



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 09:39 PM EST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

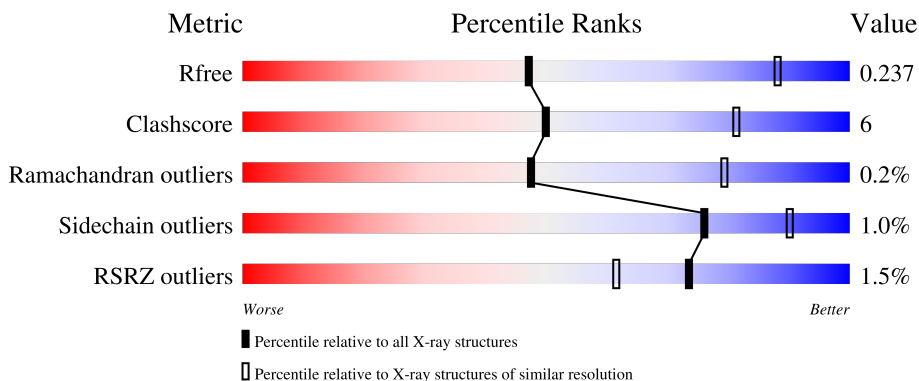
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">85% 10% 5%</p>
1	C	451	<div style="display: flex; align-items: center;"> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">82% 14% .</p>
1	G	451	<div style="display: flex; align-items: center;"> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">83% 11% 6%</p>
1	I	451	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">84% 12% .</p>
2	B	445	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">83% 13% .</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	445	<p>83% 13%</p>
2	H	445	<p>80% 16%</p>
2	J	445	<p>83% 13%</p>
3	E	554	<p>65% 23% 12%</p>
3	K	554	<p>69% 18% 12%</p>
4	F	140	<p>79% 10% 11%</p>
4	L	140	<p>77% 12% 11%</p>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 36853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Tubulin beta chain.

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

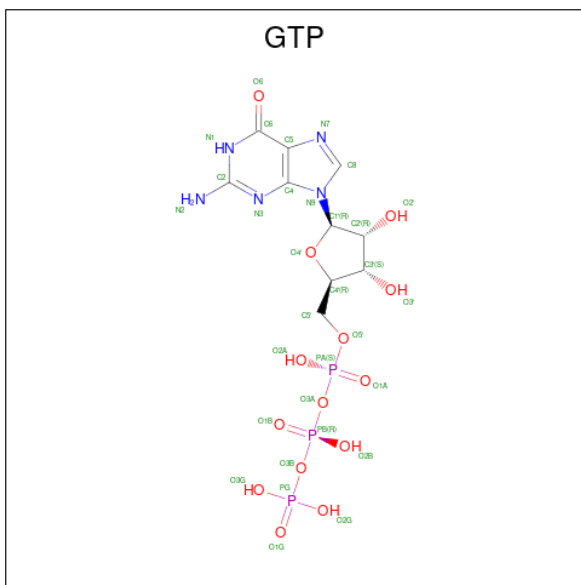
- Molecule 3 is a protein called Protein Stu2p/Alp14p.

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

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

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

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

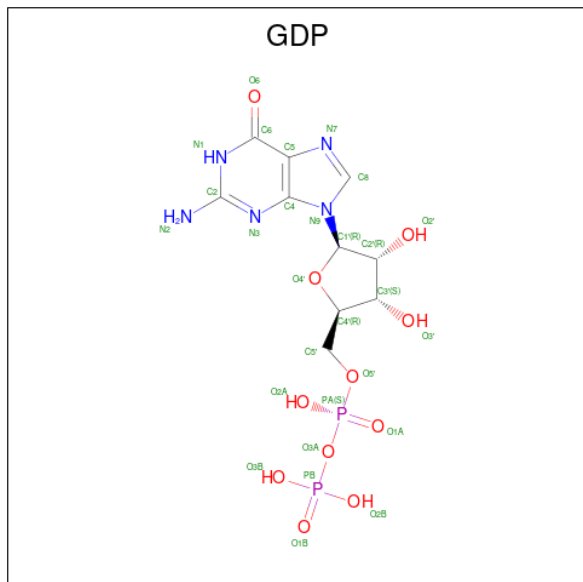
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

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




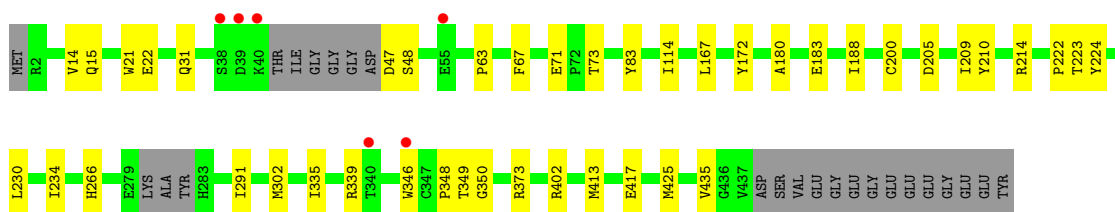
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 28 10 5 11 2	0	0
7	D	1	Total C N O P 28 10 5 11 2	0	0
7	H	1	Total C N O P 28 10 5 11 2	0	0
7	J	1	Total C N O P 28 10 5 11 2	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

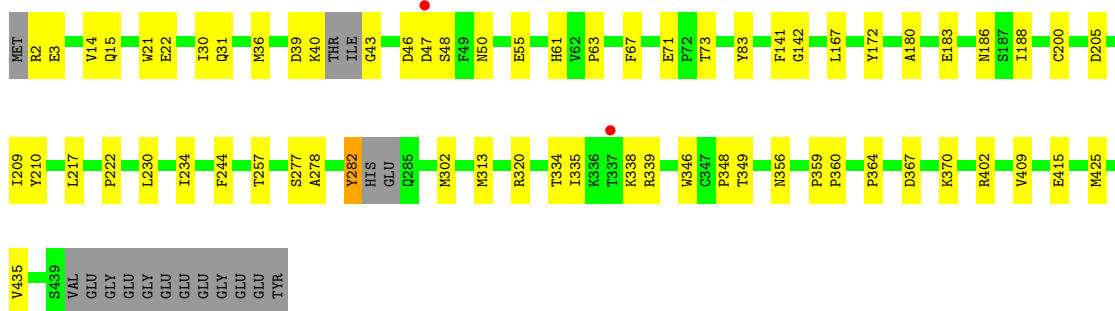
- Molecule 1: Tubulin alpha-1A chain

Chain A: 




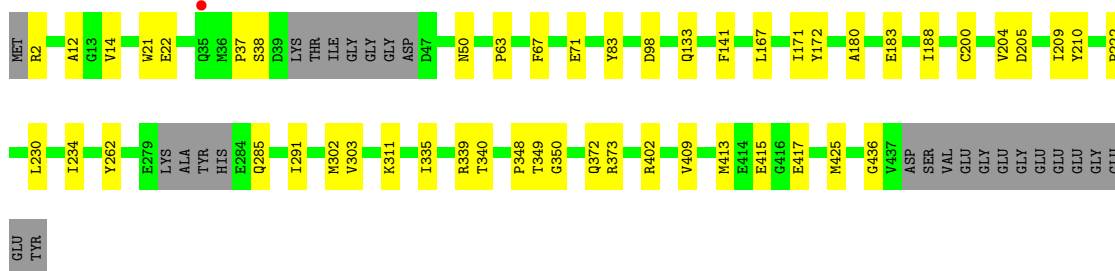
- Molecule 1: Tubulin alpha-1A chain

Chain C: 

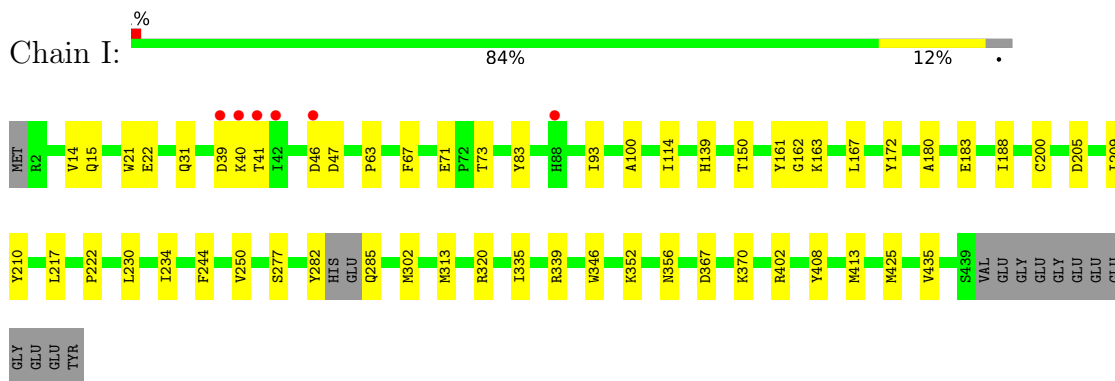


- Molecule 1: Tubulin alpha-1A chain

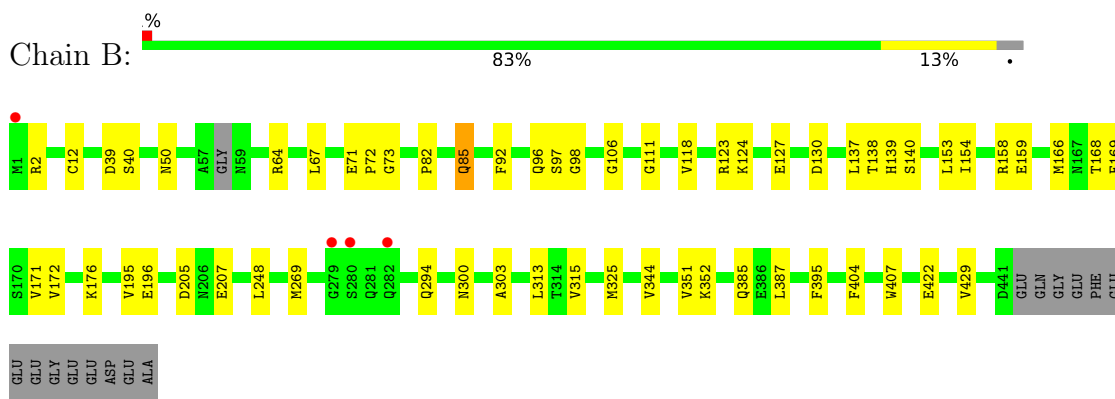
Chain G: 



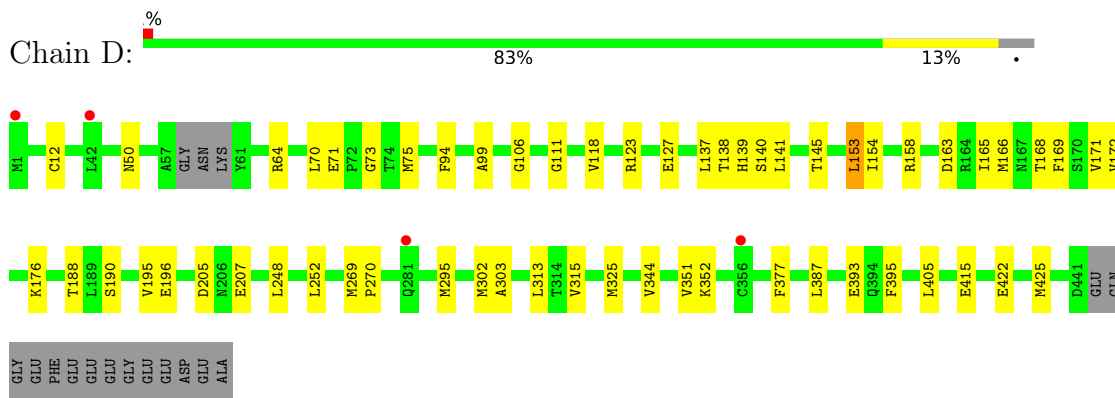
- Molecule 1: Tubulin alpha-1A chain



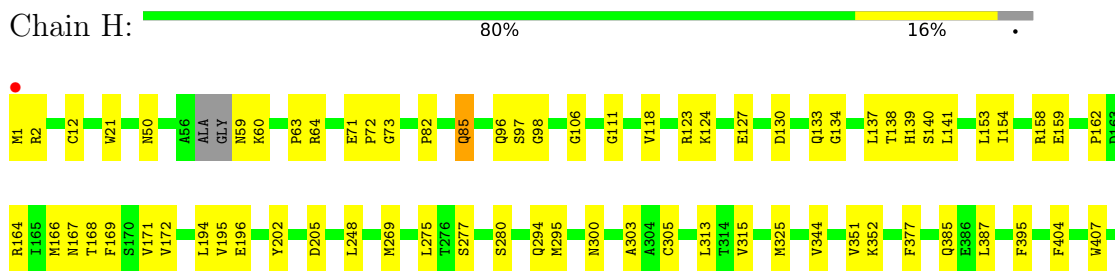
- Molecule 2: Tubulin beta chain

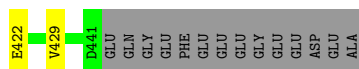


- Molecule 2: Tubulin beta chain

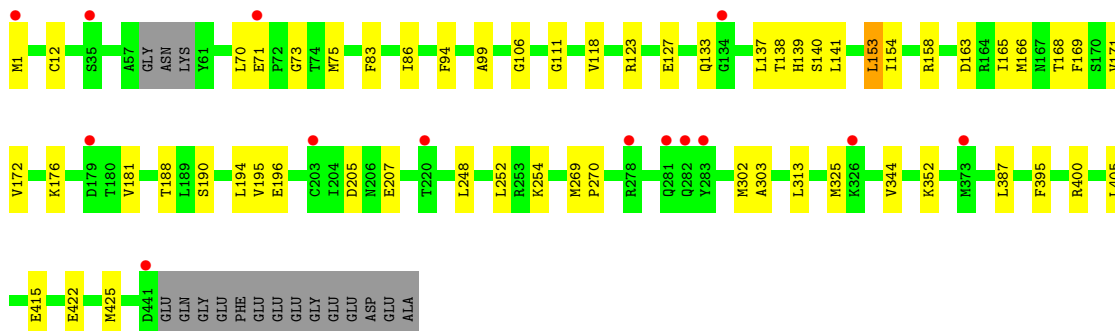
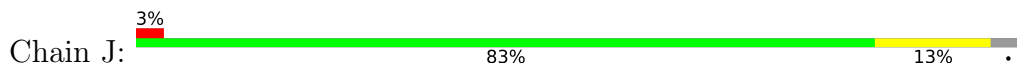


- Molecule 2: Tubulin beta chain

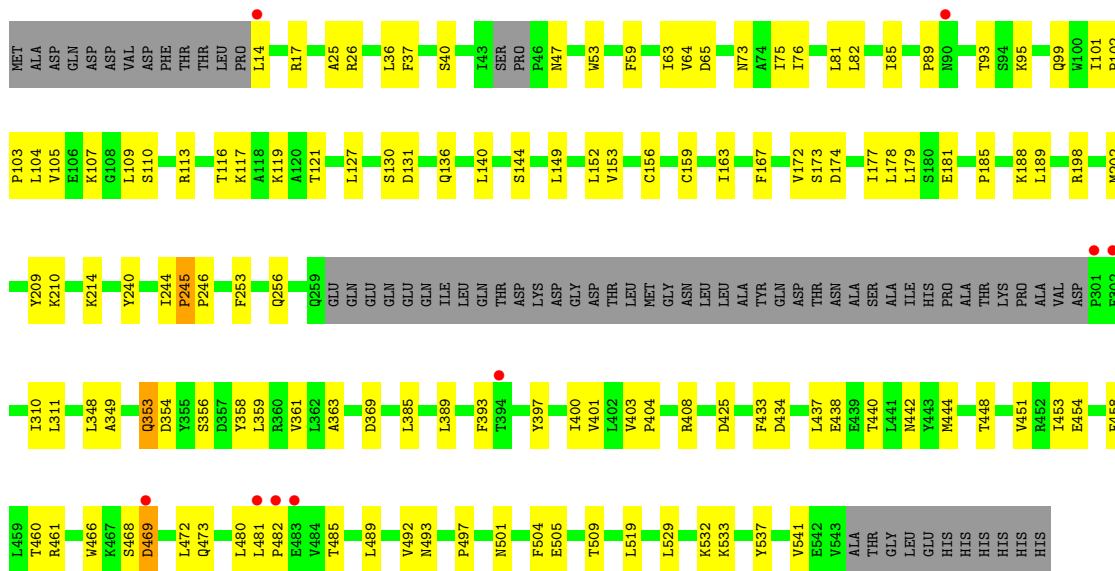




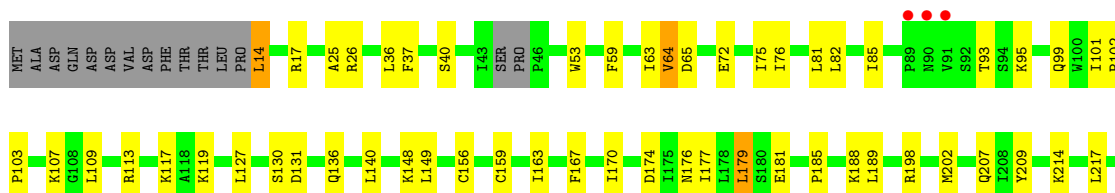
- Molecule 2: Tubulin beta chain

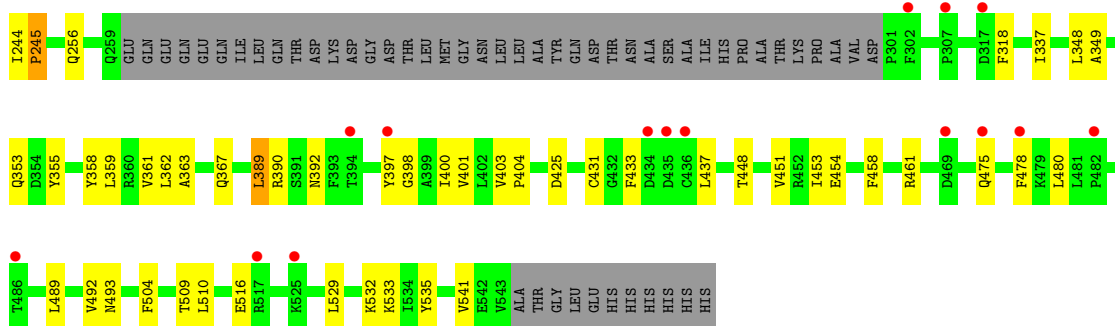


- Molecule 3: Protein Stu2p/Alp14p

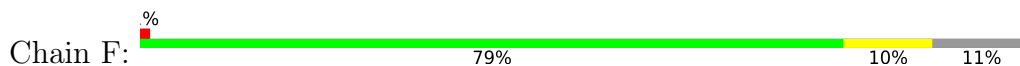


- Molecule 3: Protein Stu2p/Alp14p

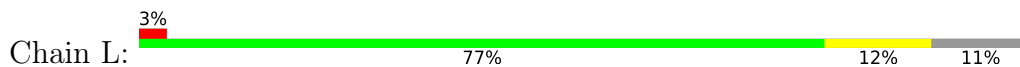




● Molecule 4: Truncated Darpin-D1



● Molecule 4: Truncated Darpin-D1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.13Å 194.99Å 149.57Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	57.56 – 3.21 57.56 – 3.21	Depositor EDS
% Data completeness (in resolution range)	81.9 (57.56-3.21) 81.9 (57.56-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.19Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.175 , 0.234 0.178 , 0.237	Depositor DCC
R_{free} test set	4370 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 9.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.410 for h,-k,-l	Xtrriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	0 of 88337 reflections	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	36853	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/3411	0.41	0/4628
1	C	0.25	0/3445	0.42	0/4671
1	G	0.25	0/3396	0.41	0/4610
1	I	0.25	0/3463	0.41	0/4698
2	B	0.25	0/3452	0.41	0/4676
2	D	0.24	0/3437	0.40	0/4657
2	H	0.25	0/3449	0.41	0/4672
2	J	0.24	0/3437	0.40	0/4657
3	E	0.24	0/3986	0.42	0/5401
3	K	0.24	0/3986	0.41	0/5401
4	F	0.23	0/951	0.38	0/1296
4	L	0.23	0/951	0.38	0/1296
All	All	0.25	0/37364	0.41	0/50663

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3338	0	3240	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3377	0	3270	47	0
1	G	3322	0	3225	27	0
1	I	3391	0	3288	37	0
2	B	3378	0	3258	33	0
2	D	3363	0	3239	31	0
2	H	3375	0	3253	40	0
2	J	3363	0	3239	31	0
3	E	3914	0	4032	80	0
3	K	3914	0	4032	69	0
4	F	935	0	935	8	0
4	L	935	0	935	10	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
5	G	32	0	12	0	0
5	I	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	B	28	0	12	1	0
7	D	28	0	12	2	0
7	H	28	0	12	1	0
7	J	28	0	12	1	0
All	All	36853	0	36042	426	0

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

All (426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLN:CG	1:C:31:GLN:NE2	2.42	0.83
1:I:31:GLN:CG	1:I:31:GLN:NE2	2.42	0.83
1:A:31:GLN:CG	1:A:31:GLN:NE2	2.42	0.83
1:C:47:ASP:CB	1:C:47:ASP:N	2.44	0.81
2:H:172:VAL:HG11	2:H:387:LEU:HD11	1.61	0.81
1:I:31:GLN:CB	1:I:31:GLN:N	2.43	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:172:VAL:HG11	2:J:387:LEU:HD11	1.64	0.80
1:I:31:GLN:CB	1:I:31:GLN:C	2.51	0.79
2:D:172:VAL:HG11	2:D:387:LEU:HD11	1.63	0.79
3:E:403:VAL:HG13	3:E:404:PRO:HD3	1.64	0.77
3:K:480:LEU:HD11	3:K:510:LEU:HD21	1.67	0.75
2:B:172:VAL:HG11	2:B:387:LEU:HD11	1.70	0.72
1:C:46:ASP:OD2	1:C:46:ASP:CB	2.38	0.71
1:C:31:GLN:CG	1:C:31:GLN:OE1	2.39	0.71
3:K:76:ILE:HG22	3:K:119:LYS:HG3	1.73	0.70
1:I:31:GLN:NE2	1:I:31:GLN:OE1	2.25	0.70
1:C:31:GLN:NE2	1:C:31:GLN:OE1	2.25	0.70
1:I:31:GLN:CG	1:I:31:GLN:OE1	2.39	0.70
1:A:31:GLN:CG	1:A:31:GLN:OE1	2.39	0.70
1:I:31:GLN:N	1:I:31:GLN:C	2.45	0.69
1:A:31:GLN:NE2	1:A:31:GLN:OE1	2.25	0.69
1:C:46:ASP:CB	1:C:46:ASP:OD1	2.39	0.69
1:C:47:ASP:O	1:C:48:SER:N	2.25	0.69
3:E:17:ARG:HD3	3:E:25:ALA:HB1	1.76	0.68
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.75	0.68
2:H:277:SER:HB3	2:H:280:SER:HB3	1.76	0.68
2:B:71:GLU:HG3	2:B:73:GLY:H	1.58	0.66
3:K:403:VAL:HG13	3:K:404:PRO:HD3	1.77	0.66
3:E:64:VAL:HG13	3:E:107:LYS:HD3	1.77	0.66
3:E:458:PHE:HA	3:E:461:ARG:HD2	1.78	0.66
1:I:172:TYR:HB3	1:I:205:ASP:HA	1.76	0.66
3:E:393:PHE:HA	3:E:397:TYR:HB2	1.79	0.65
3:K:458:PHE:HA	3:K:461:ARG:HD2	1.79	0.65
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.79	0.64
2:H:295:MET:HG3	2:H:377:PHE:HB2	1.79	0.64
2:D:71:GLU:HG3	2:D:73:GLY:H	1.62	0.64
3:E:460:THR:HG23	3:E:509:THR:HG21	1.79	0.63
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.80	0.63
2:H:313:LEU:HD23	2:H:344:VAL:HG21	1.80	0.63
4:L:46:SER:O	4:L:78:ILE:N	2.31	0.63
3:K:95:LYS:NZ	3:K:99:GLN:OE1	2.32	0.63
3:K:170:ILE:HD11	3:K:256:GLN:NE2	2.14	0.62
1:G:335:ILE:HG23	1:G:339:ARG:HD2	1.81	0.62
2:B:72:PRO:HD3	2:B:96:GLN:HA	1.79	0.62
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.80	0.62
3:E:489:LEU:O	3:E:493:ASN:ND2	2.33	0.62
2:J:118:VAL:HG11	2:J:153:LEU:HD11	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:95:LYS:NZ	3:E:99:GLN:OE1	2.33	0.61
3:E:82:LEU:HD21	3:E:127:LEU:HG	1.81	0.61
3:K:489:LEU:O	3:K:493:ASN:ND2	2.34	0.61
2:H:159:GLU:HA	3:K:149:LEU:HD13	1.83	0.61
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.81	0.61
1:C:46:ASP:OD2	1:C:46:ASP:OD1	2.19	0.61
2:H:71:GLU:HG3	2:H:73:GLY:H	1.65	0.60
2:J:248:LEU:HD21	2:J:352:LYS:HB3	1.82	0.60
2:B:313:LEU:HD23	2:B:344:VAL:HG21	1.82	0.60
1:I:346:TRP:HZ2	1:I:435:VAL:HG13	1.66	0.60
3:K:363:ALA:HB1	3:K:404:PRO:HG2	1.83	0.60
1:G:172:TYR:HB3	1:G:205:ASP:HA	1.83	0.59
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.84	0.59
2:H:269:MET:HG3	2:H:303:ALA:HB3	1.85	0.59
2:J:313:LEU:HD23	2:J:344:VAL:HG21	1.84	0.59
2:H:118:VAL:HG11	2:H:153:LEU:HD11	1.83	0.59
3:E:81:LEU:O	3:E:85:ILE:HG23	2.03	0.59
1:G:409:VAL:O	3:K:198:ARG:NH2	2.36	0.59
1:C:335:ILE:HG23	1:C:339:ARG:HD2	1.85	0.59
3:E:172:VAL:HG21	3:E:178:LEU:HD22	1.84	0.59
3:K:529:LEU:HD23	3:K:532:LYS:HE3	1.85	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.83	0.58
1:G:2:ARG:HH12	1:G:50:ASN:HB3	1.68	0.58
3:K:81:LEU:O	3:K:85:ILE:HG23	2.03	0.58
3:K:64:VAL:HG13	3:K:107:LYS:HD3	1.85	0.58
1:C:348:PRO:O	1:C:349:THR:HG22	2.03	0.58
3:E:363:ALA:HB1	3:E:404:PRO:HG2	1.84	0.58
2:D:313:LEU:HD23	2:D:344:VAL:HG21	1.86	0.58
1:I:335:ILE:HG23	1:I:339:ARG:HD2	1.86	0.58
2:H:50:ASN:O	2:H:64:ARG:NH2	2.36	0.58
1:G:285:GLN:NE2	1:G:372:GLN:OE1	2.35	0.58
1:C:15:GLN:NE2	5:C:600:GTP:O6	2.37	0.58
1:C:217:LEU:HA	1:C:277:SER:HB2	1.86	0.58
3:E:433:PHE:CE2	3:E:466:TRP:HD1	2.21	0.58
1:I:39:ASP:OD1	1:I:40:LYS:N	2.37	0.57
3:E:349:ALA:HB3	3:E:353:GLN:HG3	1.86	0.57
3:K:82:LEU:HD21	3:K:127:LEU:HG	1.84	0.57
2:B:294:GLN:O	2:B:300:ASN:ND2	2.36	0.57
1:C:409:VAL:HG12	3:E:497:PRO:HB3	1.87	0.57
3:K:101:ILE:HG22	3:K:127:LEU:HD13	1.85	0.57
3:E:433:PHE:HB3	3:E:437:LEU:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:ILE:HG23	2:H:166:MET:HG2	1.87	0.56
2:H:72:PRO:HD3	2:H:96:GLN:HA	1.87	0.56
2:B:39:ASP:HB3	3:K:478:PHE:HB3	1.85	0.56
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.41	0.56
2:D:195:VAL:HG13	2:D:196:GLU:HG2	1.87	0.56
4:F:100:LEU:HD23	4:F:104:ALA:HB3	1.87	0.56
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.89	0.55
1:A:71:GLU:HG2	1:A:73:THR:H	1.71	0.55
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.89	0.55
3:E:468:SER:OG	3:E:469:ASP:N	2.39	0.55
2:J:195:VAL:HG13	2:J:196:GLU:HG2	1.88	0.55
3:E:101:ILE:HG22	3:E:127:LEU:HD13	1.88	0.55
3:E:400:ILE:HG23	3:E:401:VAL:HG13	1.88	0.54
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.88	0.54
2:B:172:VAL:HB	2:B:205:ASP:HA	1.89	0.54
2:D:172:VAL:HG21	2:D:387:LEU:HD21	1.90	0.54
3:K:389:LEU:HD12	3:K:392:ASN:HB3	1.90	0.54
2:J:1:MET:HE3	2:J:133:GLN:HG3	1.89	0.54
3:E:481:LEU:HA	3:E:485:THR:HG22	1.90	0.54
1:I:161:TYR:O	1:I:163:LYS:N	2.40	0.54
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.90	0.54
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.89	0.54
3:E:244:ILE:HB	3:E:245:PRO:HD3	1.88	0.54
3:K:348:LEU:HB2	3:K:389:LEU:HD22	1.89	0.54
3:E:509:THR:HA	3:E:541:VAL:HG11	1.90	0.54
2:J:71:GLU:HG3	2:J:73:GLY:H	1.72	0.53
3:K:14:LEU:O	3:K:17:ARG:HG2	2.09	0.53
2:B:123:ARG:O	2:B:127:GLU:HG2	2.08	0.53
3:K:53:TRP:HE1	3:K:85:ILE:HB	1.74	0.53
2:H:195:VAL:HG13	2:H:196:GLU:HG2	1.90	0.53
2:B:50:ASN:O	2:B:64:ARG:NH2	2.42	0.53
3:E:403:VAL:CG1	3:E:404:PRO:HD3	2.36	0.53
2:J:123:ARG:O	2:J:127:GLU:HG2	2.08	0.53
1:I:180:ALA:HB3	1:I:183:GLU:HG3	1.91	0.53
1:C:71:GLU:HG2	1:C:73:THR:H	1.73	0.52
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.90	0.52
3:K:37:PHE:CD2	3:K:81:LEU:HB2	2.44	0.52
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.44	0.52
2:J:172:VAL:HG21	2:J:387:LEU:HD21	1.91	0.52
2:H:82:PRO:O	2:H:85:GLN:NE2	2.42	0.52
2:D:123:ARG:O	2:D:127:GLU:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:59:HIS:HB3	4:F:62:ILE:HD13	1.92	0.52
2:H:172:VAL:HG21	2:H:387:LEU:HD21	1.91	0.52
3:K:198:ARG:O	3:K:202:MET:HG2	2.08	0.52
3:E:209:TYR:HE1	3:E:214:LYS:HB2	1.75	0.52
2:J:154:ILE:HG23	2:J:166:MET:HG2	1.90	0.52
3:K:244:ILE:HB	3:K:245:PRO:HD3	1.92	0.52
2:B:159:GLU:HA	3:E:149:LEU:HD13	1.91	0.52
1:C:364:PRO:HG3	3:K:177:ILE:HG23	1.91	0.52
3:K:101:ILE:HD11	3:K:140:LEU:HB2	1.92	0.52
1:C:39:ASP:OD2	1:C:43:GLY:N	2.42	0.52
3:K:509:THR:HA	3:K:541:VAL:HG11	1.91	0.52
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.75	0.52
2:H:97:SER:OG	2:H:98:GLY:N	2.43	0.52
3:E:101:ILE:HD11	3:E:140:LEU:HB2	1.92	0.51
2:D:145:THR:N	7:D:600:GDP:O3B	2.30	0.51
3:E:102:PRO:HB2	3:E:103:PRO:HD3	1.92	0.51
1:C:188:ILE:HD12	1:C:425:MET:HG3	1.91	0.51
3:E:109:LEU:HA	3:E:117:LYS:HG3	1.92	0.51
1:I:217:LEU:HA	1:I:277:SER:HB2	1.92	0.51
2:H:123:ARG:O	2:H:127:GLU:HG2	2.11	0.51
2:H:385:GLN:HB2	2:H:429:VAL:HG13	1.92	0.51
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.90	0.51
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.92	0.51
3:E:311:LEU:HD12	3:E:353:GLN:HE21	1.76	0.51
3:E:76:ILE:HG22	3:E:119:LYS:HG3	1.92	0.51
3:K:174:ASP:OD1	3:K:174:ASP:N	2.43	0.51
3:E:529:LEU:HD23	3:E:532:LYS:HE3	1.93	0.51
1:G:340:THR:O	1:G:340:THR:OG1	2.25	0.51
3:E:310:ILE:HG12	3:E:348:LEU:HD22	1.92	0.50
3:E:480:LEU:HD21	3:E:519:LEU:HD11	1.92	0.50
2:H:404:PHE:HD2	2:H:407:TRP:HZ3	1.59	0.50
1:I:188:ILE:HD12	1:I:425:MET:HG3	1.92	0.50
1:C:364:PRO:HG3	3:K:177:ILE:HD12	1.93	0.50
3:E:348:LEU:HB2	3:E:389:LEU:HG	1.93	0.50
2:J:176:LYS:HD2	2:J:207:GLU:HG3	1.92	0.50
3:K:185:PRO:HB2	3:K:189:LEU:HD23	1.93	0.50
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.94	0.50
3:K:318:PHE:CE1	3:K:337:ILE:HD13	2.46	0.50
3:E:63:ILE:HD12	3:E:75:ILE:HG12	1.93	0.50
1:C:370:LYS:HZ2	3:K:181:GLU:HG2	1.77	0.50
1:G:188:ILE:HG23	1:G:425:MET:HG3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE2	1:A:222:PRO:HD2	2.47	0.49
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.93	0.49
3:E:53:TRP:HE1	3:E:85:ILE:HB	1.77	0.49
3:E:174:ASP:O	3:E:177:ILE:HG22	2.12	0.49
3:E:185:PRO:HB2	3:E:189:LEU:HD23	1.93	0.49
2:J:12:CYS:HB2	7:J:600:GDP:C8	2.47	0.49
3:K:36:LEU:O	3:K:40:SER:HB2	2.11	0.49
3:K:63:ILE:HD12	3:K:75:ILE:HG12	1.94	0.49
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.95	0.49
3:E:110:SER:HB2	3:E:152:LEU:HD13	1.95	0.49
2:J:141:LEU:HD22	2:J:190:SER:HB3	1.94	0.49
3:K:159:CYS:O	3:K:163:ILE:HG23	2.11	0.49
1:A:15:GLN:NE2	5:A:600:GTP:O6	2.43	0.49
2:B:315:VAL:HB	2:B:351:VAL:HG22	1.93	0.49
2:H:137:LEU:HB3	2:H:168:THR:HG22	1.95	0.49
2:H:294:GLN:O	2:H:300:ASN:ND2	2.44	0.49
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.93	0.48
1:G:167:LEU:HG	1:G:200:CYS:HB3	1.95	0.48
3:K:26:ARG:NH1	3:K:65:ASP:OD1	2.46	0.48
1:G:210:TYR:CE2	1:G:222:PRO:HD2	2.48	0.48
3:E:492:VAL:HG13	3:E:504:PHE:HE1	1.79	0.48
3:K:59:PHE:O	3:K:63:ILE:HG12	2.13	0.48
2:D:75:MET:HB2	2:D:94:PHE:CD1	2.48	0.48
1:C:39:ASP:OD1	1:C:40:LYS:N	2.47	0.48
1:I:244:PHE:HB2	1:I:356:ASN:HD21	1.79	0.48
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.96	0.48
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.95	0.48
1:G:234:ILE:HG21	1:G:302:MET:HE1	1.96	0.48
1:G:180:ALA:HB3	1:G:183:GLU:HG3	1.95	0.48
3:K:176:ASN:N	3:K:176:ASN:OD1	2.46	0.48
2:B:82:PRO:O	2:B:85:GLN:NE2	2.47	0.48
2:J:172:VAL:HB	2:J:205:ASP:HA	1.96	0.48
3:K:433:PHE:CE1	3:K:475:GLN:HB3	2.49	0.48
2:D:140:SER:HA	2:D:171:VAL:HG22	1.95	0.48
2:D:172:VAL:HB	2:D:205:ASP:HA	1.96	0.48
1:I:40:LYS:HG2	1:I:41:THR:H	1.79	0.48
3:E:14:LEU:O	3:E:17:ARG:HG2	2.12	0.47
3:E:481:LEU:HG	3:E:482:PRO:HD3	1.95	0.47
1:I:14:VAL:HG13	1:I:67:PHE:HD2	1.77	0.47
2:J:75:MET:HB2	2:J:94:PHE:CD1	2.49	0.47
3:K:318:PHE:HE1	3:K:337:ILE:HD13	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:425:ASP:OD2	3:K:461:ARG:NH1	2.46	0.47
1:G:209:ILE:HG23	1:G:230:LEU:HD23	1.95	0.47
2:H:172:VAL:HB	2:H:205:ASP:HA	1.96	0.47
1:I:210:TYR:CE2	1:I:222:PRO:HD2	2.50	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
1:I:188:ILE:HG23	1:I:425:MET:HG3	1.95	0.47
3:K:163:ILE:O	3:K:167:PHE:HB2	2.15	0.47
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.96	0.47
3:E:26:ARG:NH1	3:E:65:ASP:OD1	2.47	0.47
2:H:248:LEU:HD21	2:H:352:LYS:HB3	1.96	0.47
1:I:71:GLU:HG2	1:I:73:THR:H	1.80	0.47
3:E:37:PHE:CD2	3:E:81:LEU:HB2	2.50	0.47
3:E:210:LYS:HE3	3:E:240:TYR:CE1	2.50	0.47
3:E:210:LYS:O	3:E:246:PRO:HD3	2.14	0.47
3:K:102:PRO:HB2	3:K:103:PRO:HD3	1.96	0.47
3:E:198:ARG:O	3:E:202:MET:HG2	2.14	0.47
3:E:425:ASP:OD2	3:E:461:ARG:NH1	2.47	0.47
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.96	0.47
3:E:59:PHE:O	3:E:63:ILE:HG12	2.14	0.47
1:G:2:ARG:N	1:G:133:GLN:HG3	2.29	0.47
2:B:124:LYS:HB2	2:B:124:LYS:HE3	1.68	0.47
2:J:138:THR:HG22	2:J:169:PHE:HB2	1.96	0.47
4:L:100:LEU:HD23	4:L:104:ALA:HB3	1.96	0.47
3:E:163:ILE:O	3:E:167:PHE:HB2	2.14	0.47
2:J:137:LEU:HB3	2:J:168:THR:HG22	1.97	0.47
3:E:501:ASN:OD1	3:E:537:TYR:OH	2.33	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.97	0.46
3:E:159:CYS:O	3:E:163:ILE:HG23	2.14	0.46
2:H:124:LYS:HE3	2:H:124:LYS:HB2	1.73	0.46
3:K:349:ALA:HB3	3:K:353:GLN:HG3	1.97	0.46
2:B:97:SER:OG	2:B:98:GLY:N	2.49	0.46
1:I:167:LEU:HG	1:I:200:CYS:HB3	1.96	0.46
2:J:70:LEU:HD12	2:J:99:ALA:HB2	1.96	0.46
3:E:185:PRO:HA	3:E:188:LYS:HE3	1.97	0.46
3:E:253:PHE:HD2	3:E:256:GLN:HE22	1.63	0.46
3:E:311:LEU:HD12	3:E:353:GLN:NE2	2.31	0.46
1:I:100:ALA:HA	2:J:254:LYS:HG2	1.98	0.46
1:I:282:TYR:OH	1:I:370:LYS:O	2.32	0.46
2:H:2:ARG:HH21	2:H:130:ASP:HB3	1.80	0.46
2:H:162:PRO:HD2	3:K:148:LYS:HE3	1.96	0.46
2:D:50:ASN:O	2:D:64:ARG:NH2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:VAL:HG11	1:I:352:LYS:HE3	1.98	0.46
3:K:403:VAL:CG1	3:K:404:PRO:HD3	2.46	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.98	0.46
2:H:12:CYS:HB2	7:H:600:GDP:C8	2.51	0.46
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.97	0.46
1:G:171:ILE:HA	1:G:204:VAL:HG23	1.98	0.46
1:I:139:HIS:CD2	1:I:150:THR:HG21	2.50	0.46
3:K:433:PHE:HB2	3:K:437:LEU:HB2	1.97	0.46
2:B:172:VAL:HG21	2:B:387:LEU:HD21	1.98	0.46
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.98	0.46
3:E:93:THR:HG21	3:E:130:SER:HB3	1.97	0.46
1:G:413:MET:HE3	1:G:417:GLU:HB3	1.97	0.46
1:I:93:ILE:HG22	1:I:114:ILE:HD11	1.98	0.46
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.81	0.45
1:G:205:ASP:HB2	1:G:303:VAL:HA	1.98	0.45
2:D:12:CYS:HB2	7:D:600:GDP:C8	2.51	0.45
1:G:21:TRP:CZ3	1:G:63:PRO:HB3	2.51	0.45
3:K:17:ARG:HD3	3:K:25:ALA:HB1	1.97	0.45
3:K:93:THR:HG21	3:K:130:SER:HB3	1.97	0.45
2:H:315:VAL:HB	2:H:351:VAL:HG22	1.98	0.45
1:I:282:TYR:O	1:I:285:GLN:N	2.49	0.45
3:E:354:ASP:OD2	3:E:356:SER:OG	2.23	0.45
4:F:121:ALA:HB1	4:F:161:LEU:HD21	1.98	0.45
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.82	0.45
1:C:50:ASN:ND2	1:C:55:GLU:OE1	2.50	0.45
1:G:14:VAL:HG13	1:G:67:PHE:HD2	1.82	0.45
3:K:516:GLU:OE2	3:K:535:TYR:OH	2.28	0.45
1:C:313:MET:SD	1:C:435:VAL:HG11	2.57	0.45
2:D:188:THR:HG23	2:D:425:MET:HE2	1.98	0.45
2:J:269:MET:HG3	2:J:303:ALA:HB3	1.98	0.45
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.98	0.45
3:K:209:TYR:HE1	3:K:214:LYS:HB2	1.81	0.45
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.82	0.44
2:H:395:PHE:CE2	2:H:422:GLU:HB2	2.52	0.44
2:B:137:LEU:HB3	2:B:168:THR:HG22	2.00	0.44
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.52	0.44
1:G:291:ILE:HD13	1:G:373:ARG:HG3	1.99	0.44
3:K:72:GLU:OE1	3:K:113:ARG:NH2	2.47	0.44
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.98	0.44
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.83	0.44
2:D:106:GLY:O	2:D:111:GLY:HA3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:MET:HE3	2:H:133:GLN:HG3	1.99	0.44
2:J:181:VAL:HG11	4:L:90:ILE:HA	2.00	0.44
3:K:131:ASP:OD2	3:K:136:GLN:HB2	2.16	0.44
2:B:395:PHE:CE2	2:B:422:GLU:HB2	2.53	0.44
3:E:472:LEU:O	3:E:473:GLN:HG2	2.18	0.44
3:E:492:VAL:HG13	3:E:504:PHE:CE1	2.53	0.44
1:I:402:ARG:HA	1:I:402:ARG:HD3	1.88	0.44
1:C:402:ARG:NH1	1:C:415:GLU:OE2	2.49	0.44
2:D:393:GLU:OE2	4:F:156:ASN:ND2	2.49	0.44
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.99	0.44
2:J:165:ILE:HG21	2:J:252:LEU:HB3	1.99	0.44
3:K:367:GLN:HB2	3:K:404:PRO:HB3	2.00	0.44
1:A:348:PRO:O	1:A:350:GLY:N	2.50	0.44
2:B:39:ASP:OD1	2:B:40:SER:N	2.50	0.44
1:G:402:ARG:NH1	1:G:415:GLU:OE2	2.47	0.44
2:J:395:PHE:CE2	2:J:422:GLU:HB2	2.53	0.44
1:C:402:ARG:HA	1:C:402:ARG:HD3	1.86	0.43
4:F:148:THR:OG1	4:F:151:ASP:OD1	2.23	0.43
2:H:138:THR:HG22	2:H:169:PHE:HB2	2.00	0.43
2:H:167:ASN:HD21	2:H:202:TYR:HE1	1.66	0.43
1:I:15:GLN:NE2	5:I:600:GTP:O6	2.51	0.43
1:I:313:MET:SD	1:I:435:VAL:HG11	2.58	0.43
2:H:106:GLY:O	2:H:111:GLY:HA3	2.18	0.43
1:I:320:ARG:HA	1:I:356:ASN:O	2.19	0.43
3:K:109:LEU:HA	3:K:117:LYS:HG3	2.00	0.43
1:C:22:GLU:HG3	1:C:83:TYR:OH	2.18	0.43
3:E:101:ILE:HA	3:E:104:LEU:HB2	2.00	0.43
4:L:96:VAL:HG21	4:L:128:ILE:HD13	2.01	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.53	0.43
3:E:36:LEU:O	3:E:40:SER:HB2	2.19	0.43
3:E:358:TYR:CE2	3:E:385:LEU:HD11	2.53	0.43
4:F:96:VAL:HG21	4:F:128:ILE:HD13	2.00	0.43
2:H:140:SER:HA	2:H:171:VAL:HG22	2.01	0.43
1:I:22:GLU:HG3	1:I:83:TYR:OH	2.18	0.43
3:K:358:TYR:O	3:K:361:VAL:HG22	2.17	0.43
3:E:73:ASN:HA	3:E:76:ILE:HG12	2.01	0.43
1:I:21:TRP:CZ3	1:I:63:PRO:HB3	2.53	0.43
1:C:142:GLY:HA3	1:C:183:GLU:HG2	2.00	0.43
1:C:320:ARG:HA	1:C:356:ASN:O	2.19	0.43
3:E:177:ILE:O	3:E:181:GLU:HB2	2.19	0.43
1:G:12:ALA:HB1	1:G:171:ILE:HG13	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:408:TYR:HB3	1:I:413:MET:HE3	1.99	0.43
1:C:278:ALA:HA	1:C:282:TYR:OH	2.19	0.43
1:G:348:PRO:O	1:G:350:GLY:N	2.51	0.43
1:C:30:ILE:HG12	1:C:36:MET:SD	2.59	0.43
3:E:440:THR:O	3:E:444:MET:HG3	2.18	0.43
3:E:481:LEU:HA	3:E:485:THR:CG2	2.49	0.43
3:K:217:LEU:H	3:K:217:LEU:HD23	1.83	0.43
1:I:230:LEU:O	1:I:234:ILE:HD12	2.18	0.43
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.54	0.42
2:B:12:CYS:HB2	7:B:600:GDP:C8	2.53	0.42
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.53	0.42
1:G:402:ARG:HA	1:G:402:ARG:HD3	1.86	0.42
3:E:505:GLU:O	3:E:509:THR:HG23	2.18	0.42
2:H:59:ASN:HB2	2:H:60:LYS:HG3	2.01	0.42
3:K:425:ASP:OD1	3:K:461:ARG:HD3	2.19	0.42
2:B:404:PHE:HD2	2:B:407:TRP:HZ3	1.67	0.42
3:E:359:LEU:HD22	3:E:401:VAL:HG11	2.02	0.42
3:K:453:ILE:HG13	3:K:454:GLU:N	2.34	0.42
2:D:141:LEU:HD22	2:D:190:SER:OG	2.20	0.42
2:D:395:PHE:CE2	2:D:422:GLU:HB2	2.54	0.42
3:K:355:TYR:HB2	3:K:397:TYR:HE1	1.83	0.42
4:L:123:MET:HB2	4:L:125:HIS:CD2	2.54	0.42
2:B:140:SER:HA	2:B:171:VAL:HG22	2.01	0.42
2:H:134:GLY:HA2	2:H:164:ARG:HB3	2.01	0.42
4:L:121:ALA:HB1	4:L:161:LEU:HD21	2.01	0.42
1:A:234:ILE:HG21	1:A:302:MET:SD	2.59	0.42
1:C:142:GLY:O	1:C:186:ASN:ND2	2.43	0.42
2:B:407:TRP:CH2	1:C:257:THR:HA	2.55	0.42
1:C:2:ARG:HB2	1:C:3:GLU:OE1	2.19	0.42
1:C:334:THR:O	1:C:338:LYS:HB2	2.20	0.42
3:K:359:LEU:HD23	3:K:362:LEU:HD12	2.02	0.42
1:C:234:ILE:HG21	1:C:302:MET:SD	2.60	0.42
3:E:438:GLU:O	3:E:442:ASN:ND2	2.52	0.42
1:G:22:GLU:HG3	1:G:83:TYR:OH	2.20	0.42
1:I:209:ILE:HG23	1:I:230:LEU:HD23	2.02	0.42
2:J:270:PRO:HG2	2:J:302:MET:HB2	2.02	0.42
3:E:144:SER:O	3:E:153:VAL:HG12	2.19	0.42
3:E:369:ASP:O	3:E:408:ARG:NH2	2.53	0.42
1:G:71:GLU:HB2	1:G:98:ASP:HB3	2.02	0.42
3:K:448:THR:HB	3:K:451:VAL:HG22	2.02	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:HA	1:A:402:ARG:HD3	1.86	0.41
2:J:400:ARG:HD2	4:L:112:TRP:NE1	2.34	0.41
3:K:363:ALA:HB2	3:K:401:VAL:HG12	2.01	0.41
4:L:91:GLY:HA2	4:L:128:ILE:HD12	2.02	0.41
3:E:131:ASP:OD2	3:E:136:GLN:HB2	2.19	0.41
4:F:125:HIS:O	4:F:129:VAL:HG23	2.20	0.41
2:J:106:GLY:O	2:J:111:GLY:HA3	2.20	0.41
2:J:140:SER:HA	2:J:171:VAL:HG22	2.01	0.41
3:K:359:LEU:HD23	3:K:359:LEU:HA	1.86	0.41
3:K:398:GLY:HA3	3:K:431:CYS:SG	2.60	0.41
3:E:358:TYR:O	3:E:361:VAL:HG22	2.19	0.41
3:E:453:ILE:HG13	3:E:454:GLU:N	2.35	0.41
2:D:50:ASN:OD1	2:D:50:ASN:N	2.54	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.21	0.41
1:G:409:VAL:HA	1:G:413:MET:O	2.20	0.41
1:A:22:GLU:HG3	1:A:83:TYR:OH	2.21	0.41
2:D:176:LYS:HD2	2:D:207:GLU:HG3	2.01	0.41
2:H:21:TRP:CZ3	2:H:63:PRO:HB3	2.54	0.41
2:J:188:THR:HA	2:J:425:MET:HE2	2.03	0.41
1:A:47:ASP:OD1	1:A:48:SER:N	2.46	0.41
1:A:266:HIS:O	1:A:266:HIS:ND1	2.51	0.41
2:B:2:ARG:HH21	2:B:130:ASP:HB3	1.85	0.41
3:E:448:THR:HB	3:E:451:VAL:HG22	2.03	0.41
3:K:179:LEU:HD23	3:K:179:LEU:HA	1.91	0.41
3:K:397:TYR:O	3:K:400:ILE:HG22	2.20	0.41
1:C:55:GLU:HG2	1:C:61:HIS:HD2	1.86	0.41
3:E:82:LEU:O	3:E:85:ILE:HG12	2.20	0.41
3:E:105:VAL:HA	3:E:109:LEU:HG	2.03	0.41
2:H:205:ASP:HB2	2:H:303:ALA:HA	2.03	0.41
2:H:275:LEU:HD23	2:H:275:LEU:HA	1.96	0.41
2:H:303:ALA:O	2:H:305:CYS:N	2.53	0.41
2:J:141:LEU:HD21	2:J:194:LEU:HD11	2.02	0.41
2:J:405:LEU:HD21	2:J:415:GLU:HG3	2.03	0.41
4:L:43:THR:HB	4:L:47:GLY:HA2	2.02	0.41
2:D:405:LEU:HD21	2:D:415:GLU:HG3	2.02	0.41
2:H:141:LEU:HD21	2:H:194:LEU:HD11	2.03	0.41
4:F:59:HIS:HB3	4:F:62:ILE:HB	2.03	0.40
3:K:82:LEU:O	3:K:85:ILE:HG12	2.20	0.40
3:K:185:PRO:HA	3:K:188:LYS:HE3	2.03	0.40
3:E:113:ARG:HB2	3:E:116:THR:HB	2.03	0.40
3:E:425:ASP:OD1	3:E:461:ARG:HD3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:LYS:HE2	1:G:436:GLY:O	2.21	0.40
1:A:230:LEU:O	1:A:234:ILE:HD12	2.21	0.40
1:C:359:PRO:HA	1:C:360:PRO:HD3	1.98	0.40
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.04	0.40
3:K:492:VAL:HG13	3:K:504:PHE:CE1	2.56	0.40
1:A:223:THR:OG1	1:A:224:TYR:N	2.54	0.40
3:E:109:LEU:HD22	3:E:121:THR:HG23	2.03	0.40
1:I:234:ILE:HG21	1:I:302:MET:SD	2.61	0.40
2:J:83:PHE:O	2:J:86:ILE:HG22	2.22	0.40
4:L:125:HIS:O	4:L:129:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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	421/451 (93%)	407 (97%)	12 (3%)	2 (0%)	29	67
1	C	426/451 (94%)	415 (97%)	11 (3%)	0	100	100
1	G	419/451 (93%)	403 (96%)	14 (3%)	2 (0%)	29	67
1	I	431/451 (96%)	416 (96%)	14 (3%)	1 (0%)	47	79
2	B	426/445 (96%)	405 (95%)	21 (5%)	0	100	100
2	D	424/445 (95%)	405 (96%)	19 (4%)	0	100	100
2	H	425/445 (96%)	406 (96%)	19 (4%)	0	100	100
2	J	424/445 (95%)	403 (95%)	21 (5%)	0	100	100
3	E	481/554 (87%)	442 (92%)	35 (7%)	4 (1%)	19	58
3	K	481/554 (87%)	449 (93%)	30 (6%)	2 (0%)	34	69
4	F	123/140 (88%)	118 (96%)	5 (4%)	0	100	100
4	L	123/140 (88%)	116 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4604/4972 (93%)	4385 (95%)	208 (4%)	11 (0%)	47 79

All (11) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [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	358/377 (95%)	358 (100%)	0	100 100
1	C	360/377 (96%)	357 (99%)	3 (1%)	81 93
1	G	358/377 (95%)	355 (99%)	3 (1%)	81 93
1	I	363/377 (96%)	360 (99%)	3 (1%)	81 93
2	B	369/381 (97%)	365 (99%)	4 (1%)	73 88
2	D	368/381 (97%)	363 (99%)	5 (1%)	67 86
2	H	370/381 (97%)	366 (99%)	4 (1%)	73 88
2	J	368/381 (97%)	363 (99%)	5 (1%)	67 86
3	E	447/504 (89%)	441 (99%)	6 (1%)	69 87
3	K	447/504 (89%)	440 (98%)	7 (2%)	62 84
4	F	99/111 (89%)	98 (99%)	1 (1%)	76 90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	99/111 (89%)	98 (99%)	1 (1%)	76	90
All	All	4006/4262 (94%)	3964 (99%)	42 (1%)	76	90

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	85	GLN
2	B	139	HIS
2	B	158	ARG
2	B	325	MET
1	C	141	PHE
1	C	282	TYR
1	C	367	ASP
2	D	139	HIS
2	D	153	LEU
2	D	158	ARG
2	D	163	ASP
2	D	325	MET
3	E	47	ASN
3	E	156	CYS
3	E	179	LEU
3	E	353	GLN
3	E	469	ASP
3	E	533	LYS
4	F	167	LYS
1	G	38	SER
1	G	141	PHE
1	G	262	TYR
2	H	85	GLN
2	H	139	HIS
2	H	158	ARG
2	H	325	MET
1	I	46	ASP
1	I	47	ASP
1	I	367	ASP
2	J	139	HIS
2	J	153	LEU
2	J	158	ARG
2	J	163	ASP
2	J	325	MET
3	K	14	LEU
3	K	156	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	K	179	LEU
3	K	207	GLN
3	K	389	LEU
3	K	390	ARG
3	K	533	LYS
4	L	167	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	HIS
2	B	8	GLN
2	B	433	GLN
2	B	436	GLN
1	C	28	HIS
2	D	6	HIS
2	D	8	GLN
3	E	256	GLN
3	E	353	GLN
4	F	125	HIS
2	J	6	HIS
2	J	8	GLN
3	K	135	GLN
3	K	249	GLN
3	K	256	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

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GDP	H	600	6	24,30,30	0.95	1 (4%)	30,47,47	1.20	4 (13%)
5	GTP	G	600	6	26,34,34	1.11	2 (7%)	32,54,54	1.52	6 (18%)
5	GTP	A	600	6	26,34,34	1.11	2 (7%)	32,54,54	1.51	7 (21%)
7	GDP	B	600	6	24,30,30	0.92	1 (4%)	30,47,47	1.23	4 (13%)
5	GTP	I	600	6	26,34,34	1.11	2 (7%)	32,54,54	1.57	6 (18%)
7	GDP	D	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.24	4 (13%)
7	GDP	J	600	6	24,30,30	0.93	1 (4%)	30,47,47	1.21	4 (13%)
5	GTP	C	600	6	26,34,34	1.10	2 (7%)	32,54,54	1.55	6 (18%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GDP	H	600	6	-	4/12/32/32	0/3/3/3
5	GTP	G	600	6	-	5/18/38/38	0/3/3/3
5	GTP	A	600	6	-	6/18/38/38	0/3/3/3
7	GDP	B	600	6	-	5/12/32/32	0/3/3/3
5	GTP	I	600	6	-	8/18/38/38	0/3/3/3
7	GDP	D	600	6	-	4/12/32/32	0/3/3/3
7	GDP	J	600	6	-	4/12/32/32	0/3/3/3
5	GTP	C	600	6	-	7/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	GTP	C5-C6	-3.92	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	600	GTP	C5-C6	-3.91	1.39	1.47
5	I	600	GTP	C5-C6	-3.86	1.39	1.47
5	C	600	GTP	C5-C6	-3.83	1.39	1.47
7	H	600	GDP	C6-N1	-2.36	1.34	1.37
7	J	600	GDP	C6-N1	-2.28	1.34	1.37
5	G	600	GTP	C2-N3	2.27	1.38	1.33
5	C	600	GTP	C2-N3	2.26	1.38	1.33
5	A	600	GTP	C2-N3	2.21	1.38	1.33
5	I	600	GTP	C2-N3	2.20	1.38	1.33
7	B	600	GDP	C6-N1	-2.19	1.34	1.37
7	D	600	GDP	C6-N1	-2.14	1.34	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	600	GTP	PB-O3B-PG	-3.51	120.78	132.83
7	H	600	GDP	PA-O3A-PB	-3.48	120.88	132.83
5	I	600	GTP	PB-O3B-PG	-3.48	120.89	132.83
5	C	600	GTP	PB-O3B-PG	-3.47	120.91	132.83
5	A	600	GTP	PB-O3B-PG	-3.40	121.15	132.83
5	G	600	GTP	C5-C6-N1	3.30	119.78	113.95
5	C	600	GTP	PA-O3A-PB	-3.27	121.61	132.83
5	C	600	GTP	C5-C6-N1	3.26	119.70	113.95
7	B	600	GDP	PA-O3A-PB	-3.25	121.68	132.83
5	I	600	GTP	PA-O3A-PB	-3.25	121.68	132.83
5	I	600	GTP	C5-C6-N1	3.22	119.63	113.95
5	A	600	GTP	PA-O3A-PB	-3.20	121.84	132.83
5	A	600	GTP	C5-C6-N1	3.16	119.53	113.95
7	J	600	GDP	PA-O3A-PB	-3.15	122.02	132.83
5	I	600	GTP	C8-N7-C5	3.11	108.92	102.99
7	D	600	GDP	PA-O3A-PB	-3.11	122.14	132.83
5	C	600	GTP	C8-N7-C5	3.07	108.83	102.99
5	G	600	GTP	C8-N7-C5	3.06	108.81	102.99
5	G	600	GTP	PA-O3A-PB	-3.02	122.47	132.83
5	A	600	GTP	C8-N7-C5	2.95	108.60	102.99
5	G	600	GTP	C2-N1-C6	-2.92	119.72	125.10
5	I	600	GTP	C3'-C2'-C1'	2.85	105.27	100.98
5	I	600	GTP	C2-N1-C6	-2.84	119.87	125.10
5	A	600	GTP	C2-N1-C6	-2.84	119.87	125.10
5	C	600	GTP	C2-N1-C6	-2.83	119.88	125.10
5	C	600	GTP	C3'-C2'-C1'	2.73	105.08	100.98
7	D	600	GDP	C3'-C2'-C1'	2.70	105.05	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	GDP	C3'-C2'-C1'	2.44	104.65	100.98
7	H	600	GDP	C8-N7-C5	2.38	107.53	102.99
7	H	600	GDP	C3'-C2'-C1'	2.37	104.54	100.98
7	J	600	GDP	C3'-C2'-C1'	2.36	104.54	100.98
7	B	600	GDP	C8-N7-C5	2.34	107.45	102.99
7	J	600	GDP	C5-C6-N1	2.32	118.05	113.95
7	J	600	GDP	C8-N7-C5	2.31	107.39	102.99
7	D	600	GDP	C8-N7-C5	2.28	107.34	102.99
5	A	600	GTP	C3'-C2'-C1'	2.28	104.41	100.98
7	D	600	GDP	C5-C6-N1	2.26	117.95	113.95
7	B	600	GDP	C5-C6-N1	2.26	117.95	113.95
7	H	600	GDP	C5-C6-N1	2.19	117.82	113.95
5	G	600	GTP	C3'-C2'-C1'	2.12	104.17	100.98
5	A	600	GTP	O6-C6-C5	-2.06	120.34	124.37

There are no chirality outliers.

All (43) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

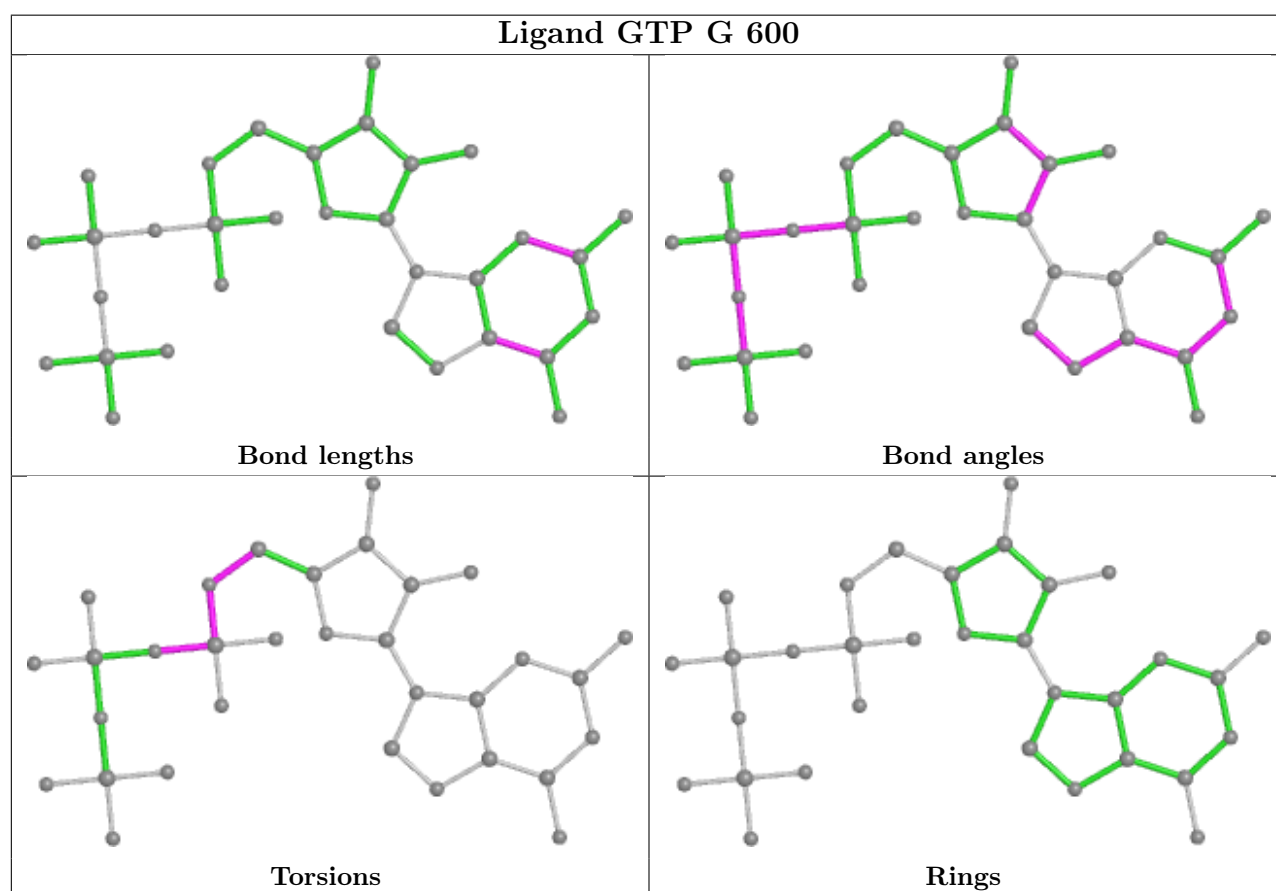
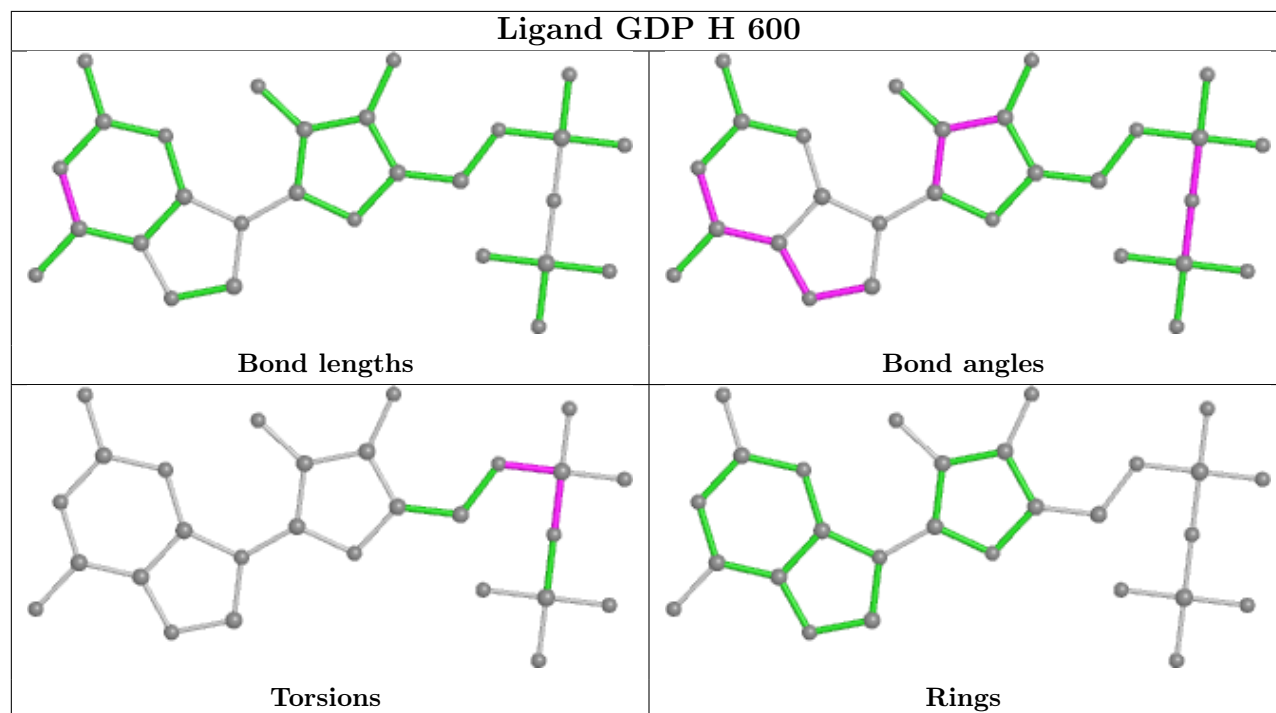
There are no ring outliers.

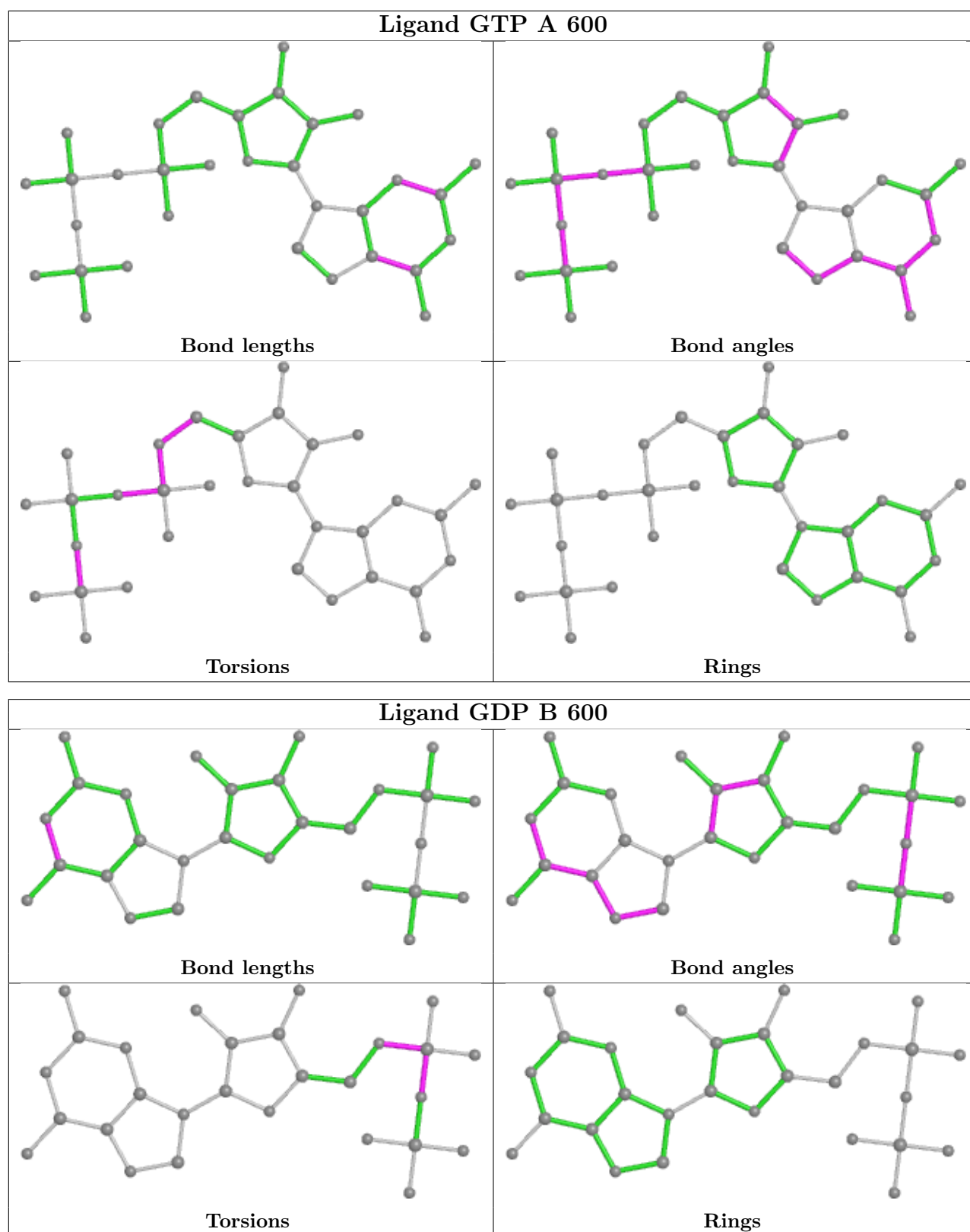
7 monomers are involved in 8 short contacts:

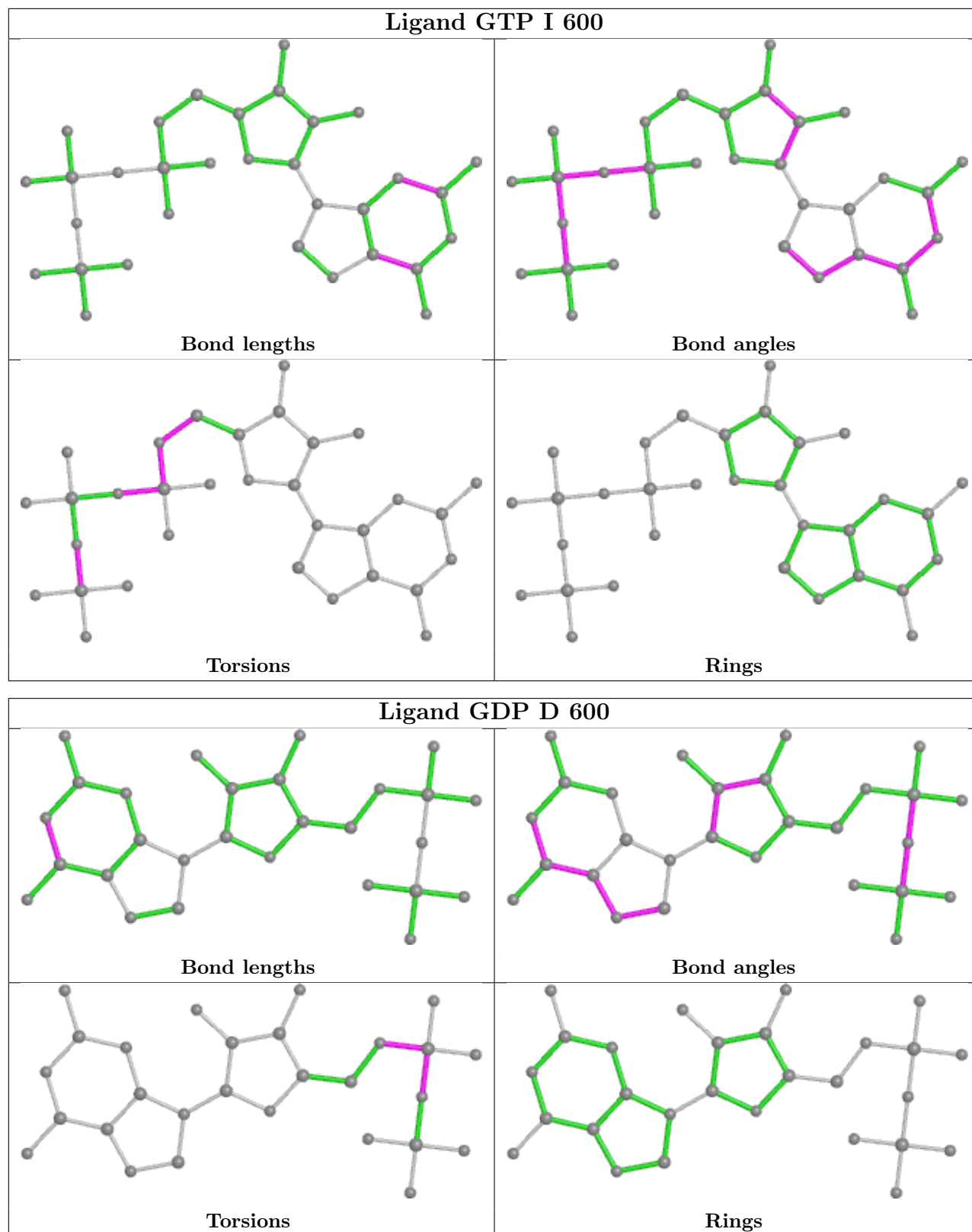
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	600	GDP	1	0
5	A	600	GTP	1	0
7	B	600	GDP	1	0
5	I	600	GTP	1	0
7	D	600	GDP	2	0
7	J	600	GDP	1	0
5	C	600	GTP	1	0

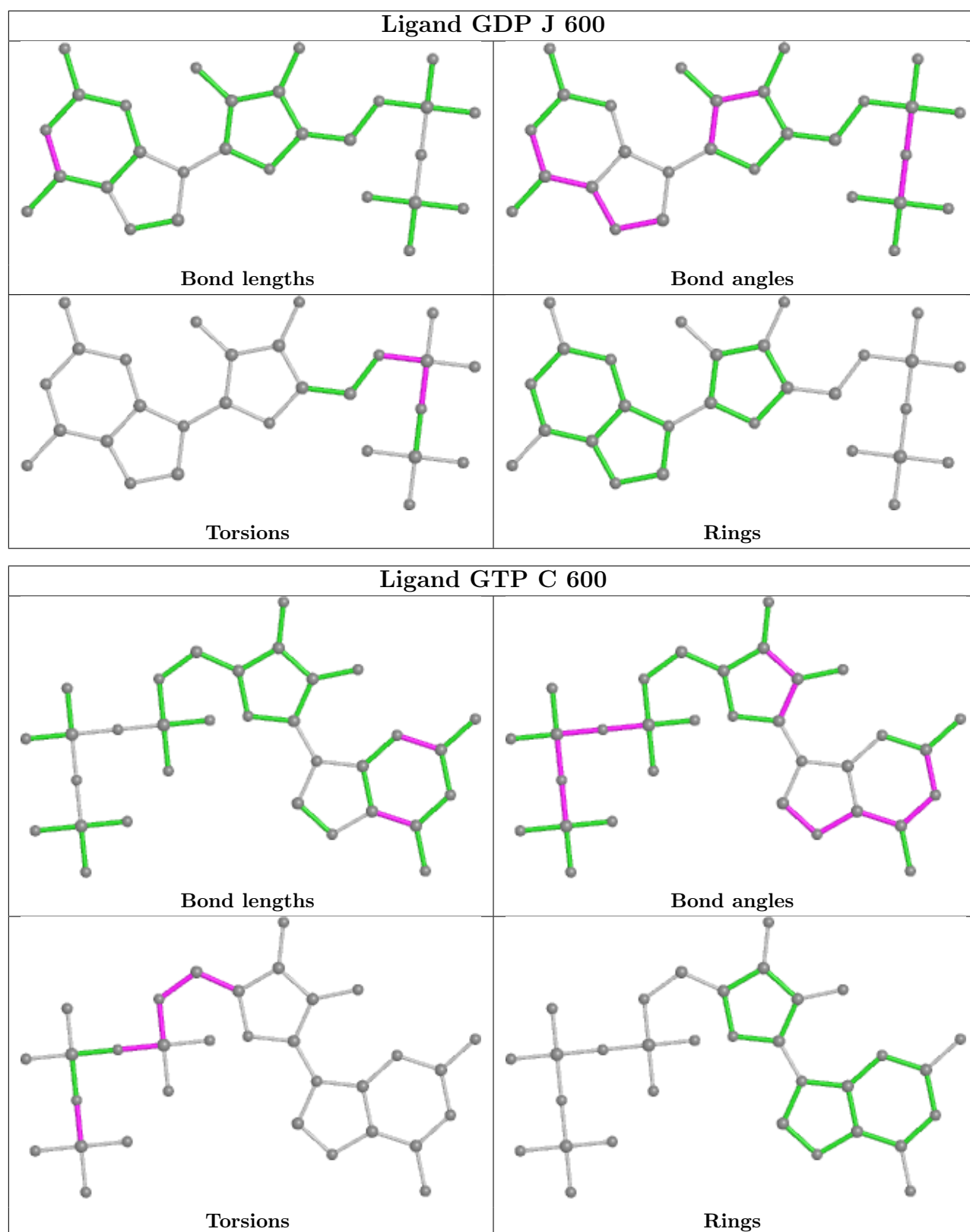
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/451 (94%)	0.04	6 (1%) 75 63	13, 44, 82, 123	0
1	C	434/451 (96%)	-0.12	2 (0%) 91 86	12, 32, 61, 80	0
1	G	425/451 (94%)	-0.02	1 (0%) 95 94	15, 40, 76, 97	0
1	I	436/451 (96%)	-0.08	6 (1%) 75 63	13, 35, 73, 122	0
2	B	430/445 (96%)	-0.00	4 (0%) 84 75	15, 43, 86, 124	0
2	D	428/445 (96%)	0.12	4 (0%) 84 75	20, 50, 92, 124	0
2	H	429/445 (96%)	-0.04	1 (0%) 95 94	17, 38, 78, 116	0
2	J	428/445 (96%)	0.23	14 (3%) 46 30	22, 56, 95, 131	0
3	E	487/554 (87%)	0.04	9 (1%) 68 55	13, 45, 95, 133	0
3	K	487/554 (87%)	0.17	18 (3%) 41 26	22, 52, 102, 127	0
4	F	125/140 (89%)	0.08	1 (0%) 86 78	17, 53, 95, 105	0
4	L	125/140 (89%)	0.24	4 (3%) 47 31	31, 53, 111, 147	0
All	All	4661/4972 (93%)	0.04	70 (1%) 73 61	12, 44, 90, 147	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	482	PRO	6.4
1	A	40	LYS	4.8
2	J	179	ASP	4.2
4	L	43	THR	4.1
2	J	283	TYR	4.0
3	K	525	LYS	3.8
3	K	435	ASP	3.7
3	K	307	PRO	3.4
1	A	38	SER	3.4
3	K	394	THR	3.3
2	J	281	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	39	ASP	3.1
1	C	337	THR	3.1
4	L	160	ASP	3.1
2	H	1	MET	3.1
3	E	301	PRO	3.1
3	E	302	PHE	3.1
3	K	517	ARG	3.1
2	J	1	MET	3.0
2	D	356	CYS	3.0
3	E	394	THR	3.0
3	E	482	PRO	3.0
4	L	161	LEU	3.0
3	K	302	PHE	2.9
1	I	39	ASP	2.9
1	C	47	ASP	2.9
3	E	469	ASP	2.9
2	J	441	ASP	2.8
2	J	220	THR	2.8
3	E	483	GLU	2.8
3	K	475	GLN	2.7
2	B	282	GLN	2.7
3	K	317	ASP	2.6
1	A	55	GLU	2.6
1	I	41	THR	2.6
2	B	1	MET	2.6
1	I	40	LYS	2.6
4	F	43	THR	2.6
4	L	165	LEU	2.6
3	K	478	PHE	2.5
2	B	280	SER	2.5
3	E	90	ASN	2.5
3	K	434	ASP	2.5
2	D	1	MET	2.5
3	K	486	THR	2.4
3	E	14	LEU	2.4
1	I	88	HIS	2.4
1	A	346	TRP	2.3
3	E	481	LEU	2.3
2	B	279	GLY	2.3
2	J	134	GLY	2.3
3	K	397	TYR	2.2
3	K	90	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	281	GLN	2.2
2	J	326	LYS	2.2
1	I	42	ILE	2.2
2	J	35	SER	2.2
2	J	203	CYS	2.2
1	I	46	ASP	2.2
3	K	91	VAL	2.2
1	G	35	GLN	2.1
2	J	373	MET	2.1
3	K	89	PRO	2.1
2	J	278	ARG	2.1
2	J	282	GLN	2.1
2	J	71	GLU	2.1
1	A	340	THR	2.1
3	K	436	CYS	2.0
2	D	42	LEU	2.0
3	K	469	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

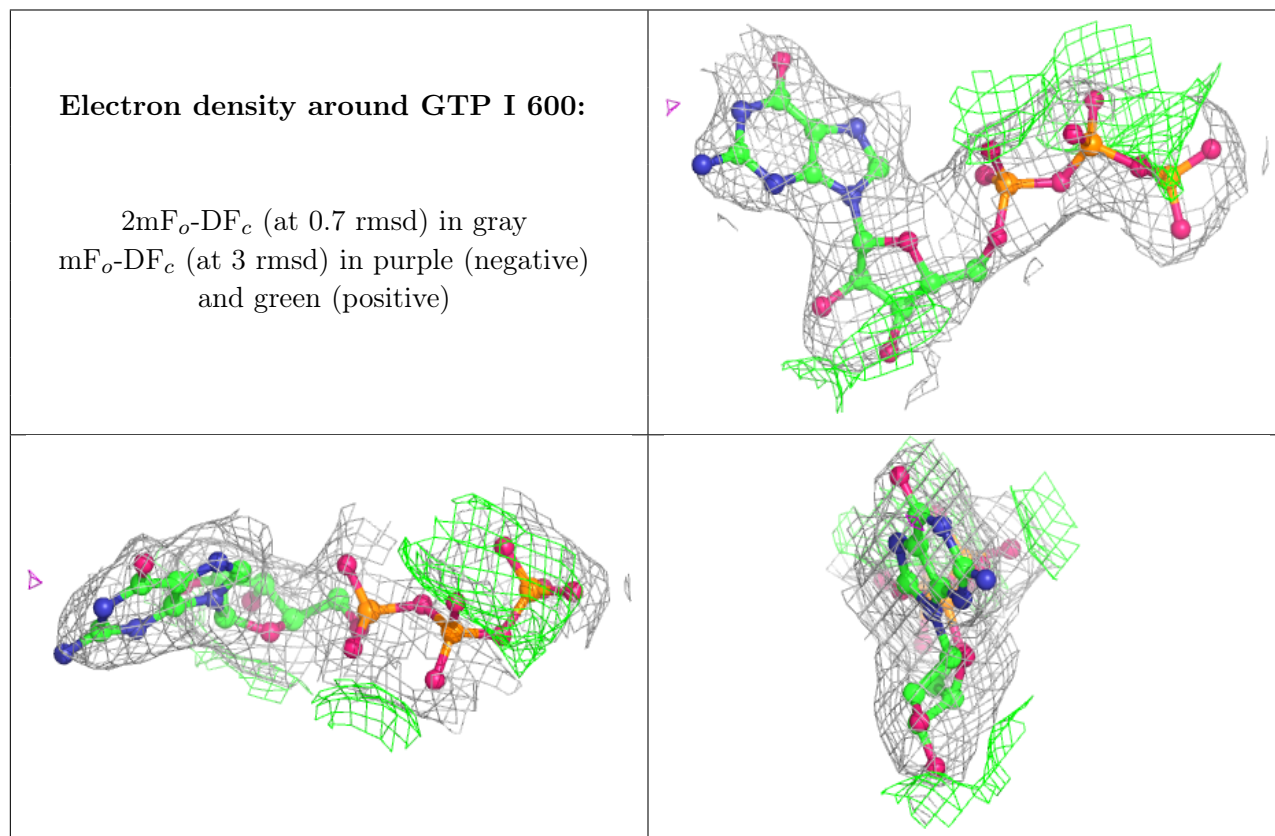
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	B	601	1/1	0.94	0.17	52,52,52,52	0
6	MG	J	601	1/1	0.95	0.11	10,10,10,10	0
6	MG	G	601	1/1	0.96	0.31	15,15,15,15	0
6	MG	H	601	1/1	0.96	0.16	13,13,13,13	0
6	MG	I	601	1/1	0.96	0.20	1,1,1,1	0
6	MG	C	601	1/1	0.96	0.23	11,11,11,11	0

Continued on next page...

Continued from previous page...

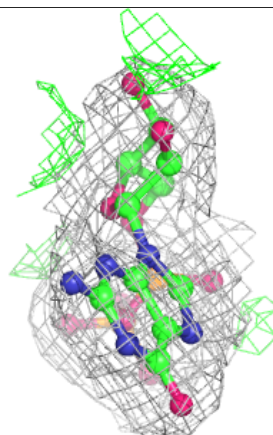
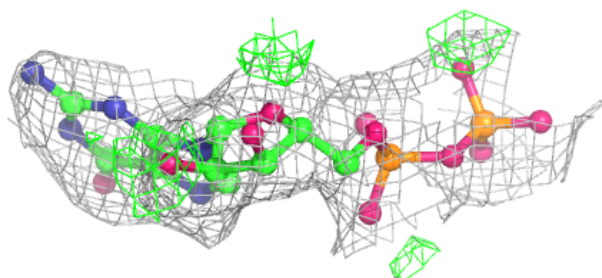
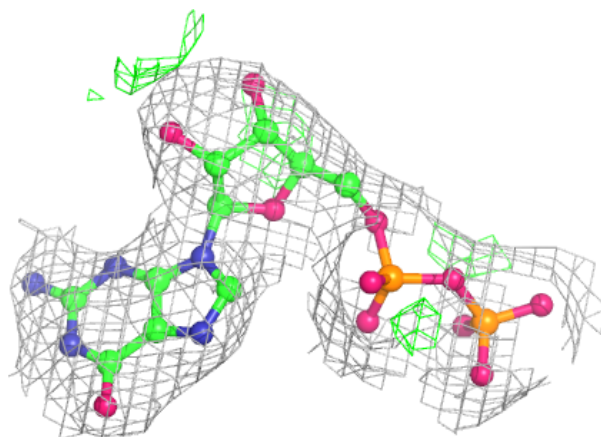
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	I	600	32/32	0.97	0.20	0,41,57,66	0
6	MG	D	601	1/1	0.97	0.17	18,18,18,18	0
7	GDP	J	600	28/28	0.97	0.16	25,42,53,61	0
5	GTP	A	600	32/32	0.98	0.21	3,30,46,61	0
5	GTP	C	600	32/32	0.98	0.19	0,30,44,51	0
7	GDP	B	600	28/28	0.98	0.18	25,47,59,62	0
7	GDP	D	600	28/28	0.98	0.19	20,46,63,68	0
7	GDP	H	600	28/28	0.98	0.18	11,29,51,71	0
5	GTP	G	600	32/32	0.98	0.21	8,33,57,60	0
6	MG	A	601	1/1	0.99	0.29	20,20,20,20	0

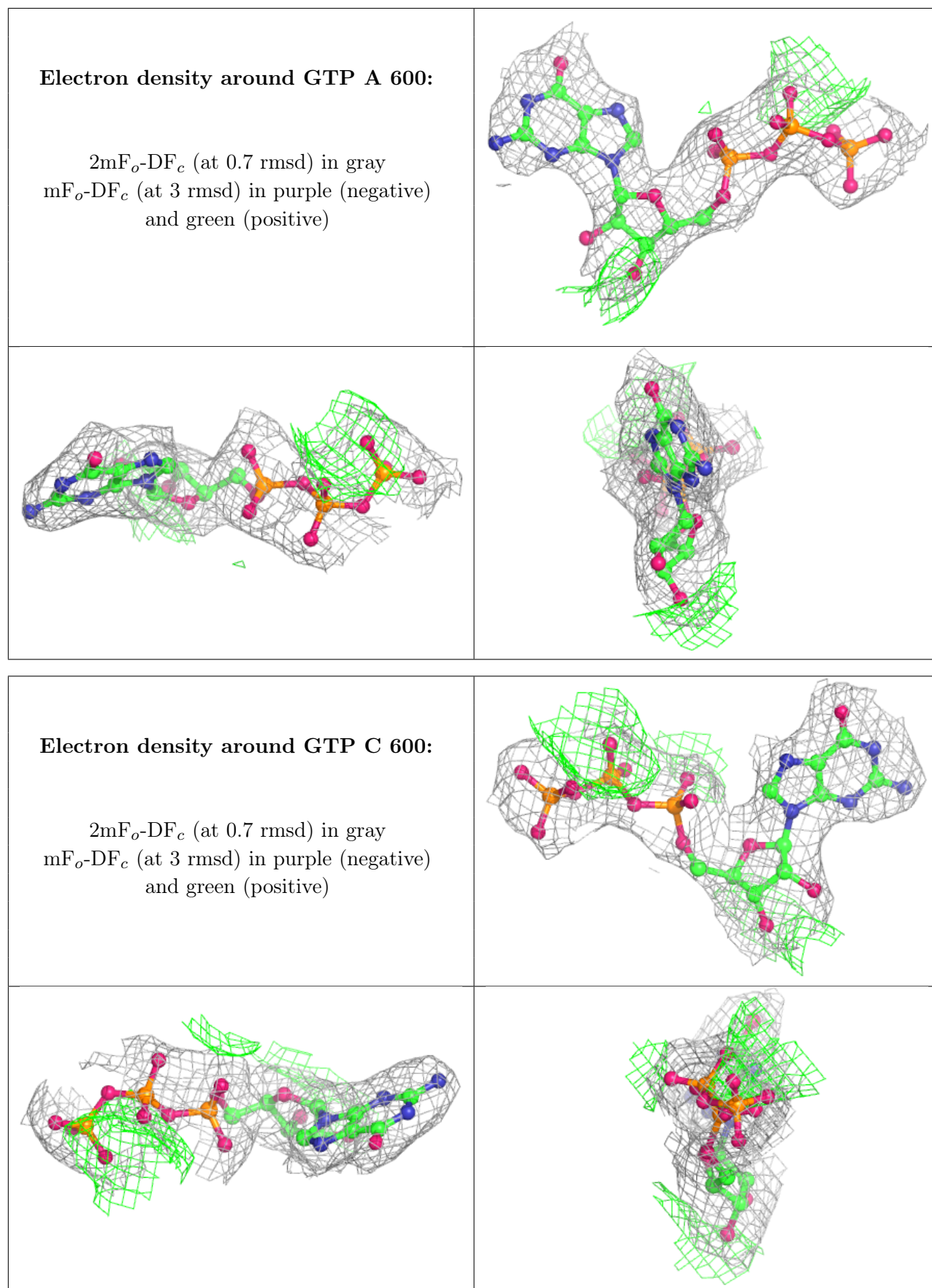
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

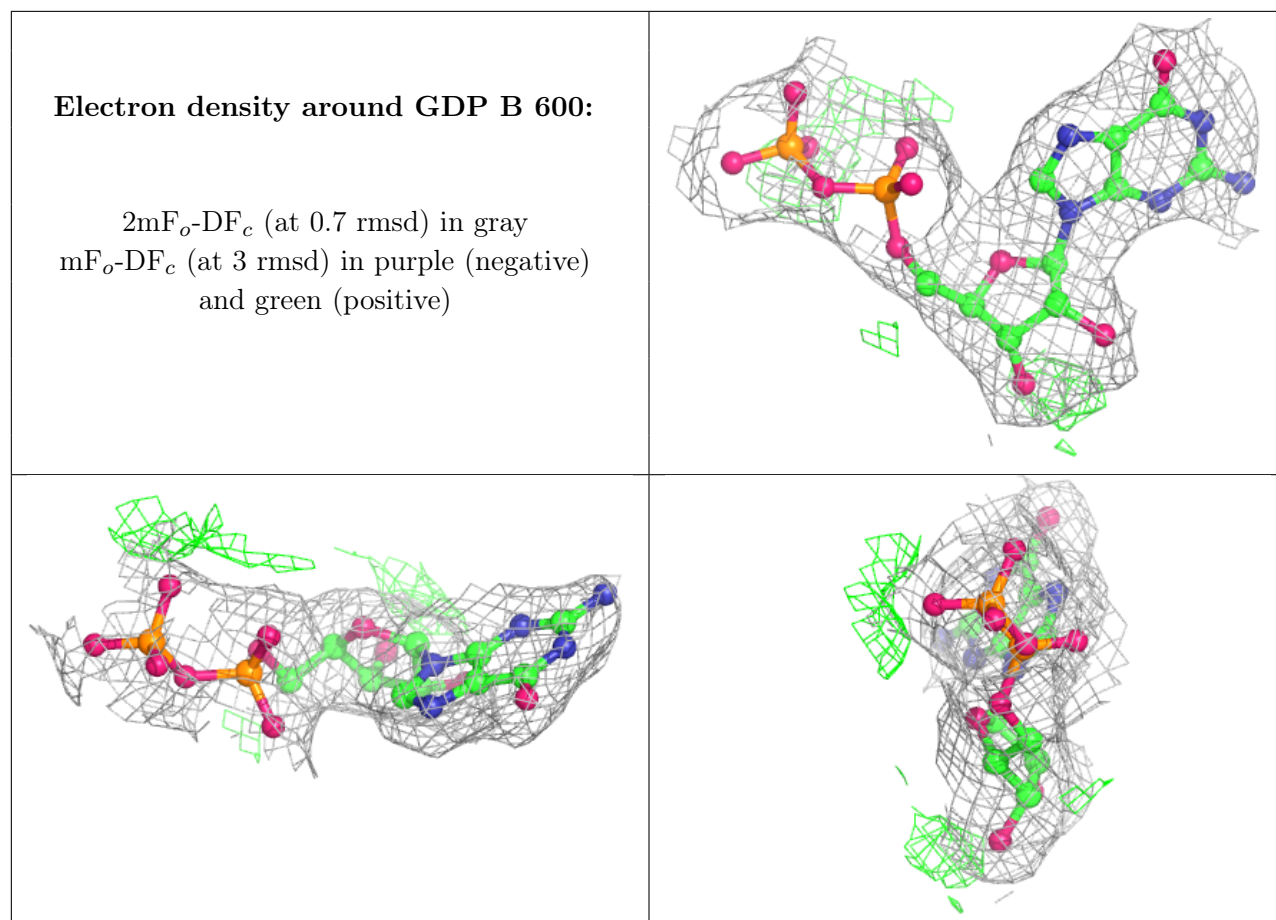


Electron density around GDP J 600:

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

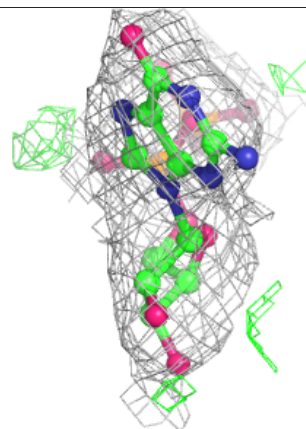
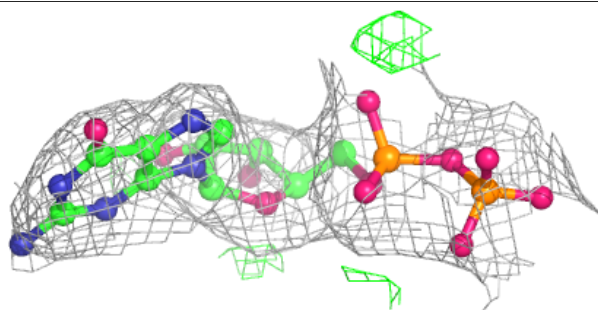
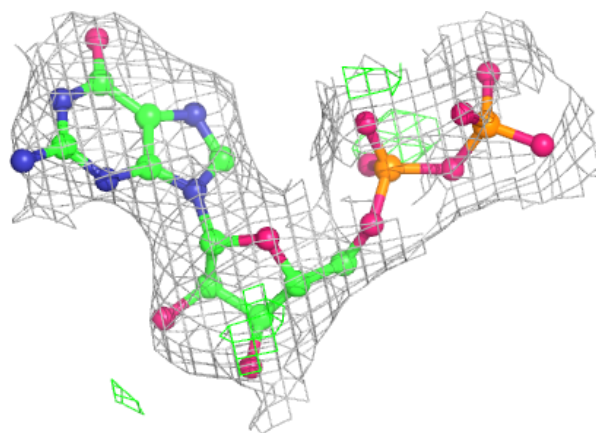






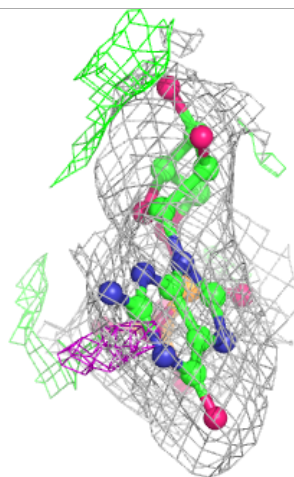
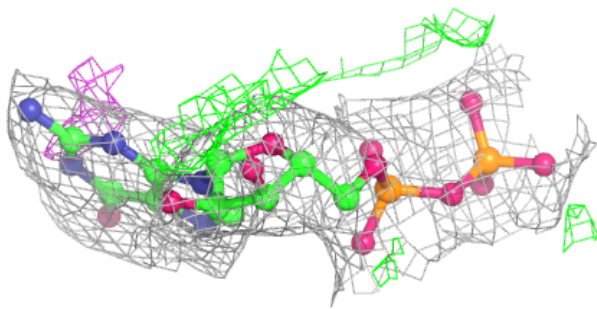
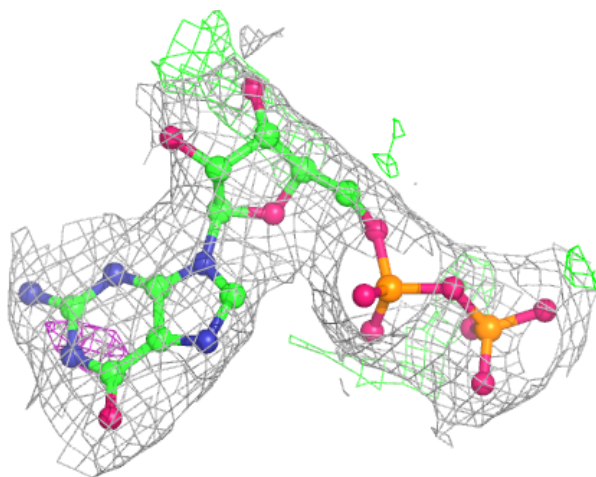
Electron density around GDP D 600:

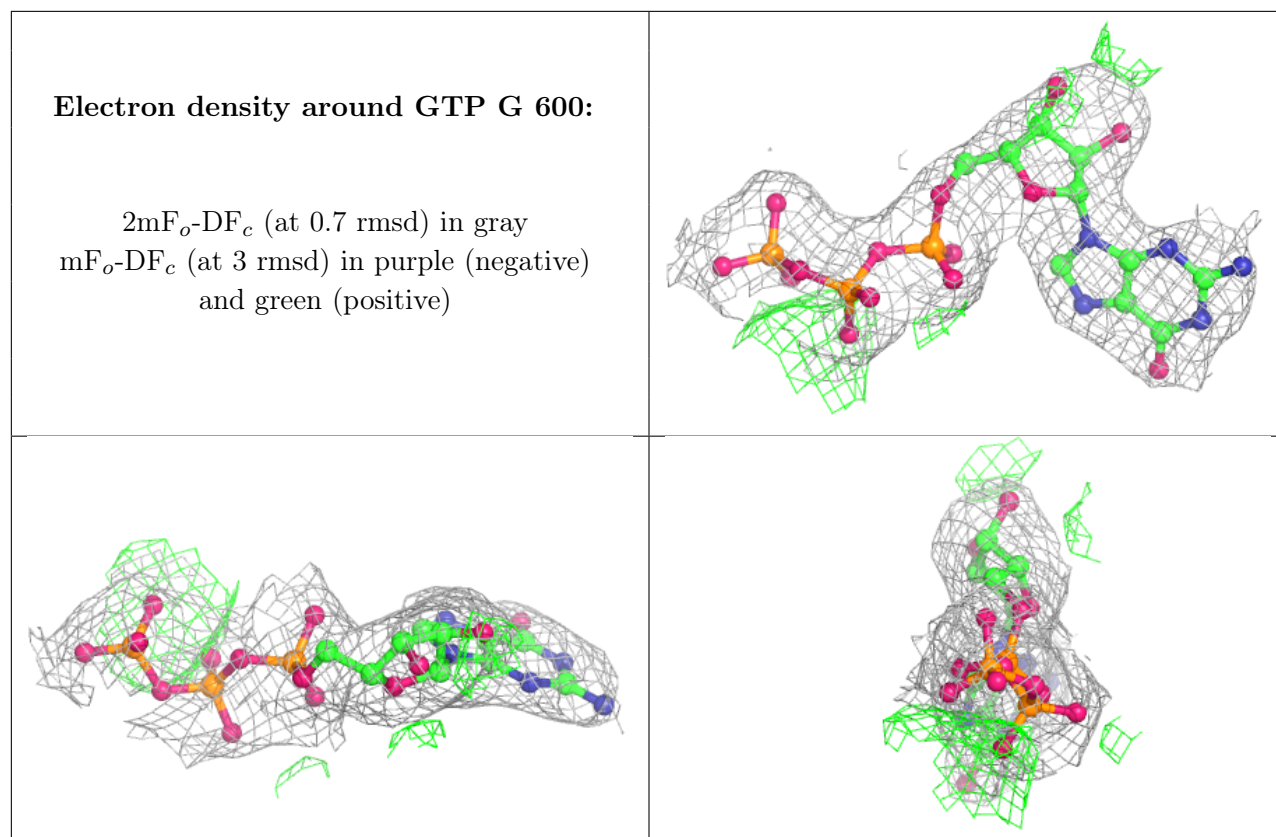
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP 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](#)

There are no such residues in this entry.