



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 04:06 am BST

PDB ID : 3RYH
Title : GMPCPP-Tubulin: RB3 Stathmin-like domain complex
Authors : Nawrotek, A.; Knossow, M.; Gigant, B.
Deposited on : 2011-05-11
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

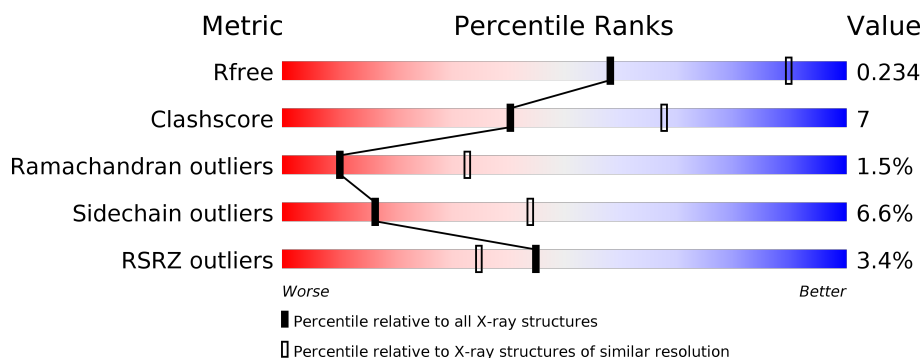
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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> <div>0%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	451	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
2	D	445	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
3	E	143	<div> <div>9%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 6%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	C	453	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15107 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
1	A	437	Total	C	N	O	S	0	1	0
			3430	2170	581	656	23			
1	C	432	Total	C	N	O	S	0	0	0
			3359	2128	571	638	22			

There are 4 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

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	7	0
			3443	2163	585	668	27			
2	D	431	Total	C	N	O	S	0	7	0
			3435	2155	588	666	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

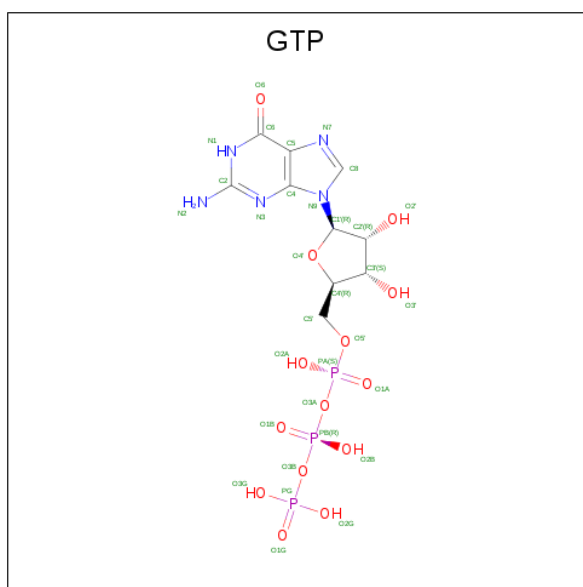
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	135	Total	C	N	O	S	0	0	0
			1076	666	195	211	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	ACE	-	SEE REMARK 999	UNP P63043
E	4	ALA	-	SEE REMARK 999	UNP P63043
E	14	ALA	CYS	ENGINEERED MUTATION	UNP P63043
E	20	TRP	PHE	ENGINEERED MUTATION	UNP P63043

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



Continued from previous page...

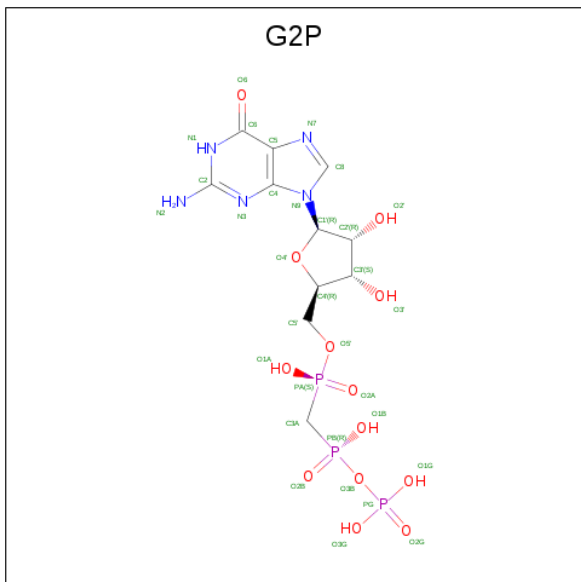
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 32	C 11	N 5	O 13	P 3	0	0
7	D	1	Total 32	C 11	N 5	O 13	P 3	0	0

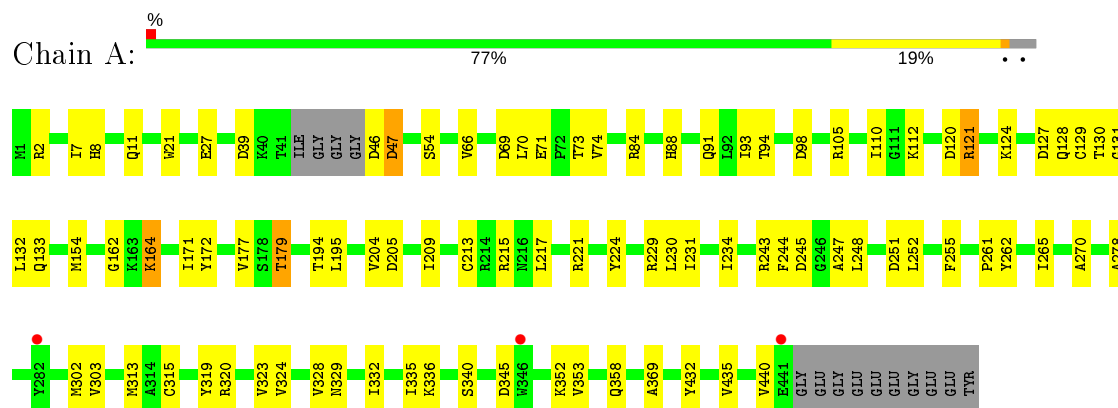
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	53	Total O 53 53	0	0
8	B	48	Total O 48 48	0	0
8	C	47	Total O 47 47	0	0
8	D	40	Total O 40 40	0	1
8	E	4	Total O 4 4	0	0

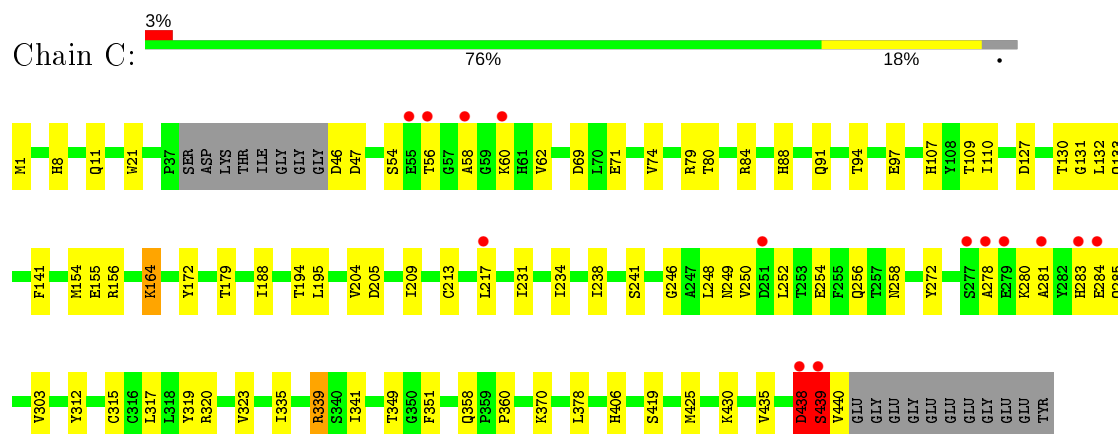
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

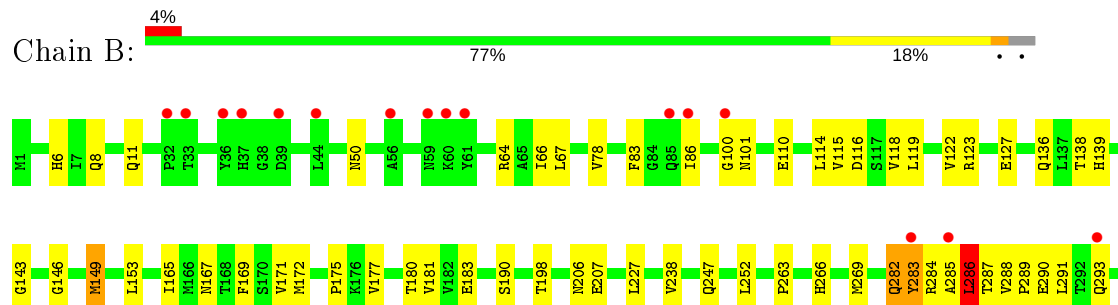
• Molecule 1: Tubulin alpha chain

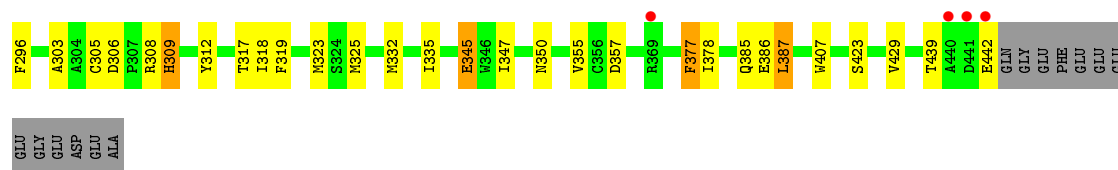


• Molecule 1: Tubulin alpha chain

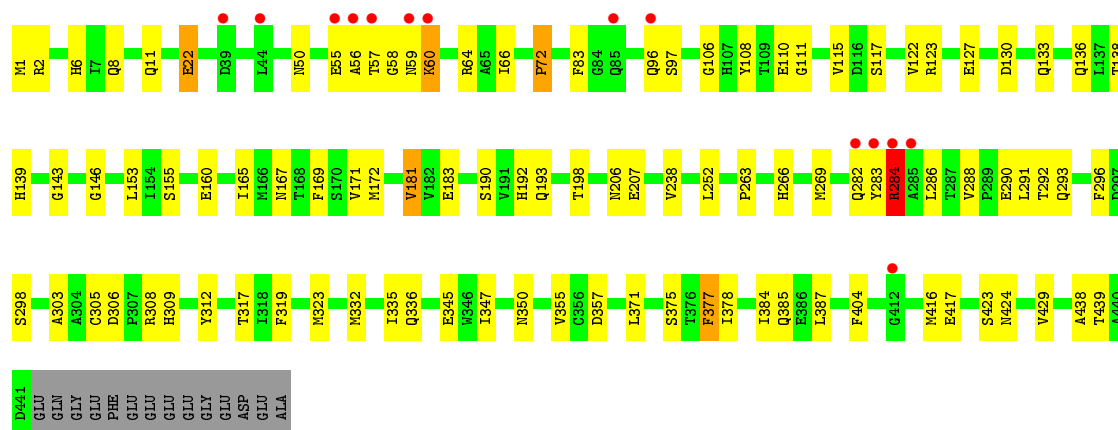


• Molecule 2: Tubulin beta chain

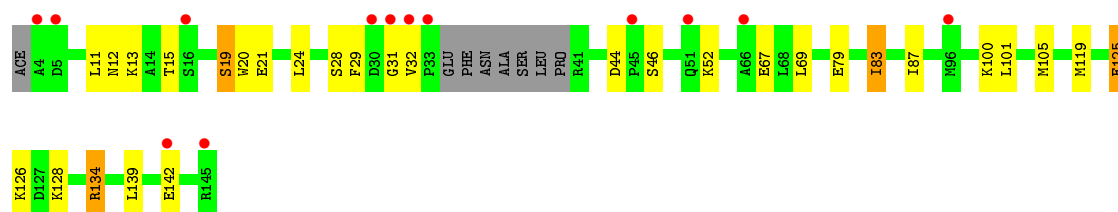
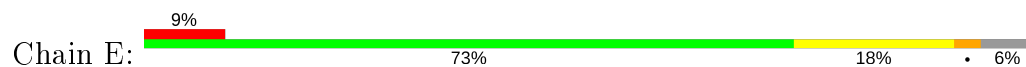




• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.27Å 128.21Å 250.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.13 – 2.80 42.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.13-2.80) 97.6 (42.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.165 , 0.217 0.183 , 0.234	Depositor DCC
R_{free} test set	2584 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.809	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15107	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, SO4, G2P

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	0.53	1/3507 (0.0%)	0.73	1/4761 (0.0%)
1	C	0.52	0/3434	0.75	1/4665 (0.0%)
2	B	0.50	0/3531	0.72	0/4782
2	D	0.49	0/3522	0.70	0/4769
3	E	0.53	0/1087	0.73	0/1450
All	All	0.51	1/15081 (0.0%)	0.73	2/20427 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	SER	CB-OG	9.07	1.54	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	ASP	C-N-CA	7.93	141.52	121.70
1	A	440	VAL	C-N-CA	5.09	134.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	142	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3331	54	0
1	C	3359	0	3262	44	0
2	B	3443	0	3293	56	0
2	D	3435	0	3293	62	0
3	E	1076	0	1063	17	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	5	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
7	B	32	0	13	4	0
7	D	32	0	13	4	0
8	A	53	0	0	3	0
8	B	48	0	0	1	0
8	C	47	0	0	0	0
8	D	40	0	0	3	0
8	E	4	0	0	0	0
All	All	15107	0	14292	211	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 7.

All (211) 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:D:2:ARG:HH21	2:D:130:ASP:HB3	1.27	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:HH21	2:D:130:ASP:CB	1.82	0.93
2:D:2:ARG:NH2	2:D:130:ASP:CG	2.25	0.89
1:A:265:ILE:HB	8:A:661:HOH:O	1.81	0.78
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.49	0.77
2:D:2:ARG:HH21	2:D:130:ASP:CG	1.88	0.77
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.51	0.76
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.22	0.75
2:D:292:THR:HG22	2:D:335:ILE:HG13	1.67	0.75
2:B:183:GLU:OE2	7:B:600:G2P:H3'	1.88	0.74
2:B:263:PRO:O	2:B:266:HIS:HD2	1.71	0.73
2:D:263:PRO:O	2:D:266:HIS:HD2	1.70	0.73
1:A:132:LEU:HD23	1:A:164:LYS:HD3	1.72	0.72
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.72	0.71
2:D:143:GLY:HA3	7:D:600:G2P:H3A1	1.72	0.70
2:B:114:LEU:HB3	2:B:149:MET:HE3	1.73	0.70
2:B:50:ASN:O	2:B:64:ARG:NH2	2.24	0.70
1:A:204:VAL:HG22	1:A:302[B]:MET:HE2	1.74	0.70
2:D:183:GLU:OE2	7:D:600:G2P:H3'	1.92	0.70
2:B:143:GLY:HA3	7:B:600:G2P:H3A1	1.75	0.68
2:D:283:TYR:O	2:D:284:ARG:HB2	1.91	0.68
2:D:206:ASN:HD21	7:D:600:G2P:H2N2	1.40	0.67
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.75	0.67
2:B:206:ASN:HD21	7:B:600:G2P:H2N2	1.42	0.67
2:D:2:ARG:NH2	2:D:130:ASP:OD2	2.28	0.67
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.76	0.66
2:B:101:ASN:HD22	1:C:258:ASN:HD21	1.43	0.66
1:A:204:VAL:HG22	1:A:302[B]:MET:CE	2.25	0.65
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.27	0.65
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.78	0.64
2:D:139:HIS:HD2	2:D:146:GLY:O	1.80	0.64
1:C:132:LEU:HD23	1:C:164:LYS:HD3	1.79	0.64
1:C:339:ARG:HD3	1:C:339:ARG:H	1.63	0.63
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.80	0.63
2:B:345:GLU:HG2	8:B:656:HOH:O	1.98	0.63
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.79	0.62
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.81	0.62
2:B:101:ASN:HB3	2:B:180:THR:HG21	1.81	0.62
1:A:247:ALA:HB1	3:E:12:ASN:HB2	1.81	0.62
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.83	0.61
1:A:127:ASP:C	1:A:129:CYS:H	2.04	0.60
2:D:296[B]:PHE:HB3	2:D:308:ARG:HE	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.83	0.60
2:B:296[B]:PHE:HB3	2:B:308:ARG:HE	1.66	0.60
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.82	0.60
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.84	0.60
2:B:114:LEU:O	2:B:118:VAL:HG23	2.03	0.59
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.85	0.59
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.85	0.59
1:C:335:ILE:HG23	1:C:341:ILE:HD13	1.86	0.58
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.39	0.58
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.86	0.57
2:D:317:THR:HG21	2:D:332:MET:HE1	1.85	0.57
2:D:50:ASN:O	2:D:64:ARG:NH2	2.32	0.57
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.70	0.57
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.39	0.56
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.70	0.56
2:D:58:GLY:C	2:D:60:LYS:H	2.09	0.56
2:D:193:GLN:HE22	3:E:126:LYS:HE2	1.71	0.56
1:A:345:ASP:HB3	3:E:29:PHE:HB3	1.89	0.55
1:C:213:CYS:HA	1:C:217:LEU:HD12	1.89	0.55
2:D:72:PRO:HG3	2:D:96:GLN:HA	1.87	0.55
1:A:261:PRO:HG3	1:A:313:MET:HG3	1.89	0.55
1:C:156:ARG:HD3	3:E:101:LEU:HD21	1.89	0.54
1:A:127:ASP:O	1:A:129:CYS:N	2.41	0.54
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.43	0.53
2:D:133:GLN:NE2	2:D:252:LEU:H	2.06	0.53
2:D:58:GLY:O	2:D:60:LYS:N	2.41	0.53
2:B:114:LEU:HB3	2:B:149:MET:CE	2.38	0.53
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.43	0.53
1:A:121:ARG:NH2	8:A:658:HOH:O	2.23	0.52
2:D:22:GLU:HB3	2:D:83:PHE:CD2	2.44	0.52
2:D:283:TYR:O	2:D:284:ARG:CB	2.57	0.52
1:A:234:ILE:HG21	1:A:302[B]:MET:HE3	1.90	0.52
1:C:56:THR:HG23	1:C:58:ALA:H	1.75	0.52
2:D:2:ARG:HH22	2:D:130:ASP:CG	2.13	0.52
1:C:141:PHE:HD1	1:C:172:TYR:HA	1.75	0.51
2:D:308:ARG:CZ	8:D:640:HOH:O	2.58	0.51
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.92	0.51
1:C:204:VAL:HG13	1:C:209:ILE:HD11	1.93	0.51
1:C:133:GLN:NE2	1:C:252:LEU:H	2.08	0.51
2:D:312:TYR:CE2	2:D:377[A]:PHE:HZ	2.29	0.51
2:D:438:ALA:O	8:D:626:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG11	1:A:231:ILE:HG12	1.93	0.51
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.57	0.51
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.29	0.51
1:A:248:LEU:HB2	3:E:19:SER:HB2	1.92	0.51
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.93	0.50
2:D:123:ARG:O	2:D:127:GLU:HG2	2.11	0.50
2:B:139:HIS:HD2	2:B:146:GLY:O	1.93	0.50
2:B:317:THR:HG21	2:B:332:MET:HE1	1.92	0.50
1:A:345:ASP:HB3	3:E:29:PHE:CB	2.42	0.50
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.47	0.50
1:C:88:HIS:O	1:C:91:GLN:HG2	2.12	0.50
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.93	0.49
1:A:244:PHE:CG	1:A:358:GLN:HG3	2.47	0.49
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.30	0.49
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.93	0.49
1:C:320:ARG:HD3	1:C:360:PRO:HB3	1.95	0.49
2:B:312:TYR:CE2	2:B:377[A]:PHE:HZ	2.31	0.49
1:A:270:ALA:HB3	1:A:302[B]:MET:SD	2.52	0.49
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.49
2:D:288:VAL:HG22	2:D:323:MET:HE3	1.95	0.49
3:E:83:ILE:O	3:E:87:ILE:HG12	2.13	0.49
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.61	0.48
1:A:121:ARG:HA	1:A:124:LYS:HG3	1.94	0.48
1:A:245:ASP:HB3	3:E:15:THR:HB	1.95	0.48
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.59	0.48
1:A:88:HIS:O	1:A:91:GLN:HG2	2.13	0.48
1:C:204:VAL:HG11	1:C:231:ILE:HG12	1.93	0.48
1:C:133:GLN:HE22	1:C:252:LEU:H	1.62	0.48
1:A:252:LEU:HA	1:A:255:PHE:HD2	1.79	0.48
1:A:262:TYR:HB2	1:A:265:ILE:HD12	1.96	0.47
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.95	0.47
2:B:319:PHE:HB2	2:B:355:VAL:HG22	1.96	0.47
2:D:308:ARG:HD2	8:D:648:HOH:O	2.15	0.47
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.97	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.46
2:B:100:GLY:HA2	1:C:254:GLU:HG2	1.97	0.46
1:C:284:GLU:CB	1:C:285:GLN:HA	2.46	0.46
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.96	0.46
1:C:56:THR:HG22	1:C:60:LYS:H	1.81	0.46
1:A:7:ILE:HG23	1:A:66:VAL:HG13	1.97	0.46
2:D:1:MET:SD	2:D:133:GLN:HA	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296[B]:PHE:HB3	2:B:308:ARG:NE	2.29	0.46
1:C:205:ASP:HB3	1:C:303:VAL:HA	1.98	0.46
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.98	0.46
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.98	0.45
2:B:282:GLN:CB	2:B:283:TYR:HA	2.46	0.45
1:C:438:ASP:HA	1:C:439:SER:HB2	1.98	0.45
2:D:296[B]:PHE:HB3	2:D:308:ARG:NE	2.29	0.45
2:B:309:HIS:CD2	2:B:386:GLU:OE1	2.64	0.45
1:C:246:GLY:H	1:C:249:ASN:HD21	1.64	0.45
2:B:67:LEU:CD2	2:B:78:VAL:HG11	2.47	0.45
2:D:2:ARG:NH2	2:D:130:ASP:CB	2.61	0.45
1:C:107:HIS:HE1	1:C:155:GLU:OE2	2.00	0.45
2:D:108:TYR:O	3:E:134:ARG:HD2	2.17	0.44
2:D:319:PHE:HB2	2:D:355:VAL:HG22	1.98	0.44
1:A:133:GLN:HE22	1:A:251:ASP:HA	1.82	0.44
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.99	0.44
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.36	0.44
1:C:79:ARG:NH2	1:C:94:THR:OG1	2.44	0.44
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.98	0.44
1:C:69:ASP:O	1:C:94:THR:HA	2.16	0.44
2:B:238:VAL:HG12	2:B:378:ILE:HG12	1.98	0.44
2:B:181:VAL:HG23	1:C:349:THR:O	2.17	0.44
1:A:332:ILE:HG22	3:E:24:LEU:HD21	1.98	0.44
1:A:204:VAL:HG22	1:A:302[B]:MET:SD	2.58	0.44
2:D:286:LEU:HD22	2:D:290:GLU:HB3	1.99	0.44
1:A:154:MET:HG3	1:A:194:THR:HG23	2.00	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
1:A:213:CYS:HA	1:A:217:LEU:HD12	2.00	0.43
2:D:238:VAL:HG12	2:D:378:ILE:HG12	2.00	0.43
2:D:291:LEU:HD12	2:D:323:MET:HE1	2.00	0.43
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.43
2:B:286:LEU:HD22	2:B:290:GLU:HB3	1.99	0.43
1:C:238:ILE:HG12	1:C:378:LEU:HD11	1.99	0.43
2:D:263:PRO:O	2:D:266:HIS:CD2	2.61	0.43
2:D:181:VAL:HG11	2:D:404:PHE:CE1	2.53	0.43
1:A:105:ARG:HG2	1:A:110:ILE:HD13	2.01	0.43
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.37	0.43
1:C:154:MET:HG3	1:C:194:THR:HG23	2.00	0.43
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.54	0.43
1:C:56:THR:HG21	1:C:60:LYS:HG2	2.00	0.43
1:A:121:ARG:NE	8:A:658:HOH:O	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:79:GLU:O	3:E:83:ILE:HG23	2.18	0.43
1:A:221:ARG:HG2	2:B:325:MET:HB3	2.00	0.42
2:B:66:ILE:HD13	2:B:122:VAL:HG12	2.01	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
3:E:101:LEU:O	3:E:105:MET:HG2	2.19	0.42
1:C:339:ARG:N	1:C:339:ARG:HD3	2.33	0.42
3:E:125:GLU:HA	3:E:128:LYS:HD2	2.02	0.42
2:B:136:GLN:HA	2:B:167:ASN:O	2.19	0.42
2:B:306:ASP:O	2:B:309:HIS:HB2	2.20	0.42
2:D:291:LEU:HD13	2:D:375:SER:HB2	2.02	0.42
2:B:293[A]:GLN:HG3	2:B:335:ILE:HD11	2.01	0.42
2:B:296[B]:PHE:CE1	2:B:312:TYR:HE1	2.37	0.42
2:D:11:GLN:HB3	7:D:600:G2P:O1A	2.20	0.42
2:B:83:PHE:O	2:B:86:ILE:HG22	2.20	0.42
2:D:139:HIS:CD2	2:D:146:GLY:O	2.68	0.42
2:D:136:GLN:HA	2:D:167:ASN:O	2.20	0.42
2:B:282:GLN:CB	2:B:283:TYR:CA	2.98	0.41
2:B:286:LEU:HA	2:B:290:GLU:OE1	2.19	0.41
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.02	0.41
2:D:332:MET:O	2:D:336:GLN:HG2	2.20	0.41
2:D:385:GLN:HB2	2:D:429:VAL:HG13	2.02	0.41
2:B:11:GLN:HB3	7:B:600:G2P:O1A	2.20	0.41
2:B:175:PRO:HB3	1:C:349:THR:HB	2.02	0.41
1:C:315:CYS:O	1:C:351:PHE:HA	2.20	0.41
1:C:438:ASP:CG	1:C:438:ASP:O	2.59	0.41
1:C:97:GLU:O	1:C:110:ILE:HG21	2.20	0.41
2:D:192:HIS:CE1	2:D:424:ASN:HD22	2.37	0.41
2:D:306:ASP:O	2:D:309:HIS:HB2	2.21	0.41
2:D:206:ASN:HD22	2:D:206:ASN:HA	1.71	0.41
3:E:11:LEU:HD11	3:E:21:GLU:HB2	2.03	0.41
2:D:296[B]:PHE:CE1	2:D:312:TYR:HE1	2.38	0.41
2:B:116:ASP:HA	2:B:119:LEU:HD12	2.03	0.41
1:A:120:ASP:O	1:A:124:LYS:HG2	2.21	0.41
1:C:234:ILE:HG13	1:C:272:TYR:HB2	2.03	0.41
1:A:179:THR:HG21	2:B:247:GLN:HB3	2.03	0.40
1:A:352:LYS:HG2	3:E:21:GLU:HG3	2.02	0.40
1:A:224:TYR:HE1	2:B:247:GLN:NE2	2.19	0.40
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.02	0.40
1:C:88:HIS:H	1:C:91:GLN:NE2	2.20	0.40
2:B:345:GLU:H	2:B:345:GLU:HG2	1.50	0.40
2:D:66:ILE:HD13	2:D:122:VAL:HG12	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293[A]:GLN:HG3	2:D:335:ILE:HD11	2.02	0.40
2:B:288:VAL:HG22	2:B:323:MET:HE3	2.02	0.40
2:B:286:LEU:CD1	2:B:291:LEU:HD23	2.52	0.40
1:A:171:ILE:HD13	1:A:204:VAL:HB	2.02	0.40
1:A:71:GLU:OE2	1:A:73:THR:HB	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	434/451 (96%)	416 (96%)	12 (3%)	6 (1%)	11	34
1	C	428/451 (95%)	408 (95%)	12 (3%)	8 (2%)	8	26
2	B	437/445 (98%)	413 (94%)	19 (4%)	5 (1%)	14	41
2	D	436/445 (98%)	414 (95%)	16 (4%)	6 (1%)	11	34
3	E	131/143 (92%)	122 (93%)	6 (5%)	3 (2%)	6	21
All	All	1866/1935 (96%)	1773 (95%)	65 (4%)	28 (2%)	10	33

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
2	B	284	ARG
1	C	47	ASP
1	C	439	SER
2	D	56	ALA
2	D	59	ASN
2	D	97	SER
2	D	282	GLN
3	E	32	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	39	ASP
2	B	282	GLN
1	C	278	ALA
2	D	284	ARG
1	A	47	ASP
1	C	281	ALA
1	C	283	HIS
3	E	44	ASP
1	A	131	GLY
1	C	280	LYS
2	D	57	THR
1	A	195	LEU
2	B	285	ALA
2	B	286	LEU
1	C	131	GLY
1	C	195	LEU
2	B	177	VAL
3	E	31	GLY
1	A	162	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/379 (98%)	353 (95%)	18 (5%)	25	57
1	C	360/379 (95%)	335 (93%)	25 (7%)	15	41
2	B	378/385 (98%)	356 (94%)	22 (6%)	20	50
2	D	378/385 (98%)	350 (93%)	28 (7%)	13	37
3	E	111/125 (89%)	98 (88%)	13 (12%)	5	16
All	All	1598/1653 (97%)	1492 (93%)	106 (7%)	16	44

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	46	ASP
1	A	47	ASP
1	A	54	SER
1	A	84	ARG
1	A	112	LYS
1	A	121	ARG
1	A	130	THR
1	A	164	LYS
1	A	177	VAL
1	A	179	THR
1	A	215	ARG
1	A	229	ARG
1	A	315	CYS
1	A	320	ARG
1	A	324	VAL
1	A	335	ILE
1	A	435	VAL
2	B	110	GLU
2	B	115	VAL
2	B	149	MET
2	B	153	LEU
2	B	171	VAL
2	B	190	SER
2	B	198	THR
2	B	207	GLU
2	B	227	LEU
2	B	283	TYR
2	B	286	LEU
2	B	305	CYS
2	B	309	HIS
2	B	318	ILE
2	B	345	GLU
2	B	357	ASP
2	B	377[A]	PHE
2	B	377[B]	PHE
2	B	387	LEU
2	B	423	SER
2	B	439	THR
2	B	442	GLU
1	C	1	MET
1	C	46	ASP
1	C	54	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	62	VAL
1	C	71	GLU
1	C	80	THR
1	C	84	ARG
1	C	109	THR
1	C	127	ASP
1	C	130	THR
1	C	164	LYS
1	C	179	THR
1	C	241	SER
1	C	248	LEU
1	C	250	VAL
1	C	317	LEU
1	C	339	ARG
1	C	358	GLN
1	C	370	LYS
1	C	419	SER
1	C	430	LYS
1	C	435	VAL
1	C	438	ASP
1	C	439	SER
1	C	440	VAL
2	D	22	GLU
2	D	55	GLU
2	D	60	LYS
2	D	72	PRO
2	D	110	GLU
2	D	115	VAL
2	D	117	SER
2	D	153	LEU
2	D	155	SER
2	D	160	GLU
2	D	171	VAL
2	D	181	VAL
2	D	190	SER
2	D	198	THR
2	D	207	GLU
2	D	284	ARG
2	D	298	SER
2	D	305	CYS
2	D	345	GLU
2	D	357	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	371	LEU
2	D	377[A]	PHE
2	D	377[B]	PHE
2	D	384	ILE
2	D	416	MET
2	D	417	GLU
2	D	423	SER
2	D	439	THR
3	E	13	LYS
3	E	19	SER
3	E	28	SER
3	E	46	SER
3	E	52	LYS
3	E	67	GLU
3	E	69	LEU
3	E	83	ILE
3	E	100	LYS
3	E	119	MET
3	E	125	GLU
3	E	134	ARG
3	E	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	GLN
1	A	61	HIS
1	A	91	GLN
1	A	249	ASN
1	A	258	ASN
1	A	301	GLN
1	A	329	ASN
1	A	372	GLN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	101	ASN
2	B	139	HIS
2	B	167	ASN
2	B	206	ASN
2	B	247	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	266	HIS
2	B	309	HIS
2	B	339	ASN
2	B	385	GLN
2	B	433	GLN
1	C	8	HIS
1	C	11	GLN
1	C	61	HIS
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	301	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	133	GLN
2	D	139	HIS
2	D	193	GLN
2	D	197	ASN
2	D	206	ASN
2	D	247	GLN
2	D	266	HIS
2	D	300	ASN
2	D	336	GLN
2	D	339	ASN
2	D	385	GLN
2	D	433	GLN
2	D	436	GLN
3	E	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
6	SO4	A	453	-	4,4,4	0.33	0	6,6,6	0.30	0
4	GTP	C	600	5	26,34,34	1.73	6 (23%)	33,54,54	2.06	10 (30%)
6	SO4	C	452	-	4,4,4	0.41	0	6,6,6	0.14	0
6	SO4	D	457	-	4,4,4	0.27	0	6,6,6	0.16	0
6	SO4	A	452	-	4,4,4	0.28	0	6,6,6	0.18	0
7	G2P	B	600	5	26,34,34	5.08	20 (76%)	30,54,54	2.93	14 (46%)
7	G2P	D	600	5	26,34,34	4.59	17 (65%)	30,54,54	2.87	13 (43%)
6	SO4	D	456	-	4,4,4	0.32	0	6,6,6	0.13	0
6	SO4	B	456	-	4,4,4	0.30	0	6,6,6	0.24	0
6	SO4	A	454	-	4,4,4	0.31	0	6,6,6	0.18	0
6	SO4	C	453	-	4,4,4	0.23	0	6,6,6	0.14	0
4	GTP	A	600	5	26,34,34	1.72	7 (26%)	33,54,54	2.34	12 (36%)

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
7	G2P	B	600	5	-	7/18/38/38	0/3/3/3
4	GTP	C	600	5	-	7/18/38/38	0/3/3/3
7	G2P	D	600	5	-	7/18/38/38	0/3/3/3
4	GTP	A	600	5	-	6/18/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	G2P	C4-N9	-16.72	1.25	1.47
7	D	600	G2P	C4-N9	-16.00	1.26	1.47
7	B	600	G2P	O3'-C3'	8.08	1.62	1.43
7	B	600	G2P	PA-O5'	6.87	1.67	1.57
7	D	600	G2P	PA-O5'	6.47	1.67	1.57
7	B	600	G2P	PA-O1A	-6.40	1.41	1.56
7	D	600	G2P	O3'-C3'	6.31	1.57	1.43
7	B	600	G2P	O2'-C2'	-6.15	1.28	1.43
7	D	600	G2P	O2'-C2'	-6.07	1.28	1.43
7	D	600	G2P	PA-O1A	-5.91	1.42	1.56
7	D	600	G2P	C8-N9	-5.16	1.27	1.45
4	C	600	GTP	O4'-C1'	4.97	1.48	1.41
7	B	600	G2P	C8-N9	-4.94	1.28	1.45
7	B	600	G2P	C6-N1	4.72	1.40	1.33
7	B	600	G2P	PA-O2A	4.58	1.62	1.51
7	B	600	G2P	O5'-C5'	-4.44	1.27	1.44
7	D	600	G2P	PA-O2A	4.38	1.62	1.51
7	B	600	G2P	PG-O2G	4.11	1.63	1.50
7	D	600	G2P	O5'-C5'	-4.09	1.29	1.44
7	B	600	G2P	PB-O2B	3.97	1.61	1.51
4	A	600	GTP	C6-N1	3.68	1.39	1.33
4	A	600	GTP	C8-N7	-3.58	1.28	1.34
7	B	600	G2P	PG-O1G	-3.39	1.41	1.54
7	B	600	G2P	C2'-C1'	3.38	1.64	1.53
4	A	600	GTP	C2'-C1'	-3.28	1.48	1.53
4	C	600	GTP	C8-N7	-3.26	1.28	1.34
7	B	600	G2P	C3'-C4'	3.16	1.61	1.53
7	D	600	G2P	PG-O2G	2.99	1.60	1.50
7	D	600	G2P	PG-O1G	-2.97	1.43	1.54
7	B	600	G2P	PB-O1B	2.94	1.63	1.56
7	B	600	G2P	C2-N2	2.85	1.50	1.36
7	B	600	G2P	O4'-C4'	2.75	1.51	1.45
4	A	600	GTP	C6-C5	2.75	1.46	1.41
7	D	600	G2P	O4'-C4'	2.66	1.50	1.45
7	B	600	G2P	O6-C6	-2.56	1.18	1.23
4	C	600	GTP	C2'-C1'	2.55	1.57	1.53
7	D	600	G2P	C2'-C1'	2.52	1.61	1.53
4	A	600	GTP	O4'-C1'	2.45	1.44	1.41
7	D	600	G2P	C2-N2	2.44	1.48	1.36
7	D	600	G2P	C3'-C4'	2.44	1.59	1.53
4	C	600	GTP	PA-O2A	2.44	1.66	1.55
7	D	600	G2P	O6-C6	-2.26	1.18	1.23
4	A	600	GTP	C4-N3	2.25	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	G2P	C2'-C3'	-2.22	1.47	1.53
7	D	600	G2P	C2'-C3'	-2.20	1.47	1.53
4	C	600	GTP	C6-N1	2.19	1.36	1.33
7	B	600	G2P	PB-O3B	2.17	1.60	1.58
4	A	600	GTP	C2-N2	2.11	1.38	1.33
4	C	600	GTP	C6-C5	2.09	1.45	1.41
7	D	600	G2P	PB-O1B	2.07	1.61	1.56

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	G2P	O4'-C4'-C3'	-7.80	89.68	105.11
7	D	600	G2P	O4'-C4'-C3'	-7.55	90.18	105.11
4	C	600	GTP	C5-C6-N1	-5.46	115.96	123.43
4	A	600	GTP	C2-N3-C4	5.16	121.25	115.36
4	A	600	GTP	N3-C2-N1	-5.14	120.37	127.22
4	A	600	GTP	C6-C5-C4	-4.97	116.05	120.80
7	B	600	G2P	O1B-PB-O2B	4.88	126.35	110.07
7	D	600	G2P	O1B-PB-O2B	4.83	126.19	110.07
7	B	600	G2P	C4-C5-N7	4.72	108.72	102.46
7	D	600	G2P	O2'-C2'-C3'	-4.72	96.57	111.82
7	D	600	G2P	C4-C5-N7	4.71	108.71	102.46
7	B	600	G2P	O1A-PA-C3A	4.68	125.73	106.58
7	D	600	G2P	O1A-PA-C3A	4.68	125.73	106.58
7	B	600	G2P	O2'-C2'-C3'	-4.49	97.30	111.82
7	B	600	G2P	C3'-C2'-C1'	-4.21	93.42	101.43
7	D	600	G2P	O2A-PA-C3A	-4.11	98.22	109.07
4	C	600	GTP	C6-N1-C2	3.95	122.20	115.93
4	A	600	GTP	C6-N1-C2	3.94	122.19	115.93
7	D	600	G2P	C3'-C2'-C1'	-3.82	94.17	101.43
7	B	600	G2P	C4'-O4'-C1'	3.76	117.78	109.47
4	A	600	GTP	PB-O3B-PG	-3.73	120.03	132.83
4	C	600	GTP	N3-C2-N1	-3.59	122.44	127.22
4	A	600	GTP	C5-C6-N1	-3.58	118.53	123.43
4	A	600	GTP	PA-O3A-PB	-3.56	120.59	132.83
7	B	600	G2P	O4'-C1'-C2'	-3.48	99.05	106.64
4	C	600	GTP	C4-C5-N7	-3.45	105.81	109.40
4	C	600	GTP	PA-O3A-PB	-3.45	120.99	132.83
7	D	600	G2P	C4'-O4'-C1'	3.33	116.83	109.47
4	A	600	GTP	O4'-C4'-C3'	-3.32	98.54	105.11
4	C	600	GTP	C2-N3-C4	3.28	119.11	115.36
7	B	600	G2P	O2A-PA-C3A	-3.27	100.43	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	G2P	O2'-C2'-C1'	3.19	120.69	110.02
4	C	600	GTP	PB-O3B-PG	-3.14	122.06	132.83
7	D	600	G2P	O4'-C1'-C2'	-3.09	99.90	106.64
4	A	600	GTP	N2-C2-N3	2.98	122.66	117.79
7	D	600	G2P	O2'-C2'-C1'	2.67	118.94	110.02
4	C	600	GTP	C6-C5-C4	-2.60	118.31	120.80
4	A	600	GTP	C3'-C2'-C1'	-2.35	97.44	100.98
4	C	600	GTP	PA-O5'-C5'	-2.29	108.26	121.68
7	B	600	G2P	O3'-C3'-C2'	2.27	119.17	111.82
4	A	600	GTP	C1'-N9-C4	-2.26	122.67	126.64
7	D	600	G2P	O3G-PG-O1G	2.23	116.17	107.64
7	D	600	G2P	O1B-PB-C3A	-2.15	97.77	106.58
7	D	600	G2P	O3'-C3'-C2'	2.14	118.74	111.82
4	C	600	GTP	C1'-N9-C4	-2.13	122.89	126.64
7	B	600	G2P	O3'-C3'-C4'	2.08	117.07	111.05
4	A	600	GTP	O3G-PG-O2G	2.06	115.53	107.64
7	B	600	G2P	O3G-PG-O1G	2.03	115.38	107.64
7	B	600	G2P	O4'-C4'-C5'	2.02	116.02	109.37

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O2A
7	B	600	G2P	PB-O3B-PG-O1G
7	B	600	G2P	C5'-O5'-PA-O2A
7	B	600	G2P	C2'-C1'-N9-C4
7	D	600	G2P	PB-O3B-PG-O1G
7	D	600	G2P	C5'-O5'-PA-O2A
7	D	600	G2P	C2'-C1'-N9-C4
4	A	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C3'-C4'-C5'-O5'
4	C	600	GTP	O4'-C4'-C5'-O5'
4	C	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3A-PA-O2A
7	D	600	G2P	C3'-C4'-C5'-O5'
7	B	600	G2P	C3'-C4'-C5'-O5'
7	B	600	G2P	C5'-O5'-PA-O1A
7	D	600	G2P	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

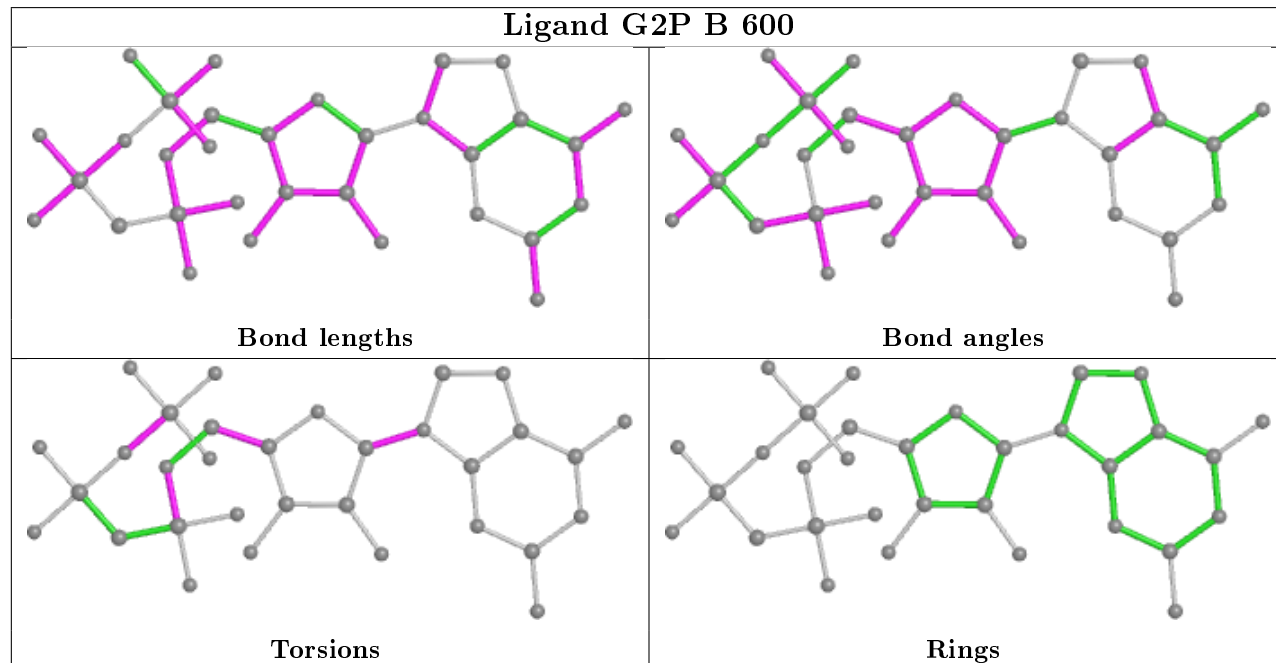
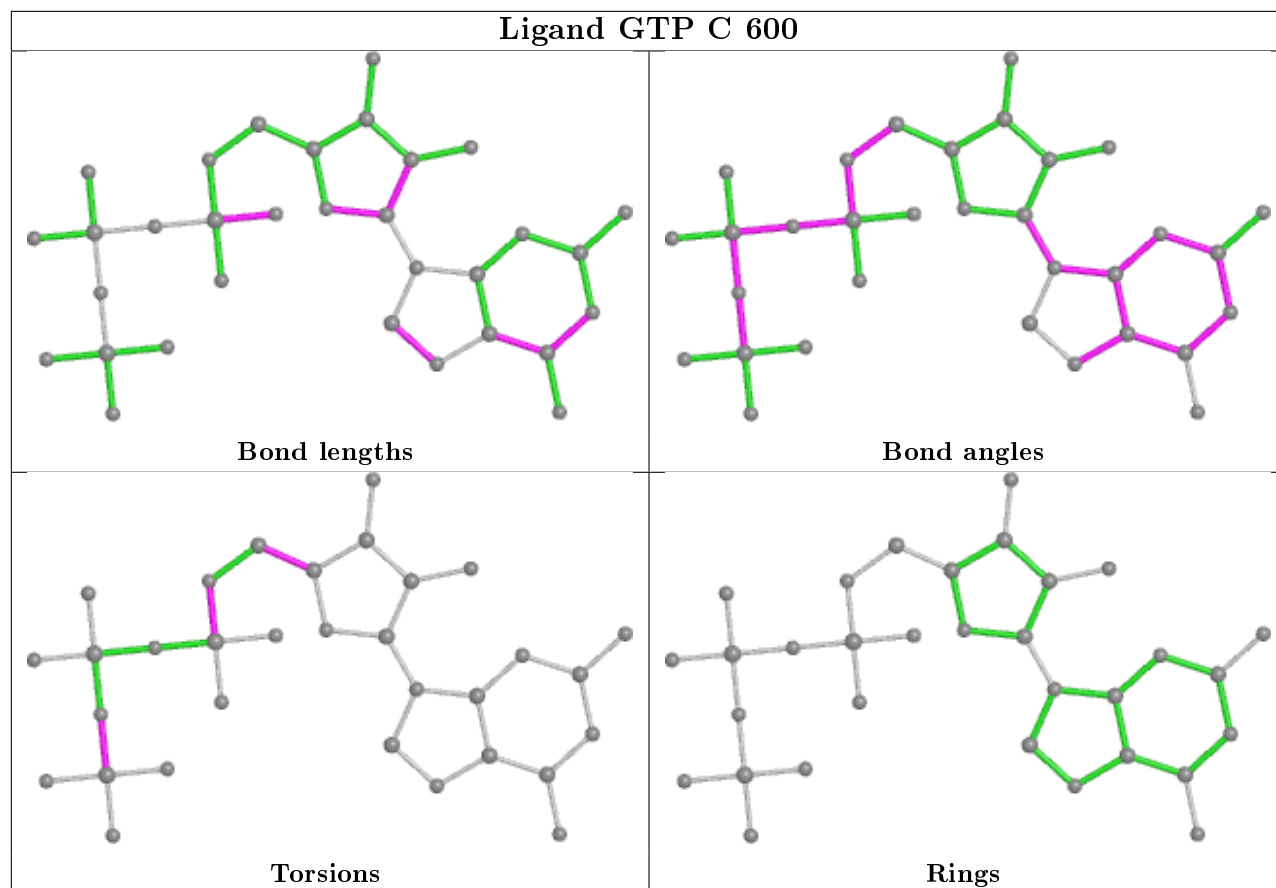
Mol	Chain	Res	Type	Atoms
7	B	600	G2P	PB-O3B-PG-O2G
7	D	600	G2P	PB-O3B-PG-O2G
4	A	600	GTP	PB-O3B-PG-O1G
4	C	600	GTP	PB-O3B-PG-O2G
4	C	600	GTP	PB-O3B-PG-O3G
7	B	600	G2P	PB-O3B-PG-O3G
7	D	600	G2P	PB-O3B-PG-O3G
4	A	600	GTP	PB-O3B-PG-O2G

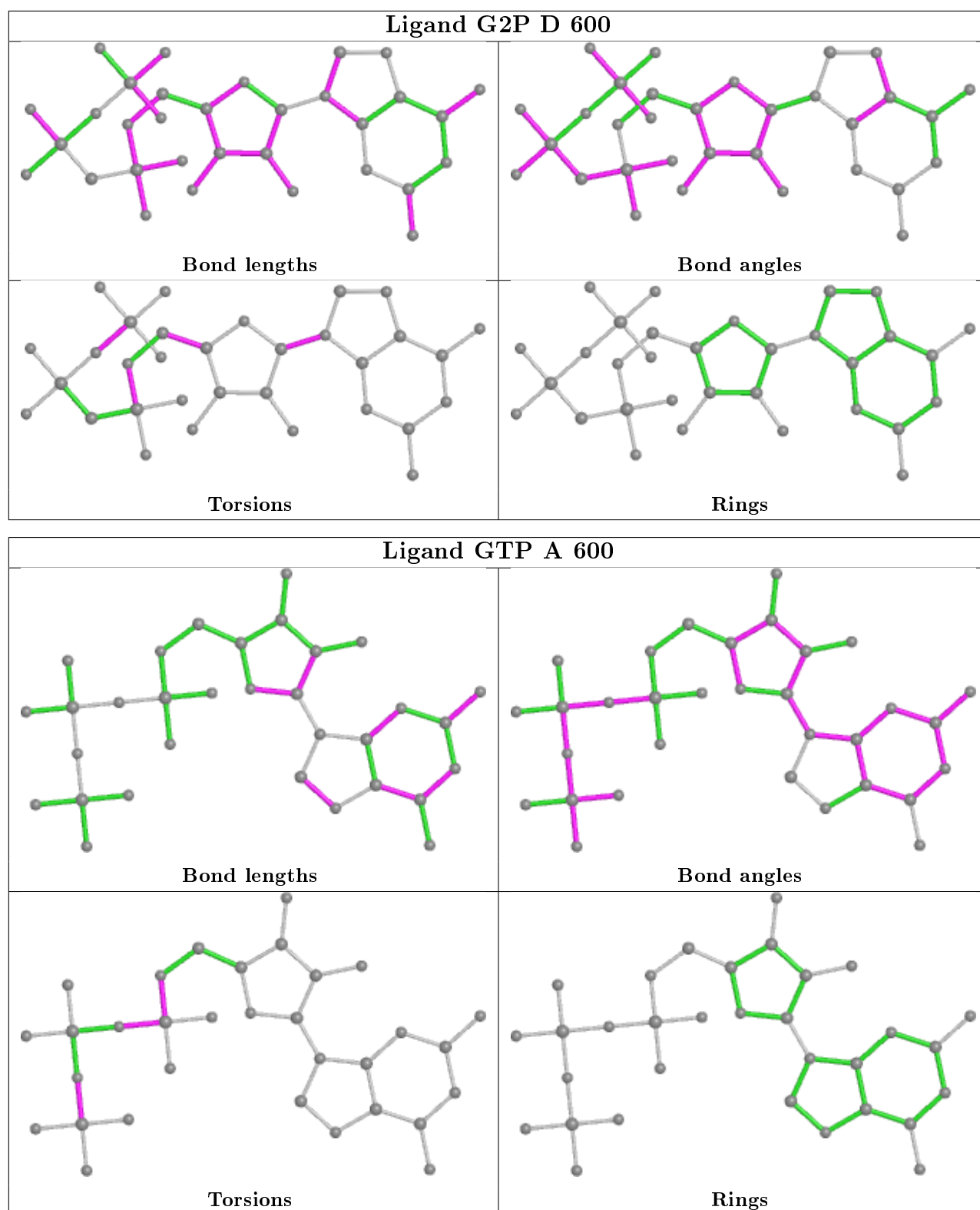
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	600	G2P	4	0
7	D	600	G2P	4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	-0.17	3 (0%) 87 84	56, 79, 115, 198	0
1	C	432/451 (95%)	0.04	14 (3%) 47 37	53, 78, 117, 156	0
2	B	432/445 (97%)	-0.01	20 (4%) 32 22	52, 75, 124, 191	4 (0%)
2	D	431/445 (96%)	0.01	14 (3%) 47 37	50, 77, 129, 212	4 (0%)
3	E	135/143 (94%)	0.54	13 (9%) 8 4	64, 102, 208, 251	0
All	All	1867/1935 (96%)	0.01	64 (3%) 45 35	50, 79, 126, 251	8 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	4	ALA	7.1
3	E	32	VAL	6.4
2	D	39	ASP	6.1
2	D	283	TYR	5.4
2	B	442	GLU	5.3
1	C	283	HIS	4.7
3	E	33	PRO	4.6
2	D	57	THR	4.4
1	A	441	GLU	4.1
3	E	31	GLY	4.1
1	C	284	GLU	4.0
1	A	282	TYR	3.9
2	B	85	GLN	3.8
3	E	30	ASP	3.7
1	C	278	ALA	3.6
2	B	32	PRO	3.5
2	D	44	LEU	3.5
3	E	5	ASP	3.2
2	B	283	TYR	3.2
1	C	58	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	85	GLN	3.1
3	E	145	ARG	3.1
2	B	37	HIS	3.1
1	C	56	THR	3.1
2	D	59	ASN	3.1
2	B	285	ALA	2.9
1	C	217	LEU	2.8
3	E	16	SER	2.8
2	D	56	ALA	2.7
2	D	282	GLN	2.7
1	C	281	ALA	2.7
2	D	55	GLU	2.6
2	B	86	ILE	2.6
2	B	441	ASP	2.6
2	B	59	ASN	2.5
2	B	44	LEU	2.5
2	D	96	GLN	2.5
1	C	438	ASP	2.5
1	C	60	LYS	2.5
2	B	56	ALA	2.5
2	B	440	ALA	2.5
2	B	33	THR	2.5
1	C	55	GLU	2.4
1	C	277	SER	2.4
3	E	142	GLU	2.3
3	E	51	GLN	2.3
1	C	439	SER	2.3
2	D	412	GLY	2.3
3	E	45	PRO	2.3
3	E	66	ALA	2.3
1	C	279	GLU	2.3
2	D	285	ALA	2.2
2	B	293[A]	GLN	2.2
2	B	39	ASP	2.2
3	E	96	MET	2.2
2	B	61	TYR	2.2
2	B	60	LYS	2.1
1	A	346	TRP	2.1
2	B	100	GLY	2.1
2	B	36	TYR	2.1
1	C	251	ASP	2.1
2	B	369	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	60	LYS	2.0
2	D	284	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

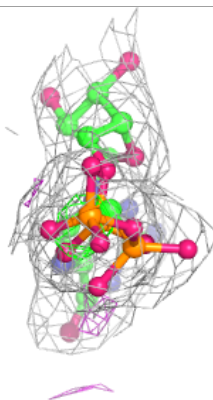
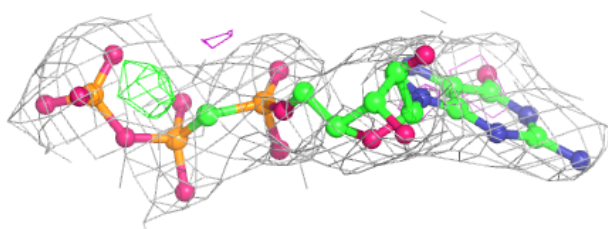
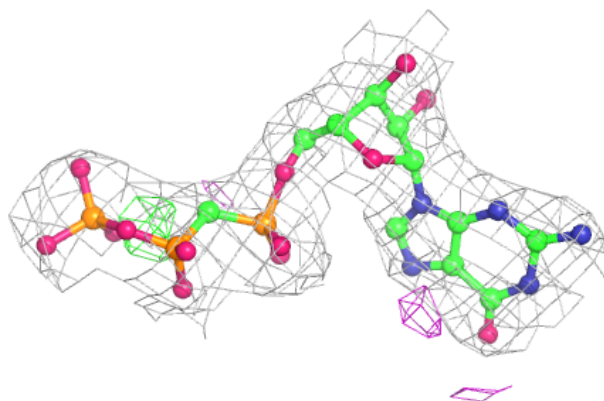
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	SO4	C	453	5/5	0.80	0.42	161,165,166,166	0
6	SO4	A	454	5/5	0.83	0.28	170,174,176,176	0
6	SO4	C	452	5/5	0.93	0.13	119,123,124,124	0
5	MG	C	601	1/1	0.93	0.14	67,67,67,67	0
6	SO4	D	457	5/5	0.94	0.20	122,127,127,127	0
6	SO4	A	453	5/5	0.94	0.13	119,123,124,125	0
6	SO4	B	456	5/5	0.95	0.12	102,106,107,107	0
6	SO4	A	452	5/5	0.95	0.12	111,115,116,117	0
5	MG	A	601	1/1	0.96	0.21	75,75,75,75	0
7	G2P	B	600	32/32	0.97	0.19	61,68,75,81	0
4	GTP	C	600	32/32	0.98	0.19	69,72,75,77	0
5	MG	B	601	1/1	0.98	0.19	50,50,50,50	0
7	G2P	D	600	32/32	0.98	0.13	58,70,81,84	0
5	MG	D	601	1/1	0.98	0.04	75,75,75,75	0
4	GTP	A	600	32/32	0.98	0.23	56,59,63,65	0
6	SO4	D	456	5/5	0.99	0.11	72,77,78,78	0

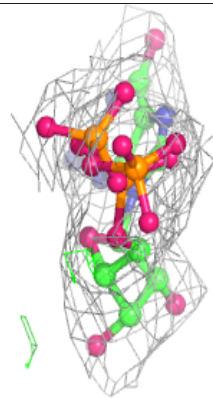
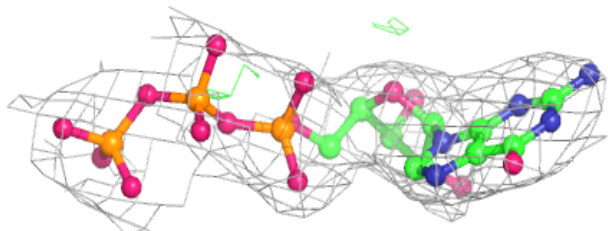
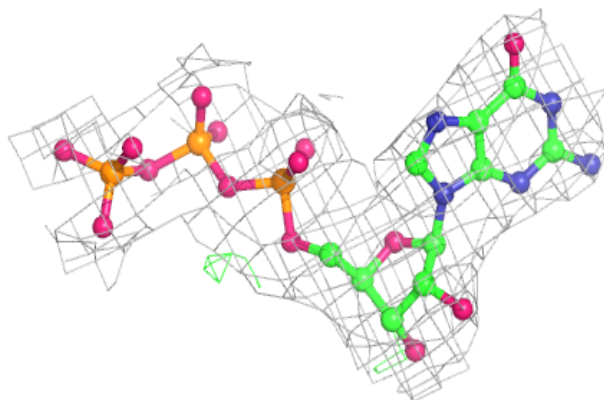
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G2P 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)

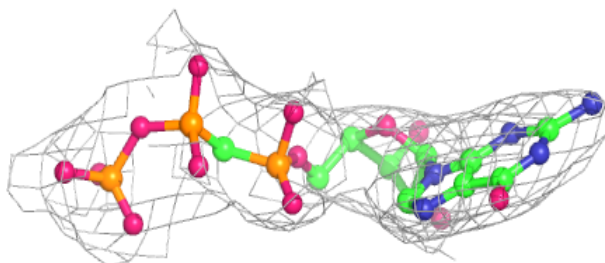
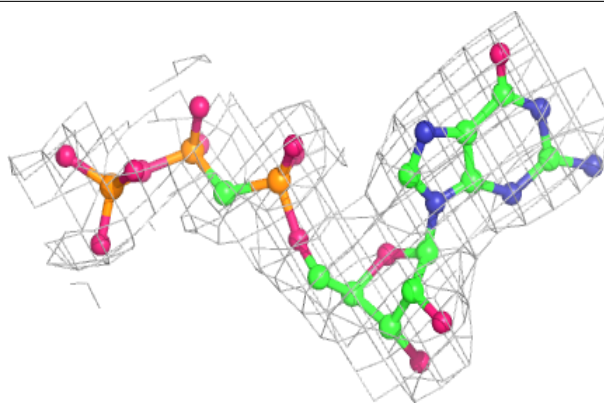
**Electron density around GTP C 600:**

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

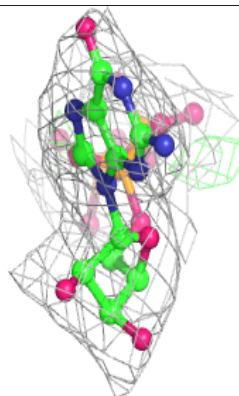
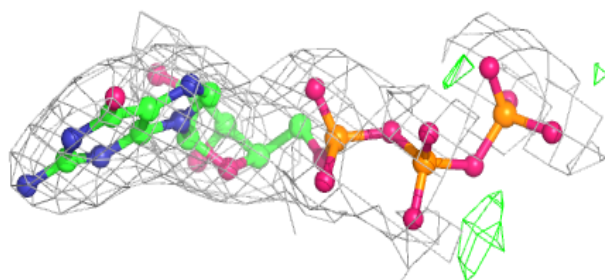
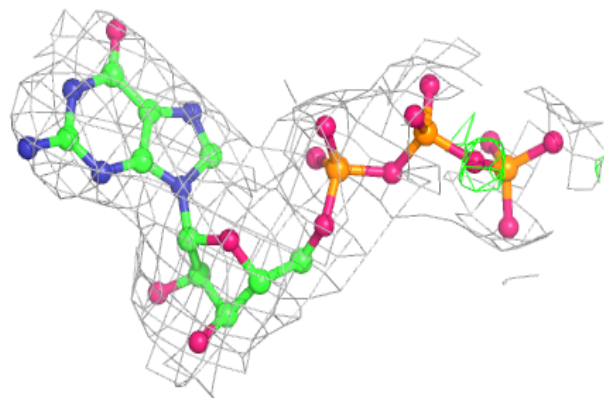


Electron density around G2P D 600:

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

**Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.