.37	0.55
2:B:286:LEU:HD12	2:B:291:LEU:HD23	1.89	0.55
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.53	0.55
3:I:52:LYS:HE2	3:I:53:LYS:HG3	1.89	0.55
1:E:56:THR:HG23	1:E:58:ALA:H	1.72	0.54
3:I:232:ALA:O	3:I:236:ARG:HD3	2.07	0.54
2:H:286:LEU:HD12	2:H:291:LEU:CD2	2.29	0.54
2:B:282:GLN:CB	2:B:283:TYR:HA	2.37	0.54
2:H:75:MET:CB	2:H:94:PHE:CE2	2.90	0.54
2:D:309:HIS:HD2	2:D:386:GLU:OE1	1.90	0.54
2:H:295:MET:HG3	2:H:377:PHE:CD1	2.42	0.54
2:F:6:HIS:HE1	2:F:8:GLN:HE21	1.55	0.54
1:A:348:PRO:HB3	3:I:27:PRO:HD3	1.89	0.54
2:F:287:THR:HG23	2:F:289:PRO:HD2	1.89	0.54
2:H:50:ASN:O	2:H:64:ARG:NH2	2.37	0.53
2:D:286:LEU:HD12	2:D:291:LEU:HD23	1.90	0.53
2:B:50:ASN:O	2:B:64:ARG:NH2	2.36	0.53
1:E:248:LEU:HB2	1:E:355:ILE:H	1.71	0.53
2:F:286:LEU:HD12	2:F:291:LEU:HD23	1.90	0.53
2:H:6:HIS:HE1	2:H:8:GLN:HE21	1.55	0.53
1:C:54:SER:OG	1:C:62:VAL:HG13	2.08	0.52
1:G:246:GLY:H	1:G:249:ASN:HD21	1.58	0.52
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.09	0.52
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.91	0.52
2:D:139:HIS:HD2	2:D:146:GLY:O	1.93	0.52
2:H:6:HIS:CE1	2:H:8:GLN:HG3	2.44	0.52
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.43	0.52
2:D:56:ALA:HB3	2:D:60:LYS:HG3	1.91	0.52
2:D:109:THR:HG23	3:I:134:ARG:NH2	2.25	0.52
2:F:269:MET:CE	2:F:305:CYS:HB2	2.39	0.52
1:G:97:GLU:HG3	2:H:1:MET:HG2	1.92	0.52
1:G:54:SER:OG	1:G:62:VAL:HG13	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLY:H	1:C:249:ASN:HD21	1.57	0.52
1:C:248:LEU:HB2	1:C:355:ILE:H	1.74	0.52
2:B:269:MET:CE	2:B:305:CYS:HB2	2.40	0.52
2:H:180:THR:HG23	2:H:183:GLU:HG3	1.92	0.51
1:A:105:ARG:HB3	1:A:110:ILE:HD12	1.93	0.51
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.93	0.51
2:F:139:HIS:HD2	2:F:146:GLY:O	1.94	0.51
2:H:274:PRO:HB3	2:H:286:LEU:HG	1.92	0.51
3:I:160:LYS:HE2	3:I:164:LYS:HD2	1.90	0.51
3:I:185:ILE:O	3:I:188:ALA:HB3	2.10	0.51
1:E:54:SER:OG	1:E:62:VAL:HG13	2.10	0.51
2:D:282:GLN:CB	2:D:283:TYR:HA	2.40	0.51
2:B:139:HIS:HD2	2:B:146:GLY:O	1.93	0.51
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.92	0.51
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.45	0.51
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.75	0.51
2:D:269:MET:CE	2:D:305:CYS:HB2	2.41	0.51
2:H:106:GLY:O	2:H:111:GLY:HA3	2.11	0.50
2:F:50:ASN:O	2:F:64:ARG:NH2	2.38	0.50
2:H:139:HIS:HD2	2:H:146:GLY:O	1.94	0.50
2:F:6:HIS:CE1	2:F:8:GLN:HG3	2.46	0.50
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.46	0.50
2:F:282:GLN:CB	2:F:283:TYR:HA	2.41	0.50
2:F:407:TRP:CH2	1:G:256:GLN:HB3	2.47	0.50
2:D:331:GLN:O	2:D:335:VAL:HG23	2.12	0.49
2:F:106:GLY:O	2:F:111:GLY:HA3	2.11	0.49
2:H:325:MET:CE	2:H:355:VAL:HG11	2.42	0.49
3:I:116:PHE:HA	3:I:119:MET:HB2	1.94	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.49
2:D:106:GLY:O	2:D:111:GLY:HA3	2.11	0.49
1:G:107:HIS:HE1	1:G:155:GLU:OE2	1.95	0.49
2:B:331:GLN:O	2:B:335:VAL:HG23	2.13	0.49
1:E:107:HIS:HE1	1:E:155:GLU:OE2	1.95	0.49
2:B:101:ASN:HB3	2:B:180:THR:HG21	1.95	0.49
1:E:246:GLY:H	1:E:249:ASN:HD21	1.61	0.49
1:G:209:ILE:HD11	1:G:302:MET:CE	2.43	0.49
2:F:331:GLN:O	2:F:335:VAL:HG23	2.12	0.49
3:I:179:GLU:O	3:I:183:GLU:HB2	2.11	0.49
2:H:133:GLN:NE2	2:H:252:LEU:H	2.10	0.49
2:B:414:ASP:HB2	3:I:85:ARG:HH22	1.78	0.48
2:H:69:ASP:HB3	2:H:94:PHE:HD1	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.31	0.48
1:A:400:ALA:HB2	2:B:442:GLU:HG2	1.96	0.48
1:A:105:ARG:NE	1:A:110:ILE:HD11	2.27	0.48
2:F:269:MET:HE1	2:F:305:CYS:HB2	1.94	0.48
3:I:150:GLU:O	3:I:154:GLN:HB2	2.12	0.48
2:D:101:ASN:HB3	2:D:180:THR:HG21	1.95	0.48
2:H:325:MET:HE1	2:H:355:VAL:HG11	1.95	0.48
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.32	0.48
2:F:101:ASN:HB3	2:F:180:THR:HG21	1.96	0.47
2:H:178:SER:HB3	2:H:183:GLU:OE2	2.14	0.47
1:A:7:ILE:HG23	1:A:66:VAL:HG13	1.96	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.96	0.47
2:F:156:LYS:HE2	3:I:178:ARG:HD2	1.96	0.47
2:H:101:ASN:HB3	2:H:180:THR:HG21	1.96	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.97	0.47
2:F:6:HIS:CE1	2:F:8:GLN:HE21	2.33	0.47
2:H:88:ARG:NH1	2:H:90:ASP:OD1	2.47	0.47
3:I:97:ALA:HA	3:I:100:LYS:HB2	1.97	0.47
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.33	0.47
3:I:133:VAL:HG12	3:I:136:ARG:HH11	1.80	0.47
2:H:411:GLU:HA	3:I:239:LYS:HD3	1.97	0.46
2:F:123:ARG:O	2:F:127:GLU:HG2	2.15	0.46
3:I:227:GLU:C	3:I:229:ASP:H	2.19	0.46
2:D:286:LEU:HD13	2:D:290:GLU:HB3	1.97	0.46
1:A:352:LYS:HG2	3:I:21:GLU:HG3	1.98	0.46
2:H:92:PHE:CD2	2:H:94:PHE:HE2	2.30	0.46
2:H:385:GLN:HE22	2:H:433:GLN:HE21	1.63	0.46
3:I:182:ARG:HA	3:I:185:ILE:HB	1.97	0.46
1:G:167:LEU:HG	1:G:200:CYS:HB3	1.98	0.46
2:H:2:ARG:NH2	2:H:3:GLU:OE1	2.46	0.46
2:H:323:MET:O	2:H:325:MET:HE3	2.15	0.46
2:H:123:ARG:O	2:H:127:GLU:HG2	2.16	0.46
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.97	0.45
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.30	0.45
2:D:123:ARG:O	2:D:127:GLU:HG2	2.17	0.45
2:H:6:HIS:CE1	2:H:8:GLN:HE21	2.32	0.45
1:G:192:HIS:CG	1:G:421:ALA:HA	2.52	0.45
3:I:192:ASN:O	3:I:194:ASN:N	2.49	0.45
2:H:331:GLN:O	2:H:335:VAL:HG23	2.17	0.45
1:A:261:PRO:HG3	1:A:313:MET:HG3	1.98	0.45
1:A:285:GLN:NE2	1:A:372:GLN:H	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.32	0.45
1:G:209:ILE:HD11	1:G:302:MET:SD	2.57	0.45
1:G:107:HIS:NE2	3:I:206:LYS:HE3	2.32	0.45
3:I:56:ALA:HB1	3:I:60:ARG:NH1	2.31	0.45
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.57	0.44
1:G:209:ILE:HG22	1:G:227:LEU:HD22	1.99	0.44
1:G:411:GLU:C	3:I:214:ARG:HG3	2.37	0.44
2:F:83:PHE:O	2:F:86:ILE:HG22	2.17	0.44
2:F:345:GLU:H	2:F:345:GLU:HG2	1.55	0.44
2:B:269:MET:HE1	2:B:305:CYS:HB2	1.99	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.44
2:D:288:VAL:HG22	2:D:323:MET:HE3	1.99	0.44
1:E:167:LEU:HG	1:E:200:CYS:HB3	1.98	0.44
1:E:209:ILE:HG22	1:E:227:LEU:HD22	1.99	0.44
2:F:312:TYR:CE2	2:F:377:PHE:HZ	2.35	0.44
2:H:288:VAL:HG22	2:H:323:MET:HE3	2.00	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.44
2:D:407:TRP:CH2	1:E:256:GLN:HB3	2.53	0.44
1:E:209:ILE:HD11	1:E:302:MET:SD	2.58	0.44
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.99	0.43
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.43
2:B:286:LEU:HD13	2:B:290:GLU:HB3	2.00	0.43
2:D:229:HIS:CE1	2:D:276:THR:HG23	2.51	0.43
2:D:269:MET:HE1	2:D:305:CYS:HB2	2.00	0.43
2:F:12:CYS:HB3	2:F:140:SER:HB3	2.00	0.43
3:I:220:ALA:O	3:I:224:ARG:HD3	2.18	0.43
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.53	0.43
1:C:209:ILE:HD11	1:C:302:MET:CE	2.49	0.43
2:D:2:ARG:HB2	2:D:2:ARG:NH1	2.33	0.43
3:I:218:PHE:HA	3:I:221:MET:HB3	2.01	0.43
1:C:217:LEU:HD21	1:C:368:LEU:HD23	2.00	0.43
2:F:66:ILE:HG12	2:F:121:VAL:HG12	2.01	0.43
3:I:192:ASN:C	3:I:194:ASN:N	2.71	0.43
1:G:88:HIS:O	1:G:91:GLN:HG2	2.18	0.43
2:B:123:ARG:O	2:B:127:GLU:HG2	2.18	0.43
1:E:88:HIS:O	1:E:91:GLN:HG2	2.18	0.43
1:E:209:ILE:HD11	1:E:302:MET:CE	2.49	0.43
1:G:217:LEU:HD21	1:G:368:LEU:HD23	2.00	0.43
1:E:97:GLU:HG3	2:F:1:MET:HG2	2.01	0.43
2:H:292:THR:CG2	2:H:335:VAL:HG21	2.41	0.43
3:I:182:ARG:O	3:I:186:GLN:HG3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:130:ALA:O	3:I:134:ARG:HB2	2.19	0.42
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.42
1:E:217:LEU:HD21	1:E:368:LEU:HD23	2.00	0.42
2:H:171:VAL:HA	2:H:204:ILE:O	2.19	0.42
2:F:286:LEU:HD13	2:F:290:GLU:HB3	2.00	0.42
2:H:312:TYR:CE2	2:H:377:PHE:HZ	2.37	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:C:12:ALA:CB	1:C:140:SER:HB3	2.50	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.42
2:H:133:GLN:HE21	2:H:133:GLN:HB3	1.31	0.42
2:D:239:THR:O	2:D:243:ARG:HG2	2.20	0.42
1:E:192:HIS:CG	1:E:421:ALA:HA	2.55	0.42
1:A:311:LYS:HG2	1:A:342:GLN:HG2	2.02	0.42
2:B:414:ASP:HB2	3:I:85:ARG:NH2	2.34	0.42
2:H:92:PHE:HD2	2:H:94:PHE:CE2	2.34	0.42
2:H:269:MET:HG3	2:H:303:ALA:HB3	2.00	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.42
1:G:12:ALA:CB	1:G:140:SER:HB3	2.49	0.42
2:H:83:PHE:O	2:H:86:ILE:HG22	2.19	0.42
1:C:141:PHE:CE2	1:C:170:SER:HB3	2.55	0.42
1:G:141:PHE:O	1:G:147:SER:HB3	2.20	0.42
3:I:32:VAL:HB	3:I:33:PRO:HD2	2.00	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:F:2:ARG:NH1	2:F:2:ARG:HB2	2.34	0.42
2:F:385:GLN:HE22	2:F:433:GLN:HE21	1.67	0.42
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.54	0.42
2:B:269:MET:HE3	2:B:305:CYS:HB2	2.02	0.42
1:C:209:ILE:HD11	1:C:302:MET:SD	2.60	0.42
3:I:134:ARG:HD2	3:I:134:ARG:HA	1.91	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.41
2:D:220:THR:HB	1:E:326:LYS:HE3	2.02	0.41
1:C:88:HIS:H	1:C:91:GLN:NE2	2.19	0.41
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.01	0.41
1:E:12:ALA:CB	1:E:140:SER:HB3	2.50	0.41
1:C:36:MET:HA	1:C:37:PRO:HD3	1.97	0.41
1:E:88:HIS:H	1:E:91:GLN:NE2	2.18	0.41
1:E:250:VAL:CG2	1:E:255:PHE:CD1	2.99	0.41
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.03	0.41
2:F:171:VAL:HA	2:F:204:ILE:O	2.20	0.41
2:F:412:GLY:O	3:I:187:ARG:NH1	2.53	0.41
2:B:66:ILE:HG12	2:B:121:VAL:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:CYS:HA	1:C:348:PRO:HD3	1.94	0.41
2:B:181:VAL:HA	1:C:349:THR:CG2	2.50	0.41
2:B:12:CYS:HB3	2:B:140:SER:HB3	2.02	0.41
1:C:271:THR:HG22	1:C:301:GLN:HA	2.03	0.41
3:I:157:GLU:HG3	3:I:161:GLU:OE1	2.20	0.41
1:E:320:ARG:HG3	1:E:360:PRO:HD3	2.03	0.41
2:H:12:CYS:HB3	2:H:140:SER:HB3	2.02	0.41
2:B:83:PHE:O	2:B:86:ILE:HG22	2.20	0.41
2:B:220:THR:HB	1:C:326:LYS:HE3	2.02	0.41
1:C:271:THR:OG1	1:C:377:MET:HB3	2.21	0.41
2:H:66:ILE:HG12	2:H:121:VAL:HG12	2.01	0.41
3:I:6:MET:SD	3:I:22:VAL:HG13	2.61	0.41
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.68	0.40
1:A:12:ALA:CB	1:A:140:SER:HB3	2.52	0.40
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.03	0.40
1:G:320:ARG:HG3	1:G:360:PRO:HD3	2.03	0.40
1:C:88:HIS:O	1:C:91:GLN:HG2	2.22	0.40
2:D:345:GLU:H	2:D:345:GLU:HG2	1.58	0.40
2:F:239:THR:O	2:F:243:ARG:HG2	2.22	0.40
2:H:239:THR:O	2:H:243:ARG:HG2	2.21	0.40
2:F:79:ARG:HH22	2:F:94:PHE:HE2	1.69	0.40
1:G:119:LEU:HD11	1:G:156:ARG:HB3	2.02	0.40
1:G:347:CYS:HA	1:G:348:PRO:HD3	1.94	0.40
1:A:209:ILE:HD11	1:A:302:MET:CE	2.51	0.40
2:H:295:MET:HG3	2:H:377:PHE:HD1	1.86	0.40
1:A:355:ILE:HD11	3:I:20:TRP:HH2	1.87	0.40
1:C:320:ARG:HG3	1:C:360:PRO:HD3	2.03	0.40
1:G:210:TYR:CZ	1:G:222:PRO:HD2	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ALA:CB	2:H:89:PRO:O[2_556]	2.04	0.16

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/451 (95%)	410 (96%)	15 (4%)	2 (0%)	29	68
1	C	427/451 (95%)	405 (95%)	17 (4%)	5 (1%)	13	50
1	E	427/451 (95%)	406 (95%)	16 (4%)	5 (1%)	13	50
1	G	427/451 (95%)	405 (95%)	17 (4%)	5 (1%)	13	50
2	B	430/445 (97%)	413 (96%)	15 (4%)	2 (0%)	29	68
2	D	430/445 (97%)	413 (96%)	14 (3%)	3 (1%)	22	62
2	F	430/445 (97%)	412 (96%)	15 (4%)	3 (1%)	22	62
2	H	429/445 (96%)	412 (96%)	14 (3%)	3 (1%)	22	62
3	I	230/240 (96%)	192 (84%)	32 (14%)	6 (3%)	5	35
All	All	3657/3824 (96%)	3468 (95%)	155 (4%)	34 (1%)	17	55

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	282	GLN
1	C	348	PRO
2	D	282	GLN
1	E	348	PRO
2	F	282	GLN
1	G	348	PRO
1	A	47	ASP
1	A	437	VAL
1	C	47	ASP
1	C	339	ARG
1	E	47	ASP
1	E	339	ARG
1	G	47	ASP
1	G	339	ARG
2	H	98	GLY
3	I	193	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	280	LYS
1	E	280	LYS
1	G	280	LYS
2	H	280	SER
1	C	283	HIS
2	D	280	SER
2	D	284	ARG
1	E	283	HIS
1	G	283	HIS
3	I	35	PHE
2	B	284	ARG
2	F	280	SER
2	F	284	ARG
2	H	278	ARG
3	I	30	ASP
3	I	96	MET
3	I	97	ALA
3	I	44	ASP

5.3.2 Protein sidechains (i)

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	365/379 (96%)	348 (95%)	17 (5%)	26	53
1	C	359/379 (95%)	342 (95%)	17 (5%)	26	53
1	E	359/379 (95%)	343 (96%)	16 (4%)	27	54
1	G	359/379 (95%)	342 (95%)	17 (5%)	26	53
2	B	369/383 (96%)	358 (97%)	11 (3%)	41	63
2	D	369/383 (96%)	358 (97%)	11 (3%)	41	63
2	F	369/383 (96%)	358 (97%)	11 (3%)	41	63
2	H	369/383 (96%)	353 (96%)	16 (4%)	29	55
3	I	198/212 (93%)	165 (83%)	33 (17%)	2	14
All	All	3116/3260 (96%)	2967 (95%)	149 (5%)	25	52

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	4	CYS
1	A	46	ASP
1	A	73	THR
1	A	84	ARG
1	A	113	GLU
1	A	163	LYS
1	A	215	ARG
1	A	250	VAL
1	A	316	CYS
1	A	324	VAL
1	A	345	ASP
1	A	358	GLN
1	A	370	LYS
1	A	414	GLU
1	A	434	GLU
2	B	115	VAL
2	B	122	VAL
2	B	128	SER
2	B	158	ARG
2	B	171	VAL
2	B	178	SER
2	B	241	CYS
2	B	298	SER
2	B	325	MET
2	B	341	SER
2	B	377	PHE
1	C	1	MET
1	C	4	CYS
1	C	46	ASP
1	C	62	VAL
1	C	73	THR
1	C	84	ARG
1	C	127	ASP
1	C	164	LYS
1	C	241	SER
1	C	250	VAL
1	C	271	THR
1	C	316	CYS
1	C	324	VAL
1	C	339	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	340	SER
1	C	414	GLU
1	C	430	LYS
2	D	115	VAL
2	D	128	SER
2	D	158	ARG
2	D	171	VAL
2	D	178	SER
2	D	181	VAL
2	D	241	CYS
2	D	298	SER
2	D	325	MET
2	D	341	SER
2	D	377	PHE
1	E	1	MET
1	E	4	CYS
1	E	62	VAL
1	E	73	THR
1	E	84	ARG
1	E	127	ASP
1	E	164	LYS
1	E	241	SER
1	E	250	VAL
1	E	271	THR
1	E	316	CYS
1	E	324	VAL
1	E	339	ARG
1	E	340	SER
1	E	414	GLU
1	E	430	LYS
2	F	122	VAL
2	F	128	SER
2	F	158	ARG
2	F	171	VAL
2	F	178	SER
2	F	241	CYS
2	F	298	SER
2	F	325	MET
2	F	341	SER
2	F	377	PHE
2	F	442	GLU
1	G	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	4	CYS
1	G	46	ASP
1	G	62	VAL
1	G	73	THR
1	G	84	ARG
1	G	127	ASP
1	G	241	SER
1	G	250	VAL
1	G	271	THR
1	G	316	CYS
1	G	324	VAL
1	G	339	ARG
1	G	340	SER
1	G	401	LYS
1	G	414	GLU
1	G	430	LYS
2	H	115	VAL
2	H	122	VAL
2	H	128	SER
2	H	147	SER
2	H	158	ARG
2	H	171	VAL
2	H	179	ASP
2	H	241	CYS
2	H	276	THR
2	H	284	ARG
2	H	286	LEU
2	H	295	MET
2	H	325	MET
2	H	341	SER
2	H	377	PHE
2	H	406	HIS
3	I	5	ASP
3	I	21	GLU
3	I	29	PHE
3	I	49	GLU
3	I	50	ILE
3	I	52	LYS
3	I	53	LYS
3	I	54	LEU
3	I	100	LYS
3	I	113	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	120	LEU
3	I	125	GLU
3	I	145	ILE
3	I	150	GLU
3	I	152	LEU
3	I	158	SER
3	I	163	ARG
3	I	166	GLN
3	I	172	LYS
3	I	177	LYS
3	I	201	GLU
3	I	203	LEU
3	I	208	GLU
3	I	221	MET
3	I	222	LEU
3	I	223	GLU
3	I	225	LEU
3	I	227	GLU
3	I	229	ASP
3	I	236	ARG
3	I	240	GLU
3	I	241	LEU
3	I	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	91	GLN
1	A	107	HIS
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	358	GLN
1	A	372	GLN
2	B	6	HIS
2	B	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	14	ASN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	309	HIS
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	15	GLN
1	C	91	GLN
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	301	GLN
1	C	358	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	136	GLN
2	D	139	HIS
2	D	206	ASN
2	D	229	HIS
2	D	266	HIS
2	D	309	HIS
2	D	385	GLN
2	D	433	GLN
1	E	8	HIS
1	E	15	GLN
1	E	91	GLN
1	E	107	HIS
1	E	133	GLN
1	E	139	HIS
1	E	197	HIS
1	E	249	ASN
1	E	301	GLN
1	E	358	GLN
2	F	6	HIS
2	F	8	GLN
2	F	14	ASN
2	F	139	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	206	ASN
2	F	229	HIS
2	F	266	HIS
2	F	309	HIS
2	F	385	GLN
2	F	433	GLN
1	G	8	HIS
1	G	15	GLN
1	G	91	GLN
1	G	107	HIS
1	G	133	GLN
1	G	139	HIS
1	G	197	HIS
1	G	249	ASN
1	G	301	GLN
1	G	329	ASN
1	G	358	GLN
2	H	6	HIS
2	H	8	GLN
2	H	14	ASN
2	H	133	GLN
2	H	139	HIS
2	H	206	ASN
2	H	247	GLN
2	H	266	HIS
2	H	385	GLN
2	H	433	GLN
3	I	205	GLN

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 12 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	GTP	A	600	5	26,34,34	0.73	0	32,54,54	0.58	0
6	GDP	B	600	-	24,30,30	0.80	1 (4%)	30,47,47	0.60	0
4	GTP	E	600	5	26,34,34	0.71	0	32,54,54	0.63	0
4	GTP	G	600	5	26,34,34	0.76	0	32,54,54	0.69	0
6	GDP	H	600	-	24,30,30	0.92	2 (8%)	30,47,47	0.82	0
6	GDP	F	600	-	24,30,30	0.73	0	30,47,47	0.69	0
4	GTP	C	600	5	26,34,34	0.70	0	32,54,54	0.57	0
6	GDP	D	600	-	24,30,30	0.93	1 (4%)	30,47,47	0.66	0

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
4	GTP	A	600	5	-	6/18/38/38	0/3/3/3
6	GDP	B	600	-	-	5/12/32/32	0/3/3/3
4	GTP	E	600	5	-	5/18/38/38	0/3/3/3
4	GTP	G	600	5	-	5/18/38/38	0/3/3/3
6	GDP	H	600	-	-	4/12/32/32	0/3/3/3
6	GDP	F	600	-	-	4/12/32/32	0/3/3/3
4	GTP	C	600	5	-	6/18/38/38	0/3/3/3
6	GDP	D	600	-	-	5/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	GDP	PB-O1B	3.17	1.60	1.50
6	H	600	GDP	C5-C6	-2.45	1.42	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	600	GDP	PB-O2B	2.13	1.63	1.54
6	B	600	GDP	C8-N7	-2.03	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	C5'-O5'-PA-O1A
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
4	E	600	GTP	PB-O3B-PG-O3G
4	E	600	GTP	C5'-O5'-PA-O1A
4	E	600	GTP	C5'-O5'-PA-O2A
4	G	600	GTP	PB-O3B-PG-O3G
4	G	600	GTP	C5'-O5'-PA-O1A
4	G	600	GTP	C5'-O5'-PA-O2A
6	B	600	GDP	C5'-O5'-PA-O1A
6	B	600	GDP	C5'-O5'-PA-O2A
6	D	600	GDP	C5'-O5'-PA-O1A
6	D	600	GDP	C5'-O5'-PA-O2A
6	F	600	GDP	C5'-O5'-PA-O1A
6	F	600	GDP	C5'-O5'-PA-O2A
6	H	600	GDP	C5'-O5'-PA-O1A
6	H	600	GDP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3B-PG-O3G
4	C	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
4	E	600	GTP	PB-O3A-PA-O2A
4	G	600	GTP	PB-O3A-PA-O2A
6	H	600	GDP	PB-O3A-PA-O2A
6	B	600	GDP	PB-O3A-PA-O2A
6	F	600	GDP	PB-O3A-PA-O2A
4	A	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O3A
4	E	600	GTP	C5'-O5'-PA-O3A
4	G	600	GTP	C5'-O5'-PA-O3A
6	B	600	GDP	C5'-O5'-PA-O3A
6	D	600	GDP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	F	600	GDP	C5'-O5'-PA-O3A
6	H	600	GDP	C5'-O5'-PA-O3A
4	A	600	GTP	PB-O3A-PA-O1A
4	C	600	GTP	PB-O3A-PA-O1A
6	B	600	GDP	PB-O3A-PA-O1A
6	D	600	GDP	PB-O3A-PA-O1A
6	D	600	GDP	PB-O3A-PA-O2A

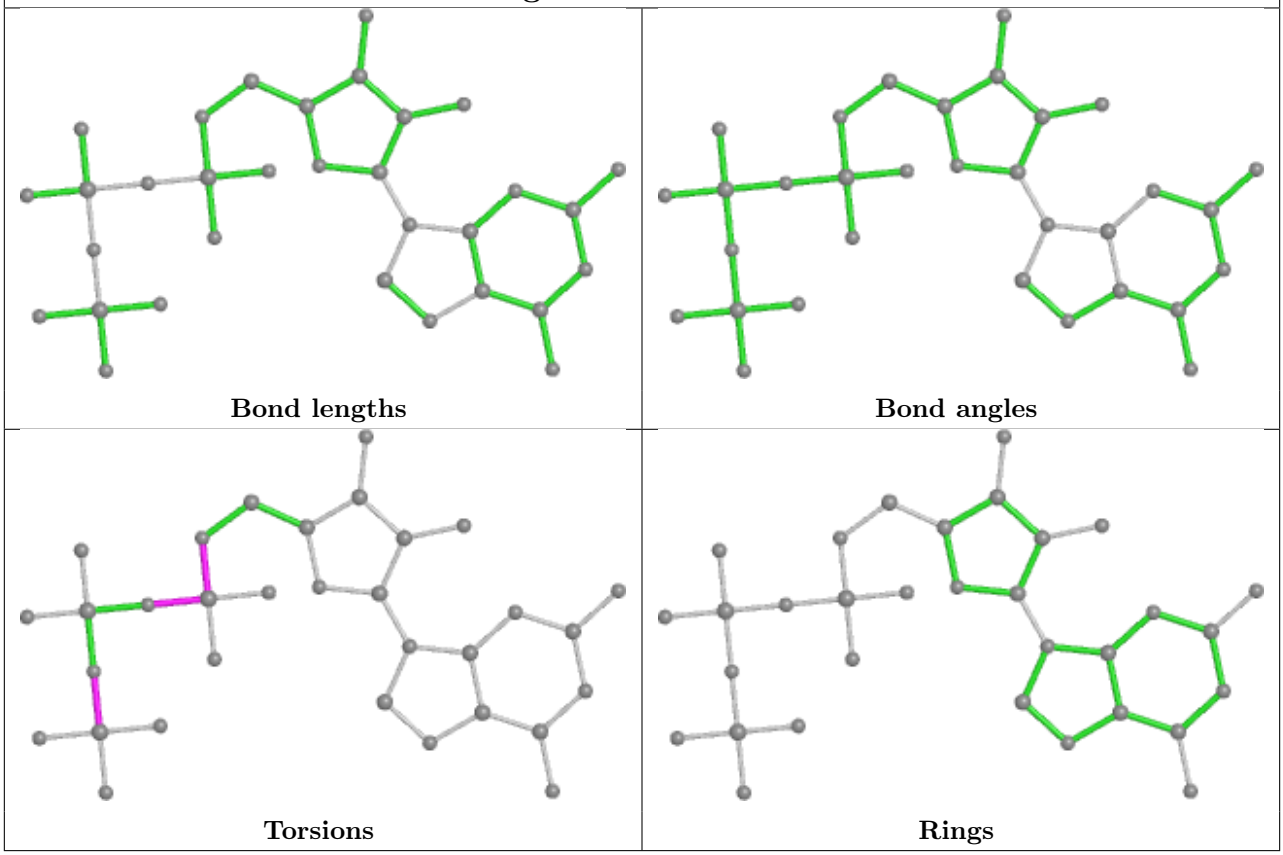
There are no ring outliers.

4 monomers are involved in 4 short contacts:

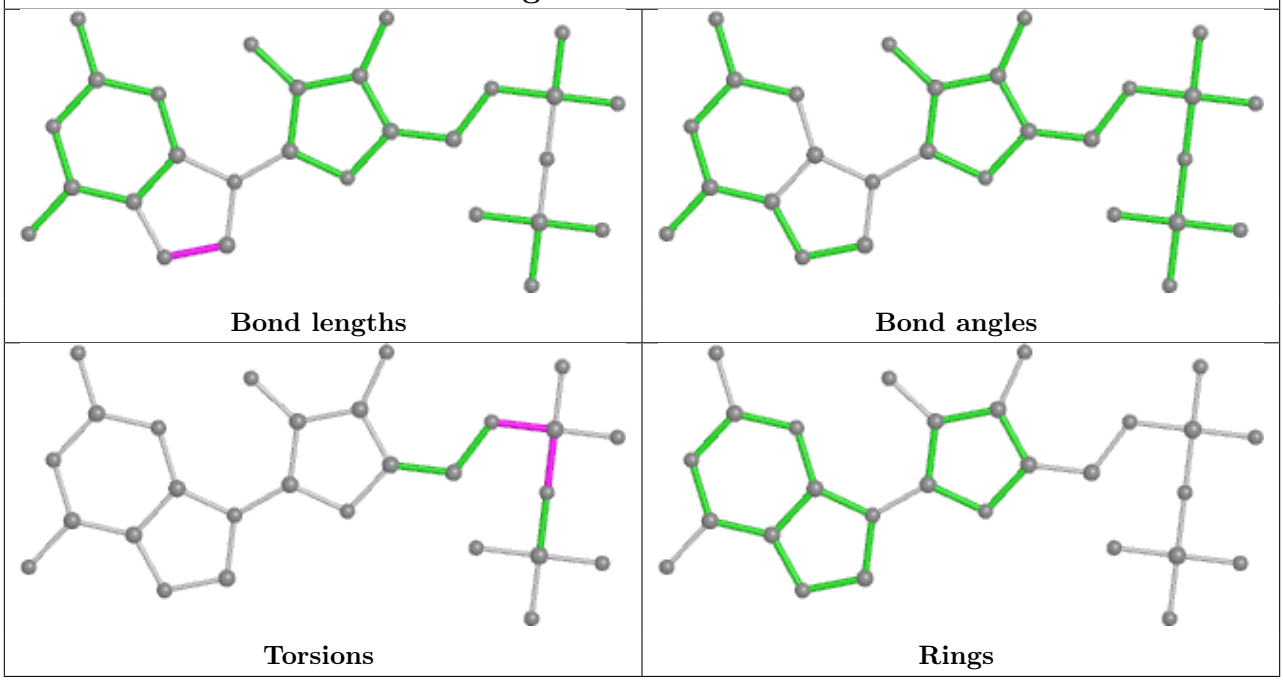
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	600	GDP	1	0
6	H	600	GDP	1	0
6	F	600	GDP	1	0
6	D	600	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

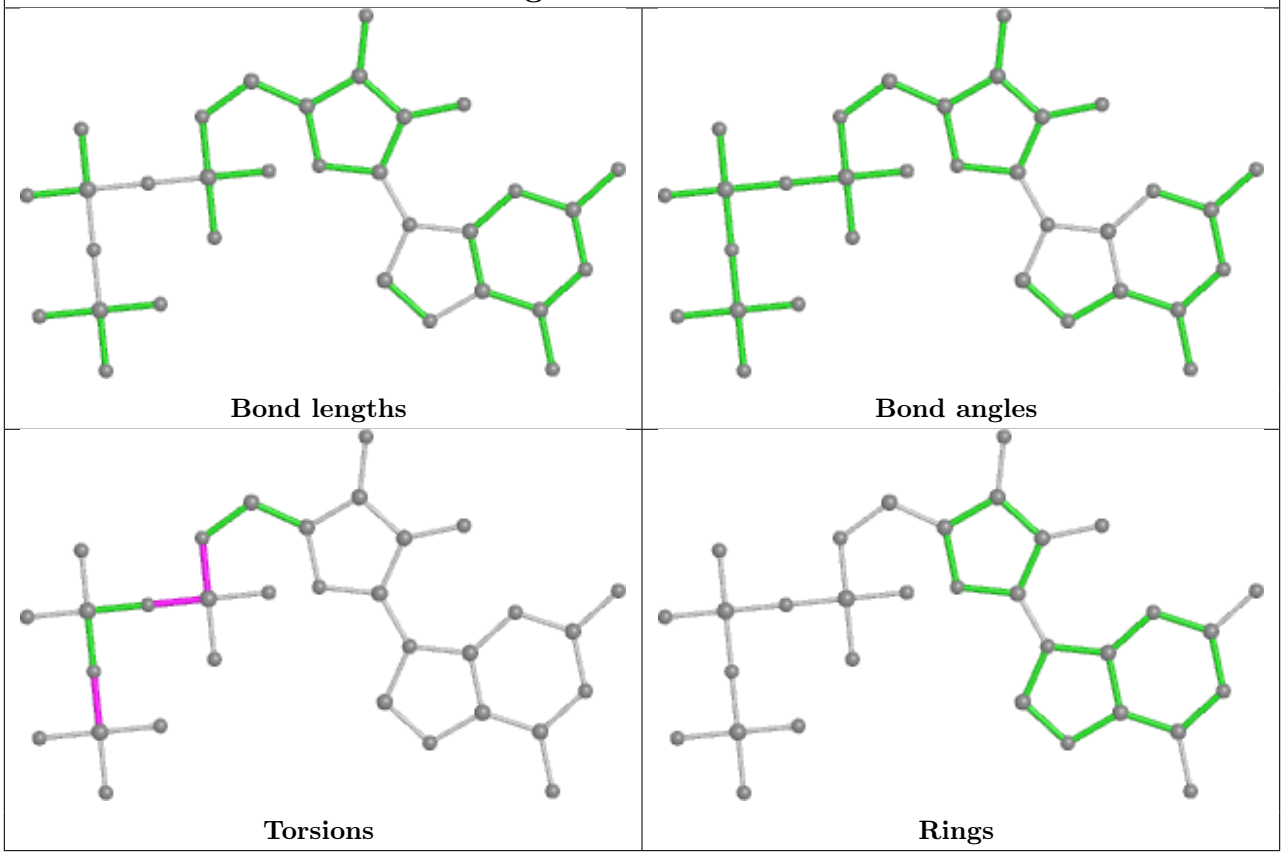
Ligand GTP A 600



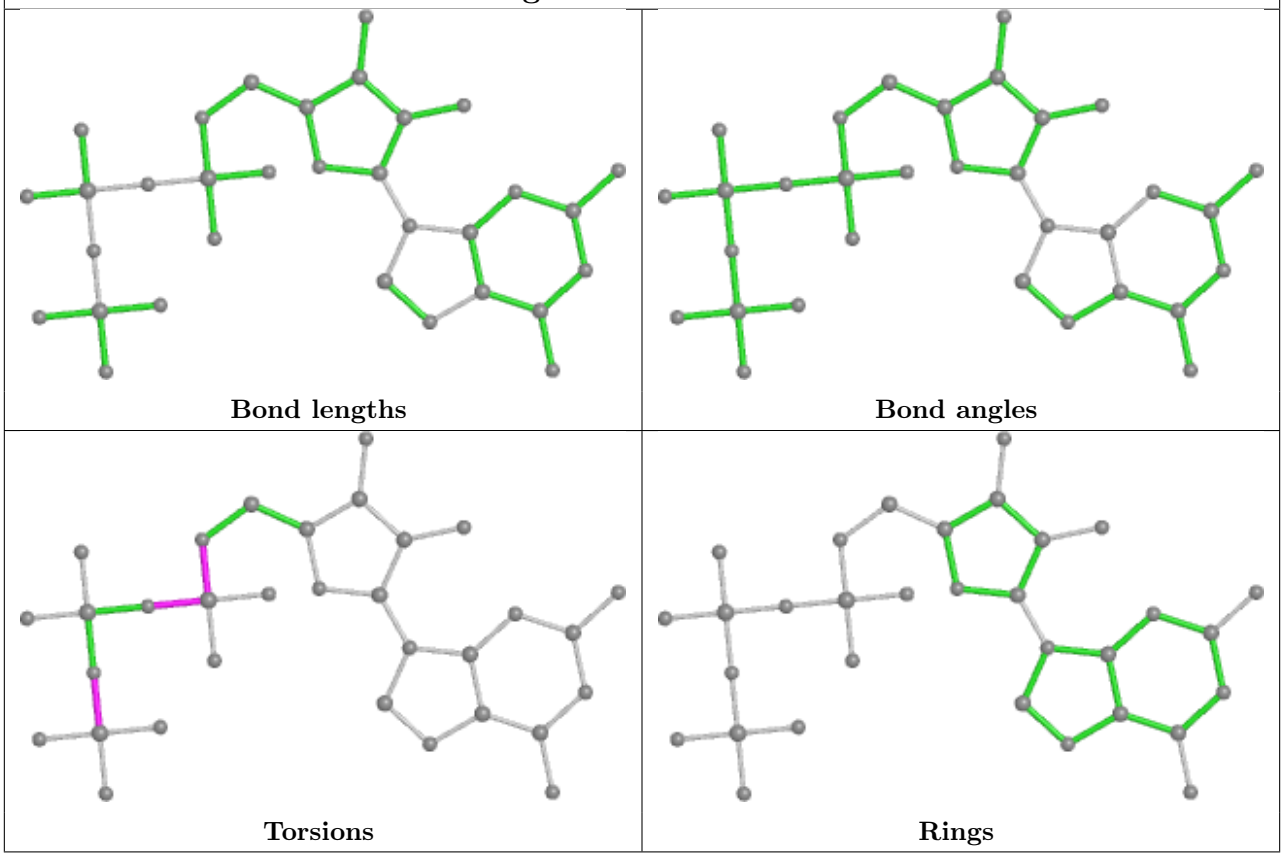
Ligand GDP B 600



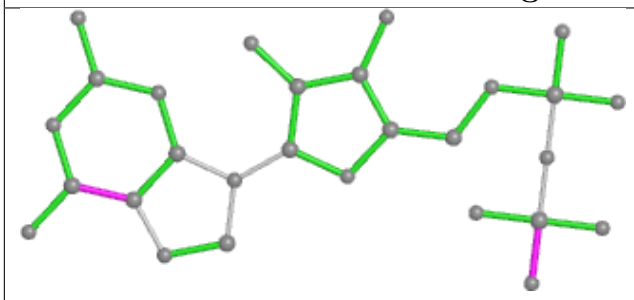
Ligand GTP E 600



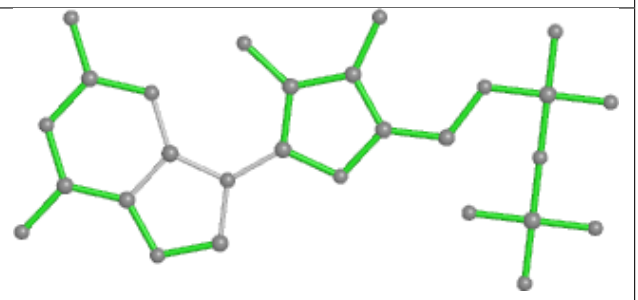
Ligand GTP G 600



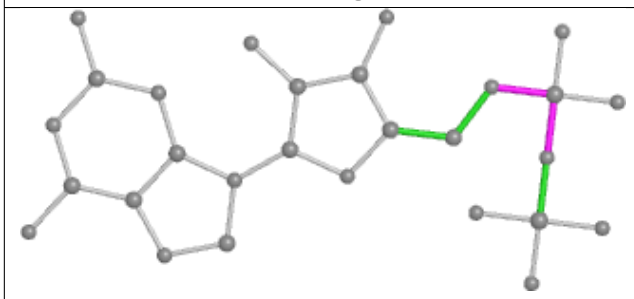
Ligand GDP H 600



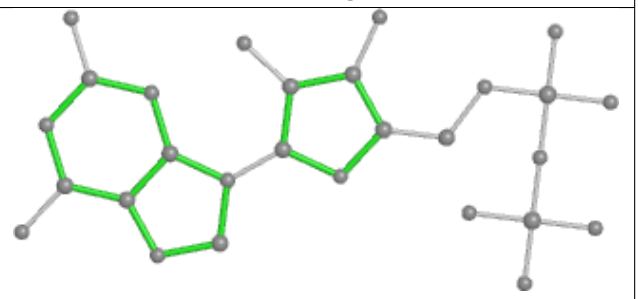
Bond lengths



Bond angles

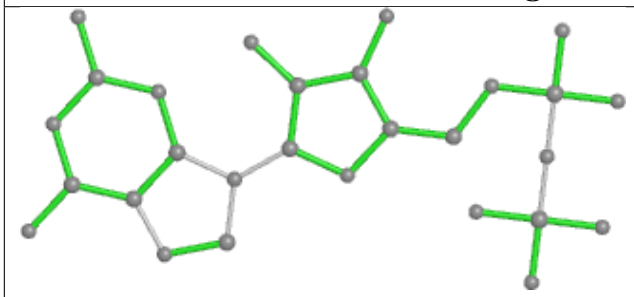


Torsions

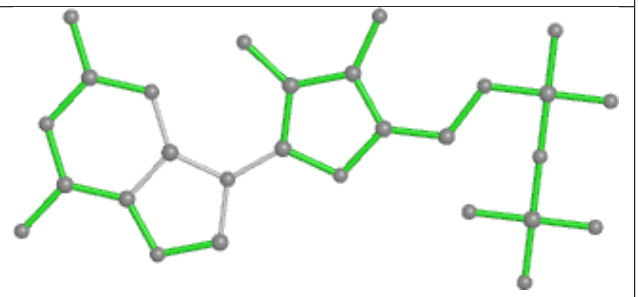


Rings

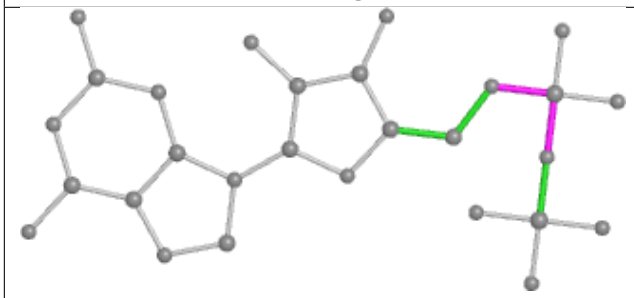
Ligand GDP F 600



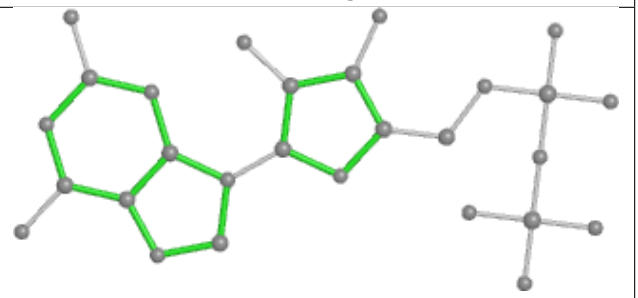
Bond lengths



Bond angles

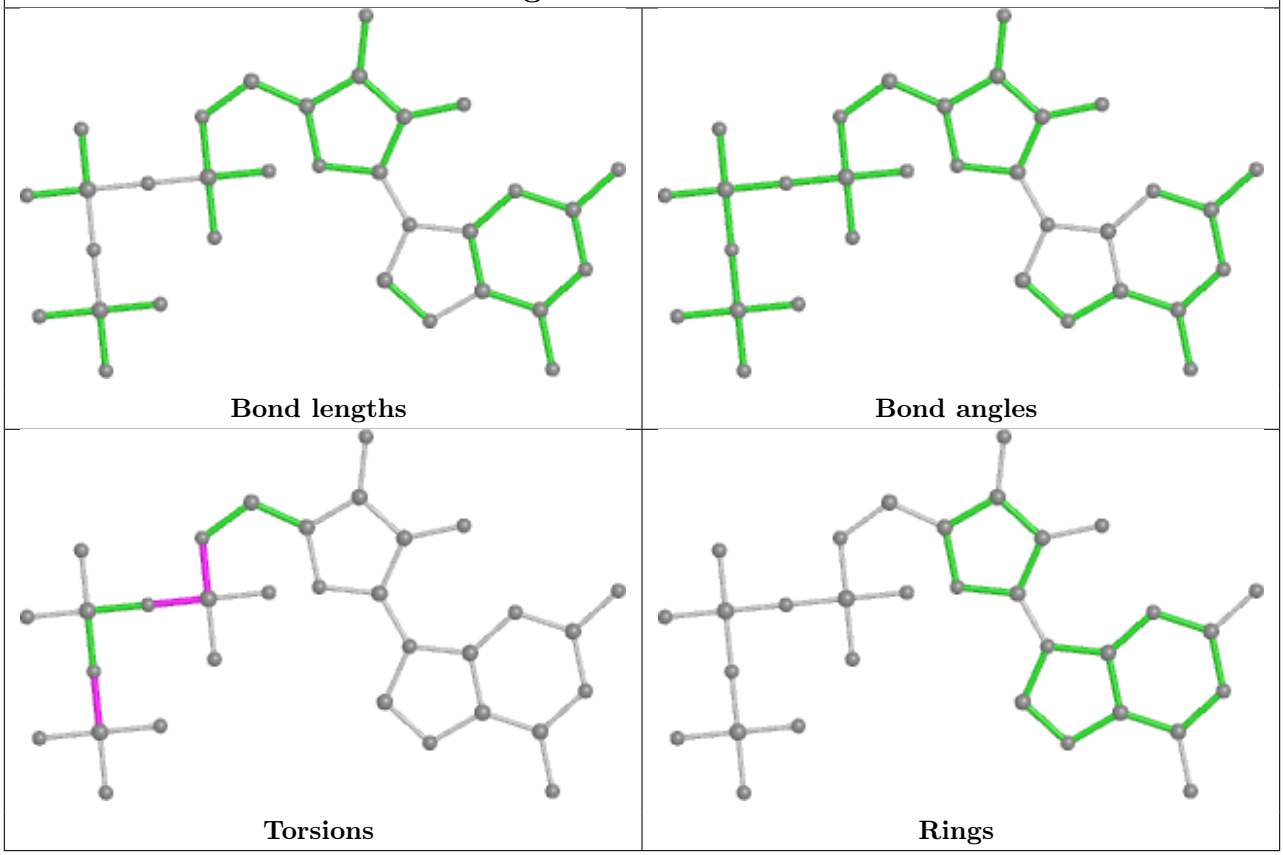


Torsions

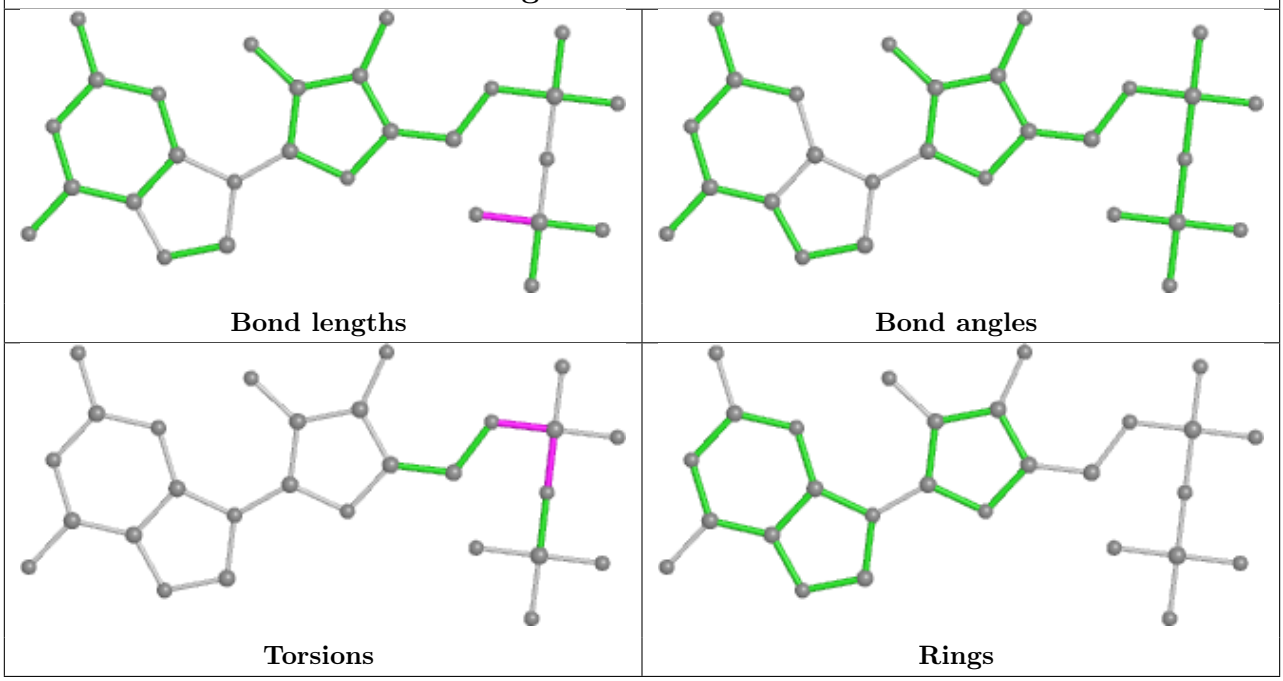


Rings

Ligand GTP C 600



Ligand GDP D 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

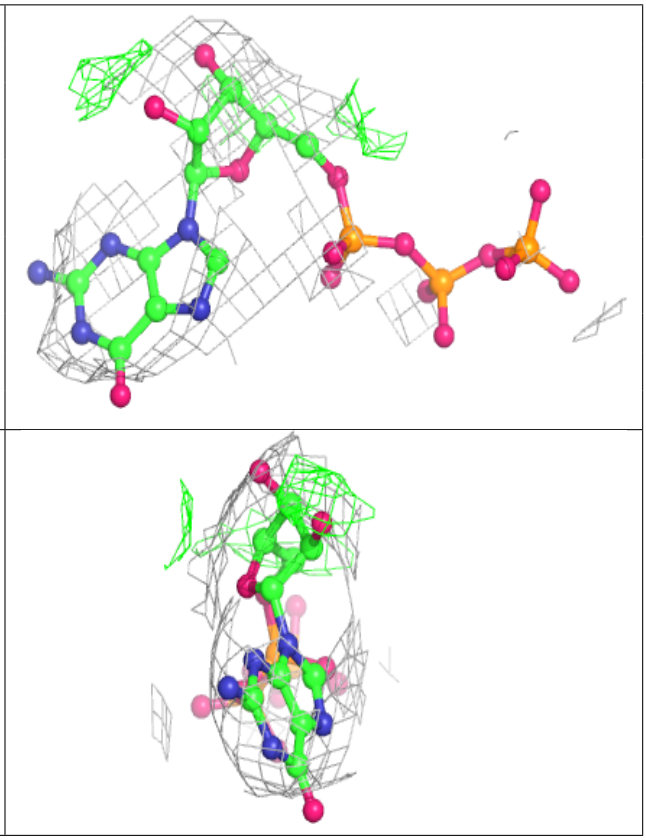
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

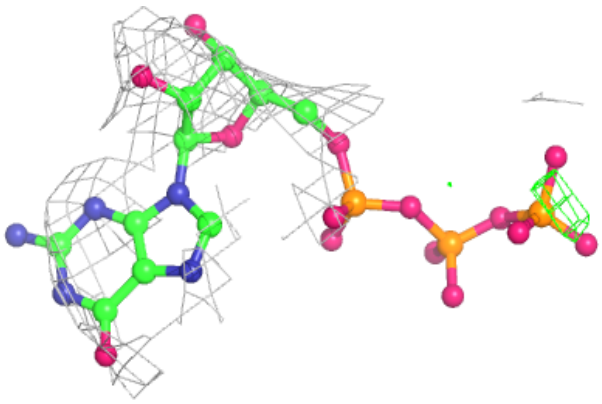
Electron density around GTP A 600:

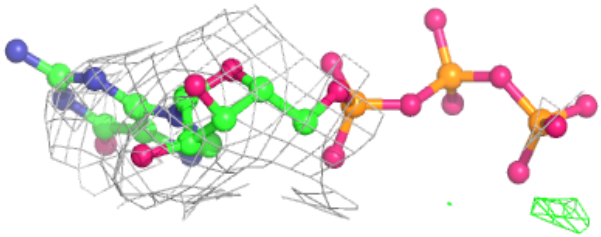
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

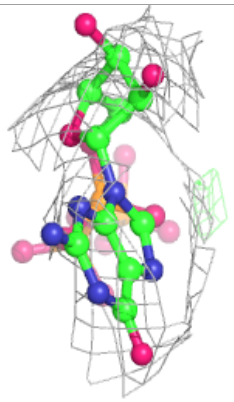


Electron density around GTP C 600:

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

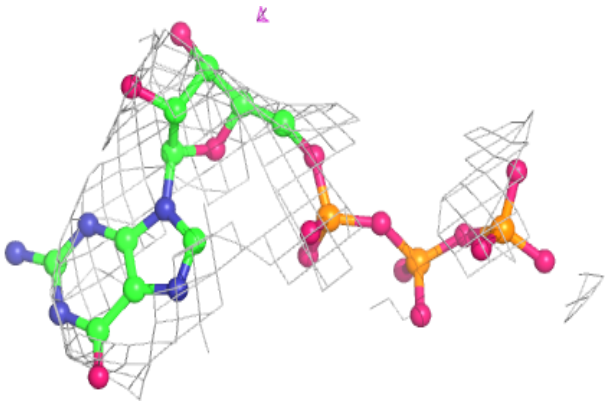


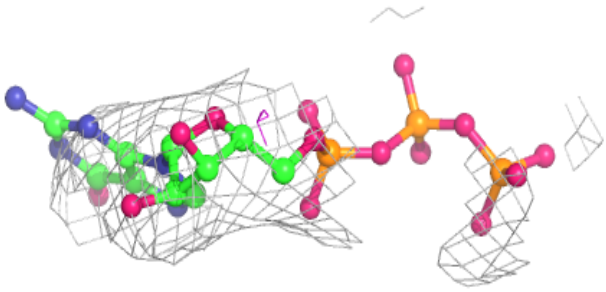


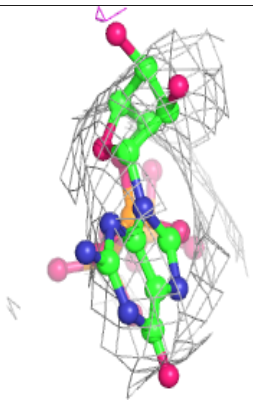


Electron density around GTP E 600:

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

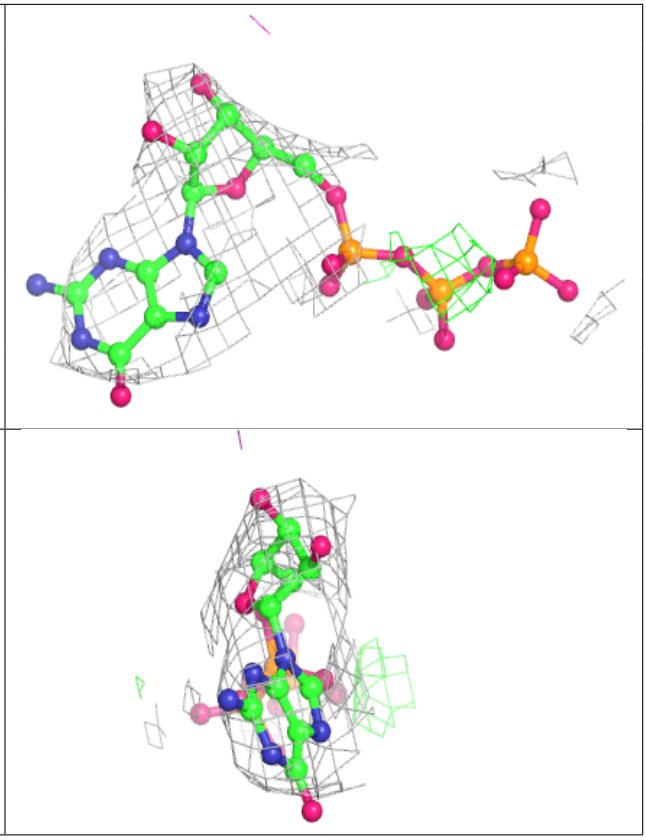






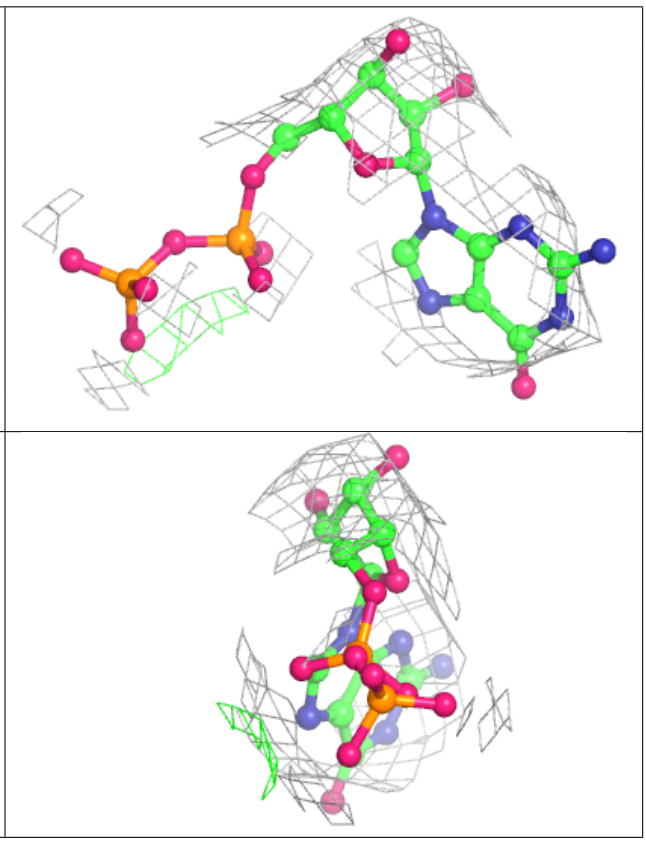
Electron density around GTP G 600:

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



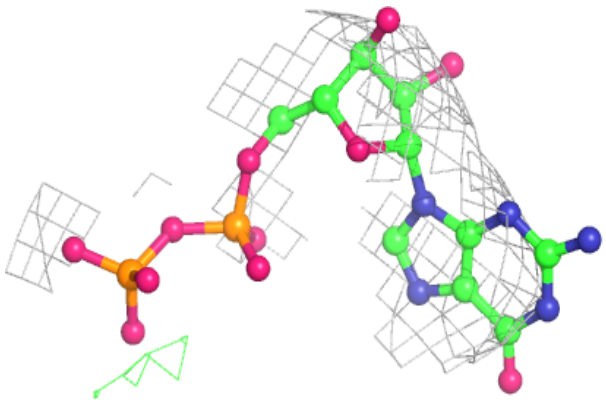
Electron density around GDP B 600:

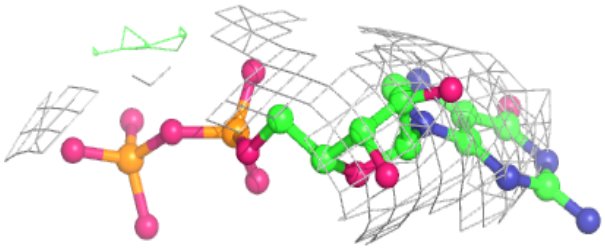
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

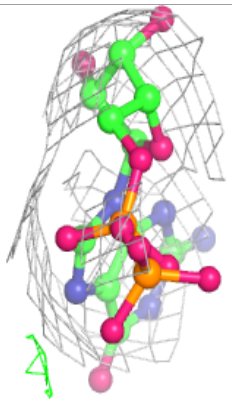


Electron density around GDP D 600:

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

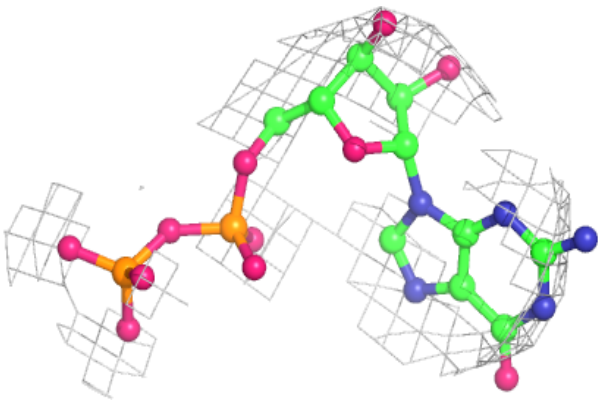


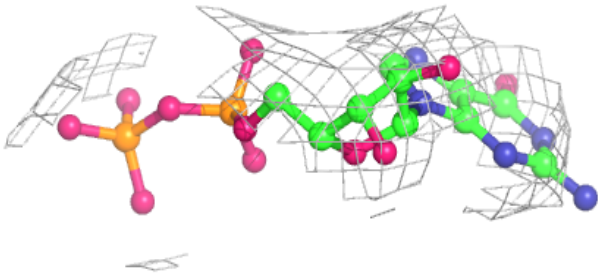


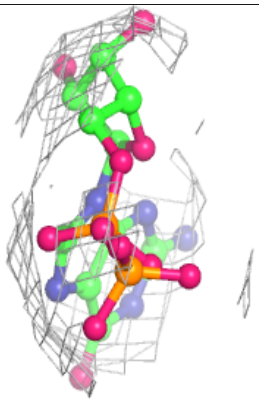


Electron density around GDP F 600:

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

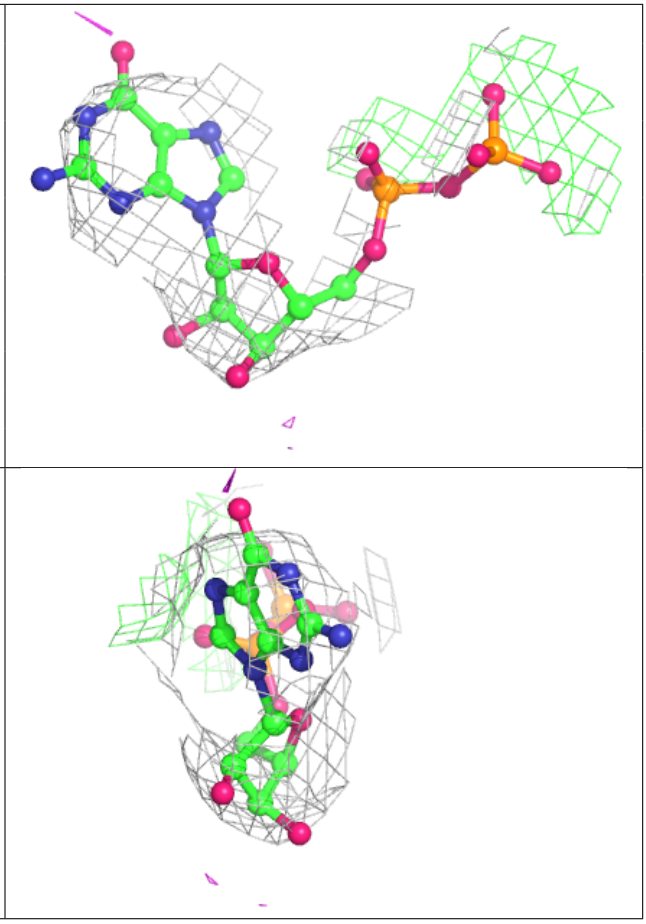






Electron density around GDP H 600:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.