



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:31 pm BST

PDB ID : 6PC4
Title : Tubulin-RB3_SLD-TTL in complex with compound ABI-274
Authors : Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on : 2019-06-15
Resolution : 2.60 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

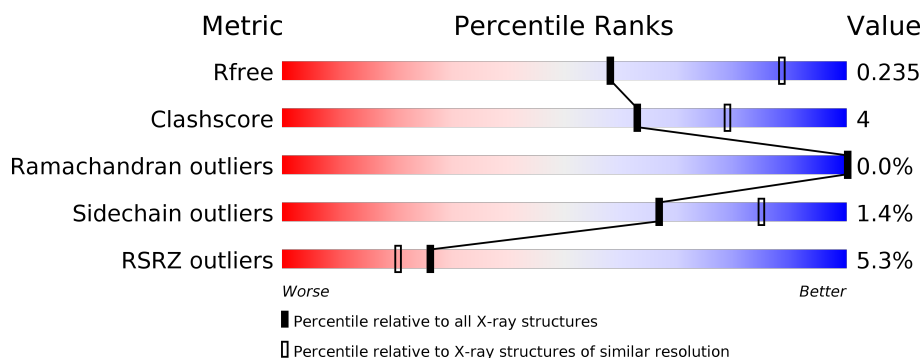
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	450	<div> <div>89%</div> <div>7%</div> <div>•</div> </div>
1	C	450	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>
2	B	445	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
2	D	445	<div> <div>6%</div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div>
3	E	143	<div> <div>%</div> <div>73%</div> <div>11%</div> <div>• 15%</div> </div>
4	F	384	<div> <div>20%</div> <div>73%</div> <div>13%</div> <div>• 14%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17742 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			997	614	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2617	1686	446	471	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- 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		

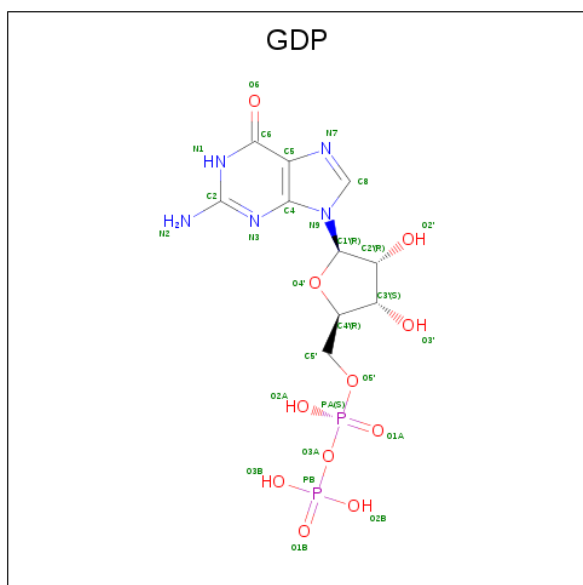
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



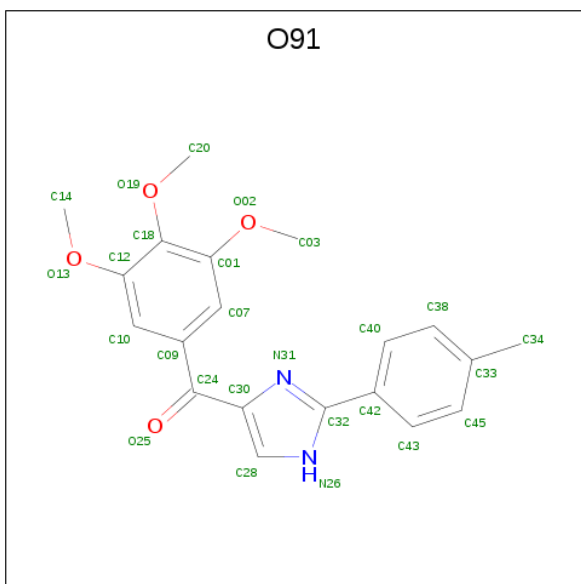
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is [2-(4-methylphenyl)-1H-imidazol-4-yl](3,4,5-trimethoxyphenyl)methanone (three-letter code: O91) (formula: C₂₀H₂₀N₂O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			26	20	2	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			26	20	2	4		

- Molecule 11 is water.

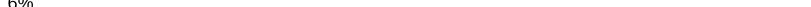
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	96	Total	O	0	0
			96	96		
11	B	76	Total	O	0	0
			76	76		
11	C	124	Total	O	0	0
			124	124		
11	D	41	Total	O	0	0
			41	41		
11	E	21	Total	O	0	0
			21	21		
11	F	46	Total	O	0	0
			46	46		

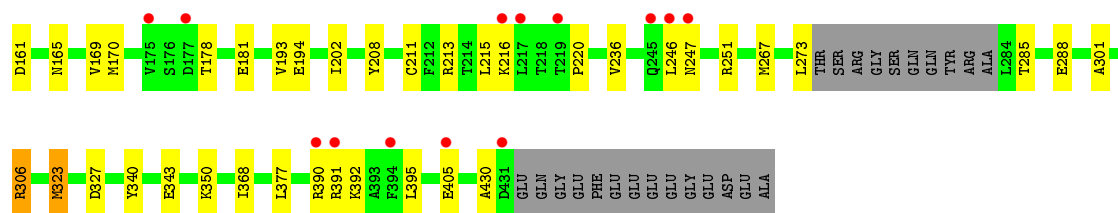
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Chain A:
-
- 89% 7%
- Q372 Y399 E402 M425 K430 V437 ASP SER VAL GLU GLY GLY GLU GLU GLU GLY GLU GLU S147 E155 G162 K163 Y172 I188 L189 T190 D205 I209 Y210 D211 R221 P222 L230 I234 A247 Y262 Q285 K304 K336

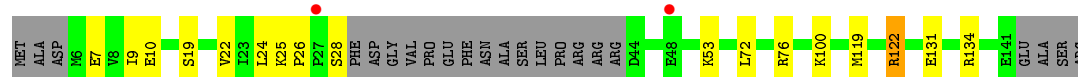
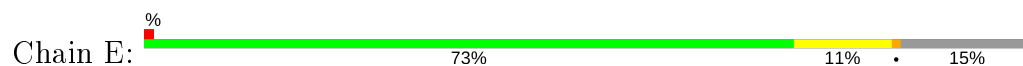
- [illegible]

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 2.00). The x-axis lists amino acids: MET, R2, H6, G12, K19, F20, W21, H37, S40, Q43, A54, T55, G56, N57, K58, P61, D67, M73, D74, S75, Y76, R77, F92, S126, Q134, H137, I163, M164, M165, M170, H190, C201, T218, T219, Q245, L246, N247, A248, P249, L250. A horizontal bar at the top shows the overall conservation: 29% (red), 87% (green), and 9% (yellow).

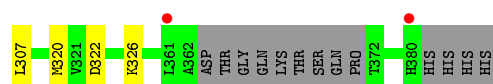
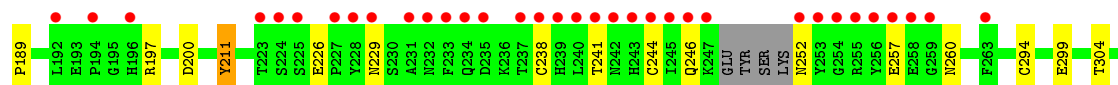
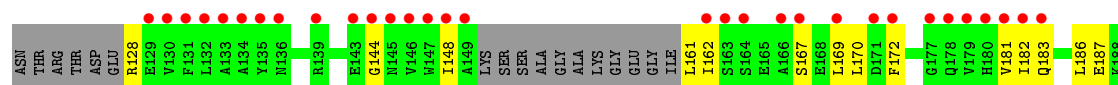
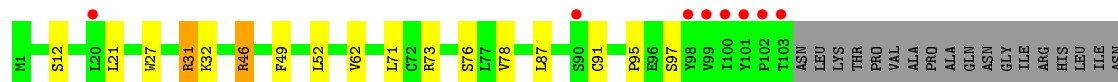
- Chain D: 



● Molecule 3: Stathmin-4



● Molecule 4: Tubulin Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.14Å 157.53Å 181.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.74 – 2.60 48.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.74-2.60) 98.7 (48.09-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.234 0.190 , 0.235	Depositor DCC
R_{free} test set	4594 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17742	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: GDP, MG, CA, O91, GTP, MES

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	0.27	0/3494	0.48	2/4743 (0.0%)
1	C	0.27	0/3515	0.46	0/4772
2	B	0.26	0/3436	0.44	0/4654
2	D	0.32	0/3382	0.59	9/4581 (0.2%)
3	E	0.25	0/1005	0.37	0/1333
4	F	0.26	0/2677	0.44	0/3629
All	All	0.28	0/17509	0.48	11/23712 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	306	ARG	NE-CZ-NH1	10.68	125.64	120.30
2	D	306	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	A	372	GLN	CA-CB-CG	6.98	128.75	113.40
2	D	306	ARG	CD-NE-CZ	6.40	132.56	123.60
2	D	86	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	D	24	ILE	CG1-CB-CG2	-5.90	98.42	111.40
2	D	86	ARG	CG-CD-NE	5.69	123.74	111.80
1	A	30	ILE	C-N-CA	5.54	135.56	121.70
2	D	24	ILE	CB-CA-C	-5.29	101.02	111.60
2	D	24	ILE	CA-CB-CG1	5.28	121.03	111.00
2	D	24	ILE	N-CA-CB	5.05	122.41	110.80

There are no chirality outliers.

There are no planarity outliers.

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	3416	0	3331	28	0
1	C	3437	0	3348	17	0
2	B	3361	0	3238	21	0
2	D	3309	0	3189	45	0
3	E	997	0	1009	11	0
4	F	2617	0	2516	29	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	24	0	24	1	0
10	B	26	0	0	1	0
10	D	26	0	0	3	0
11	A	96	0	0	0	0
11	B	76	0	0	1	0
11	C	124	0	0	0	0
11	D	41	0	0	3	0
11	E	21	0	0	1	0
11	F	46	0	0	1	0
All	All	17742	0	16703	146	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 4.

All (146) 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:A:285:GLN:HG3	1:A:372:GLN:NE2	1.40	1.32
1:A:285:GLN:CG	1:A:372:GLN:HE22	1.48	1.23
1:A:285:GLN:CG	1:A:372:GLN:NE2	2.11	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:HG3	1:A:372:GLN:HE22	0.83	0.97
1:A:90:GLU:OE2	1:A:124:LYS:NZ	2.03	0.91
1:A:285:GLN:CB	1:A:372:GLN:HE22	1.93	0.81
4:F:52:LEU:HD13	4:F:62:VAL:HG21	1.63	0.79
2:D:1:MET:HG3	2:D:2:ARG:HG2	1.65	0.79
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.68	0.76
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.18	0.74
4:F:97:SER:OG	4:F:183:GLN:NE2	2.22	0.73
1:A:163:LYS:HD2	1:A:163:LYS:H	1.55	0.71
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.74	0.70
1:C:221:ARG:NH2	2:D:323:MET:HE1	2.06	0.69
2:D:306:ARG:HD3	2:D:340:TYR:CZ	2.27	0.69
2:D:246:LEU:HD22	2:D:350:LYS:HZ1	1.56	0.69
2:D:323:MET:HE1	2:D:327:ASP:OD2	1.94	0.67
1:C:381:THR:HG22	1:C:383:ALA:H	1.60	0.66
2:B:324:LYS:O	2:B:328:GLU:HG3	1.96	0.65
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.78	0.65
4:F:161:LEU:HD23	4:F:172:PHE:HZ	1.62	0.65
2:D:392:LYS:NZ	11:D:601:HOH:O	2.30	0.64
3:E:119:MET:HA	3:E:122:ARG:HE	1.63	0.62
2:D:21:TRP:CZ3	2:D:24:ILE:HD11	2.34	0.62
2:D:236:VAL:HG22	2:D:368:ILE:HD11	1.82	0.61
2:D:246:LEU:HD22	2:D:350:LYS:NZ	2.15	0.60
1:A:285:GLN:CB	1:A:372:GLN:NE2	2.60	0.60
4:F:167:SER:HA	4:F:170:LEU:HB2	1.84	0.59
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.84	0.59
2:D:97:ALA:HB2	2:D:143:THR:OG1	2.03	0.58
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.85	0.58
2:D:134:GLN:HA	2:D:165:ASN:O	2.04	0.58
3:E:25:LYS:HD3	3:E:26:PRO:O	2.04	0.58
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.24	0.56
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.85	0.56
2:D:46:ARG:NH2	11:D:603:HOH:O	2.38	0.56
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.38	0.56
2:B:134:GLN:HA	2:B:165:ASN:O	2.05	0.56
2:D:306:ARG:HD3	2:D:340:TYR:CE2	2.41	0.56
1:C:2:ARG:HA	1:C:131:GLY:O	2.06	0.55
2:D:246:LEU:HD12	2:D:247:ASN:H	1.70	0.55
4:F:95:PRO:HB2	4:F:183:GLN:NE2	2.22	0.55
2:B:280:GLN:NE2	2:B:280:GLN:H	2.05	0.54
1:C:230:LEU:O	1:C:234:ILE:HD12	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.88	0.54
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.73	0.54
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.42	0.54
2:D:36:TYR:CD1	2:D:44:LEU:HD21	2.43	0.53
2:D:2:ARG:NH2	11:D:604:HOH:O	2.42	0.53
2:D:161:ASP:O	2:D:251:ARG:NH2	2.42	0.52
2:D:246:LEU:HD21	10:D:502:O91:C30	2.39	0.52
2:D:178:THR:O	2:D:181:GLU:HG3	2.08	0.52
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.90	0.52
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.91	0.52
4:F:226:GLU:OE1	4:F:252:ASN:HA	2.10	0.51
2:D:193:VAL:HG13	2:D:194:GLU:HG2	1.93	0.51
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.92	0.51
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.93	0.50
4:F:161:LEU:HD23	4:F:172:PHE:CZ	2.46	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.50
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.94	0.49
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.47	0.49
4:F:169:LEU:HA	4:F:172:PHE:HB3	1.93	0.49
2:D:208:TYR:CE1	2:D:220:PRO:HD2	2.48	0.49
2:B:389:PHE:O	2:B:392:LYS:NZ	2.38	0.49
2:D:141:GLY:HA3	8:D:501:GDP:O3A	2.13	0.49
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.52	0.49
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.95	0.48
3:E:100:LYS:NZ	11:E:201:HOH:O	2.45	0.48
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.48	0.48
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.48
4:F:87:LEU:O	4:F:91:CYS:HB2	2.14	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.47
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.50	0.47
4:F:189:PRO:HA	4:F:322:ASP:HA	1.96	0.47
2:D:211:CYS:HB2	2:D:220:PRO:HG3	1.97	0.47
2:B:248:ALA:HB1	10:B:505:O91:C10	2.45	0.47
4:F:31:ARG:HA	4:F:31:ARG:NE	2.30	0.47
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.18	0.47
2:D:390:ARG:HG3	2:D:391:ARG:HG3	1.96	0.46
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.96	0.46
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.98	0.46
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.46
1:A:247:ALA:HB3	3:E:19:SER:OG	2.15	0.46
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.96	0.46
2:B:219:THR:HG21	1:C:326:LYS:HA	1.98	0.46
4:F:46:ARG:NH2	11:F:403:HOH:O	2.49	0.46
1:A:155:GLU:OE1	3:E:53:LYS:NZ	2.46	0.45
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.98	0.45
1:C:241:SER:HA	1:C:249:ASN:OD1	2.16	0.45
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.97	0.45
1:A:285:GLN:CD	1:A:372:GLN:NE2	2.70	0.45
2:B:74:ASP:OD1	2:B:77:ARG:NH2	2.49	0.45
2:B:379:LYS:HE3	2:B:379:LYS:HB2	1.78	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.52	0.45
9:B:504:MES:H81	9:B:504:MES:H51	1.59	0.45
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.49	0.45
4:F:31:ARG:HD3	4:F:32:LYS:N	2.32	0.45
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.52	0.45
2:B:73:MET:N	11:B:604:HOH:O	2.48	0.45
1:A:285:GLN:HG3	1:A:372:GLN:HE21	1.61	0.44
1:A:163:LYS:CD	1:A:163:LYS:H	2.22	0.44
4:F:21:LEU:O	4:F:27:TRP:HB2	2.18	0.44
4:F:73:ARG:HB3	4:F:76:SER:OG	2.17	0.44
3:E:9:ILE:HG22	3:E:10:GLU:HB2	1.99	0.44
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.52	0.44
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.34	0.44
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.00	0.44
2:D:61:PRO:HD3	2:D:84:ILE:HG13	1.99	0.44
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.99	0.44
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.00	0.44
2:D:285:THR:HG23	2:D:288:GLU:H	1.82	0.44
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.52	0.44
2:B:246:LEU:HD21	2:B:350:LYS:HE2	2.00	0.43
1:A:97:GLU:OE1	2:B:2:ARG:NH2	2.51	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.00	0.43
2:D:395:LEU:HD21	2:D:405:GLU:HG3	2.01	0.43
4:F:186:LEU:HD13	4:F:320:MET:SD	2.58	0.43
1:C:209:ILE:HD11	1:C:302:MET:SD	2.58	0.43
3:E:7:GLU:O	3:E:22:VAL:HA	2.19	0.43
4:F:182:ILE:HD12	4:F:182:ILE:HA	1.88	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.43
2:D:44:LEU:HA	2:D:47:ILE:HB	2.00	0.43
2:B:67:ASP:O	2:B:92:PHE:HA	2.19	0.43
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LYS:HB3	1:A:430:LYS:HE2	1.79	0.42
2:D:246:LEU:HD21	10:D:502:O91:C24	2.49	0.42
2:D:323:MET:CE	2:D:327:ASP:OD2	2.66	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.42
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.42
2:D:213:ARG:O	2:D:216:LYS:HE3	2.20	0.42
2:D:116:VAL:O	2:D:120:VAL:HG23	2.19	0.42
3:E:25:LYS:CE	3:E:26:PRO:O	2.67	0.42
2:B:40:SER:HB3	2:B:43:GLN:HE21	1.85	0.42
2:D:9:ALA:HA	2:D:66:VAL:O	2.20	0.42
1:A:399:TYR:O	1:A:402:ARG:NH1	2.46	0.41
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.53	0.41
1:A:230:LEU:O	1:A:234:ILE:HD12	2.20	0.41
2:D:273:LEU:HD23	2:D:273:LEU:HA	1.88	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
2:D:350:LYS:HD3	10:D:502:O91:C40	2.51	0.41
2:D:211:CYS:CB	2:D:220:PRO:HG3	2.51	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.22	0.40
1:C:320:ARG:HA	1:C:356:ASN:O	2.20	0.40
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	426 (98%)	8 (2%)	1 (0%)	47	71
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	D	417/445 (94%)	405 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	322/384 (84%)	305 (95%)	17 (5%)	0	100	100
All	All	2154/2317 (93%)	2092 (97%)	61 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	368/378 (97%)	366 (100%)	2 (0%)	88	96
1	C	371/378 (98%)	368 (99%)	3 (1%)	81	92
2	B	369/383 (96%)	362 (98%)	7 (2%)	57	79
2	D	364/383 (95%)	361 (99%)	3 (1%)	81	92
3	E	108/127 (85%)	106 (98%)	2 (2%)	57	79
4	F	272/342 (80%)	263 (97%)	9 (3%)	38	64
All	All	1852/1991 (93%)	1826 (99%)	26 (1%)	67	85

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LYS
1	A	221	ARG
2	B	19	LYS
2	B	75	SER
2	B	126	SER
2	B	137	HIS
2	B	190	HIS
2	B	218	THR
2	B	282	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2	ARG
1	C	218	ASP
1	C	221	ARG
2	D	92	PHE
2	D	137	HIS
2	D	323	MET
3	E	28	SER
3	E	122	ARG
4	F	12	SER
4	F	31	ARG
4	F	46	ARG
4	F	128	ARG
4	F	211	TYR
4	F	229	ASN
4	F	238	CYS
4	F	244	CYS
4	F	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
2	B	43	GLN
2	B	48	ASN
2	B	280	GLN
2	B	424	GLN
2	D	247	ASN
2	D	335	ASN
3	E	12	ASN
4	F	183	GLN
4	F	196	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 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
10	O91	D	502	-	28,28,28	1.24	5 (17%)	34,39,39	1.39	7 (20%)
9	MES	B	503	-	12,12,12	2.20	1 (8%)	14,16,16	1.89	5 (35%)
9	MES	B	504	-	12,12,12	2.28	1 (8%)	14,16,16	1.95	7 (50%)
8	GDP	D	501	-	24,30,30	1.21	2 (8%)	31,47,47	1.95	8 (25%)
5	GTP	A	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.72	6 (18%)
8	GDP	B	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.90	7 (22%)
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.78	7 (21%)
10	O91	B	505	-	28,28,28	1.22	5 (17%)	34,39,39	1.25	5 (14%)

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
10	O91	D	502	-	-	4/14/18/18	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
8	GDP	D	501	-	-	6/12/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
10	O91	B	505	-	-	0/14/18/18	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.61	1.66	1.77
9	B	503	MES	C8-S	-7.37	1.67	1.77
8	D	501	GDP	C6-C5	4.34	1.48	1.41
8	B	501	GDP	C6-C5	4.04	1.48	1.41
5	C	501	GTP	C6-N1	3.27	1.38	1.33
5	A	501	GTP	C6-N1	3.07	1.38	1.33
10	D	502	O91	C28-N26	-2.96	1.31	1.36
10	B	505	O91	C28-N26	-2.78	1.32	1.36
8	D	501	GDP	C5-C4	2.45	1.47	1.40
8	B	501	GDP	C5-C4	2.36	1.47	1.40
10	D	502	O91	O13-C12	2.26	1.40	1.37
10	B	505	O91	O13-C12	2.23	1.40	1.37
10	D	502	O91	O25-C24	-2.19	1.18	1.22
10	B	505	O91	O25-C24	-2.16	1.18	1.22
10	D	502	O91	C09-C24	2.15	1.53	1.49
10	B	505	O91	C09-C24	2.14	1.53	1.49
10	B	505	O91	O02-C01	2.05	1.40	1.37
10	D	502	O91	O02-C01	2.02	1.40	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.44	119.96	127.22
5	A	501	GTP	N3-C2-N1	-5.19	120.29	127.22
8	D	501	GDP	C2-N3-C4	4.92	120.97	115.36
8	B	501	GDP	C2-N3-C4	4.74	120.77	115.36
8	B	501	GDP	C6-N1-C2	4.17	122.56	115.93
5	A	501	GTP	C2-N3-C4	4.14	120.09	115.36
5	C	501	GTP	C2-N3-C4	4.12	120.06	115.36
8	D	501	GDP	C6-N1-C2	4.02	122.31	115.93
8	B	501	GDP	C6-C5-C4	-3.99	116.99	120.80
8	B	501	GDP	C5-C6-N1	-3.98	117.98	123.43
8	D	501	GDP	C5-C6-N1	-3.95	118.03	123.43
9	B	504	MES	C5-N4-C3	3.92	117.65	108.83
8	D	501	GDP	C6-C5-C4	-3.88	117.09	120.80
9	B	503	MES	C5-N4-C3	3.65	117.04	108.83
8	B	501	GDP	N3-C2-N1	-3.46	122.61	127.22
8	D	501	GDP	N3-C2-N1	-3.29	122.84	127.22
10	D	502	O91	O13-C12-C18	3.09	120.59	115.16
9	B	504	MES	C6-C5-N4	-3.07	105.45	110.10
8	B	501	GDP	PA-O3A-PB	-3.04	122.40	132.83
5	A	501	GTP	PB-O3B-PG	-3.02	122.45	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C5-C6-N1	-3.00	119.33	123.43
10	D	502	O91	O02-C01-C18	2.92	120.30	115.16
5	A	501	GTP	C5-C6-N1	-2.90	119.46	123.43
9	B	503	MES	O3S-S-C8	2.83	110.34	105.77
8	D	501	GDP	C4-C5-N7	-2.83	106.45	109.40
5	A	501	GTP	PA-O3A-PB	-2.81	123.17	132.83
5	C	501	GTP	PB-O3B-PG	-2.79	123.25	132.83
8	B	501	GDP	C4-C5-N7	-2.74	106.54	109.40
5	C	501	GTP	C6-N1-C2	2.74	120.28	115.93
5	C	501	GTP	PA-O3A-PB	-2.70	123.56	132.83
9	B	503	MES	C7-N4-C5	2.68	118.08	111.23
10	B	505	O91	O02-C01-C18	2.62	119.77	115.16
10	B	505	O91	O13-C12-C18	2.59	119.71	115.16
10	D	502	O91	O13-C12-C10	-2.53	119.76	124.12
5	A	501	GTP	C6-N1-C2	2.52	119.94	115.93
10	B	505	O91	C42-C32-N26	2.51	126.85	123.71
9	B	503	MES	C6-C5-N4	-2.50	106.31	110.10
8	D	501	GDP	C3'-C2'-C1'	2.49	104.73	100.98
8	D	501	GDP	PA-O3A-PB	-2.39	124.63	132.83
9	B	504	MES	O3S-S-C8	2.29	109.47	105.77
10	D	502	O91	O02-C01-C07	-2.23	120.28	124.12
10	D	502	O91	C14-O13-C12	-2.22	114.18	117.53
10	D	502	O91	C03-O02-C01	-2.19	114.23	117.53
10	D	502	O91	C42-C32-N26	2.15	126.39	123.71
9	B	504	MES	C7-N4-C5	2.13	116.69	111.23
9	B	503	MES	O1S-S-C8	2.13	109.48	106.92
10	B	505	O91	O13-C12-C10	-2.07	120.55	124.12
9	B	504	MES	O2S-S-C8	2.07	109.40	106.92
9	B	504	MES	C7-N4-C3	2.05	116.47	111.23
5	C	501	GTP	N2-C2-N1	2.03	120.41	117.25
9	B	504	MES	O1S-S-C8	2.00	109.33	106.92
10	B	505	O91	O02-C01-C07	-2.00	120.67	124.12

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
10	D	502	O91	C18-C12-O13-C14
10	D	502	O91	C10-C12-O13-C14
10	D	502	O91	C18-C01-O02-C03
10	D	502	O91	C07-C01-O02-C03
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	503	MES	C7-C8-S-O1S
8	D	501	GDP	PA-O3A-PB-O1B
8	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
8	D	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C4'-C5'-O5'-PA

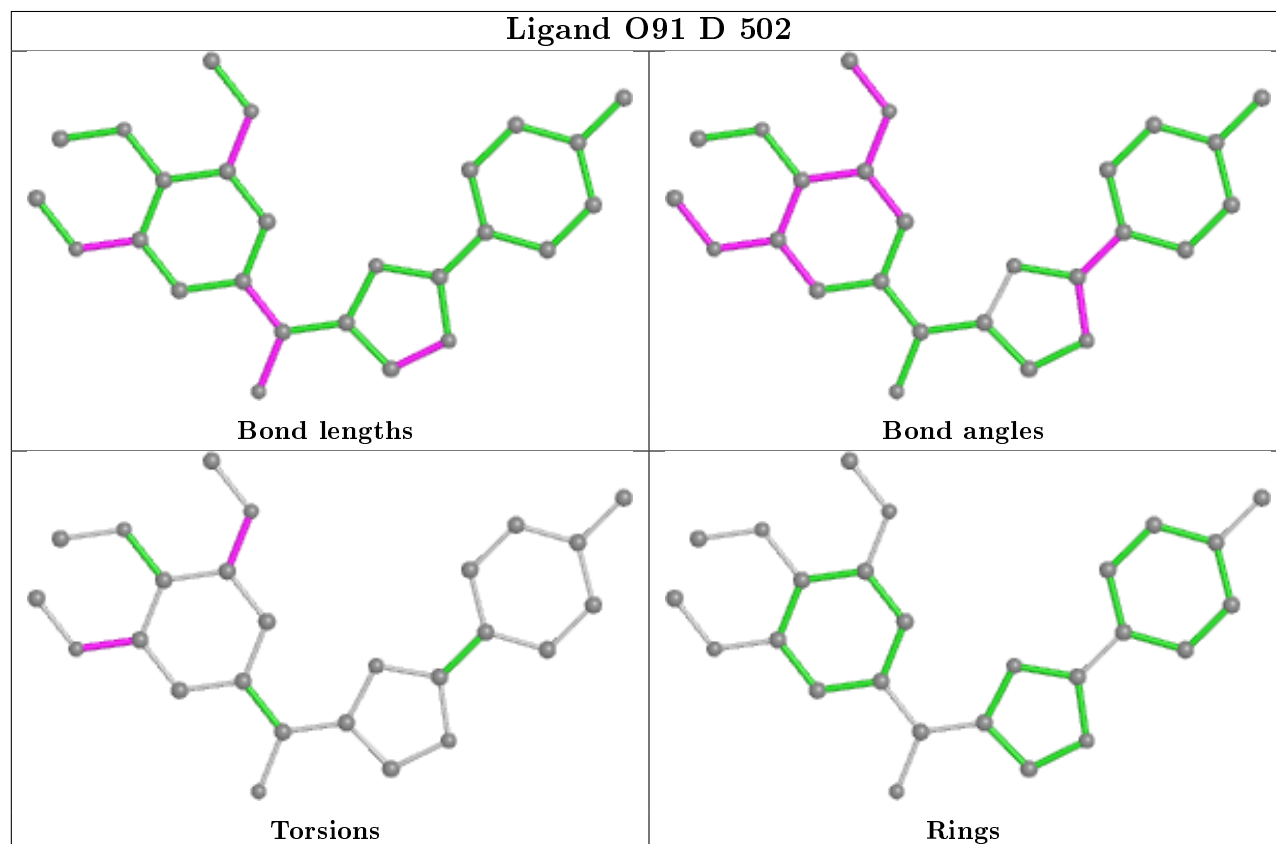
There are no ring outliers.

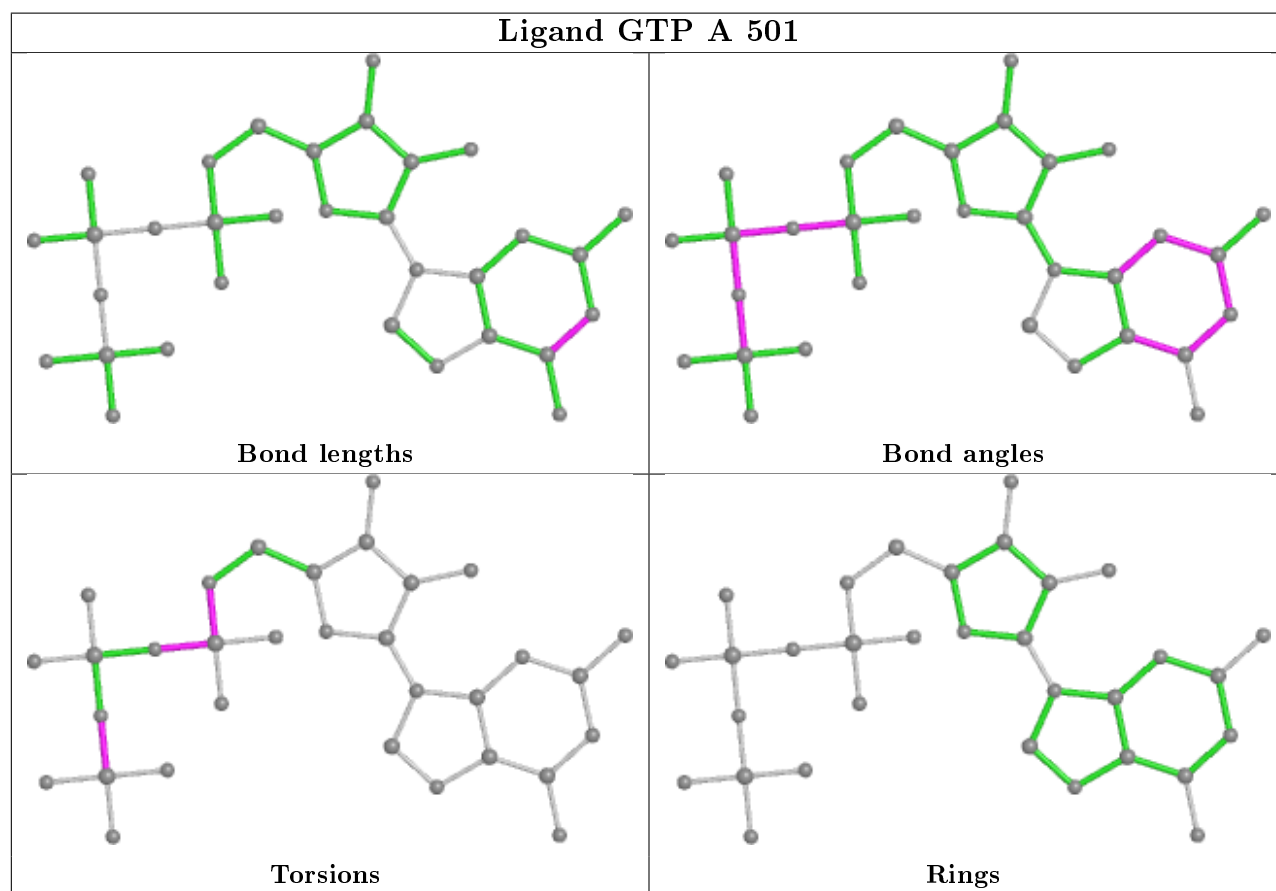
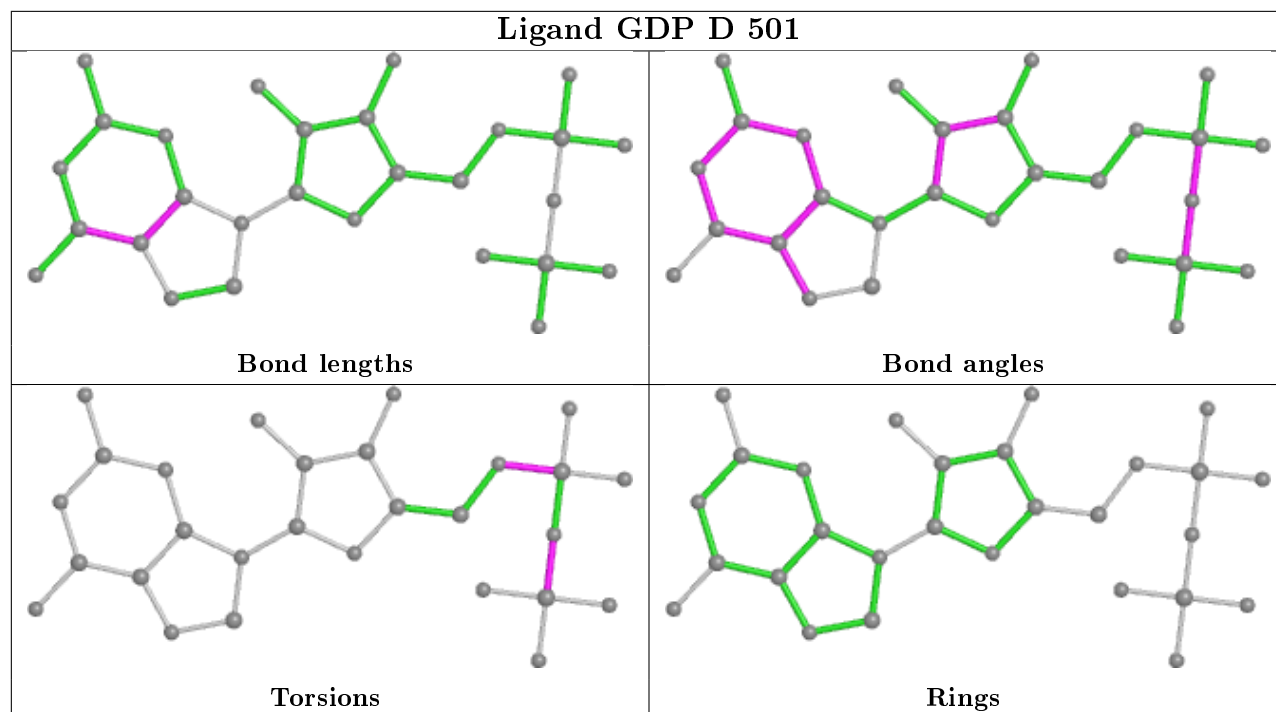
5 monomers are involved in 8 short contacts:

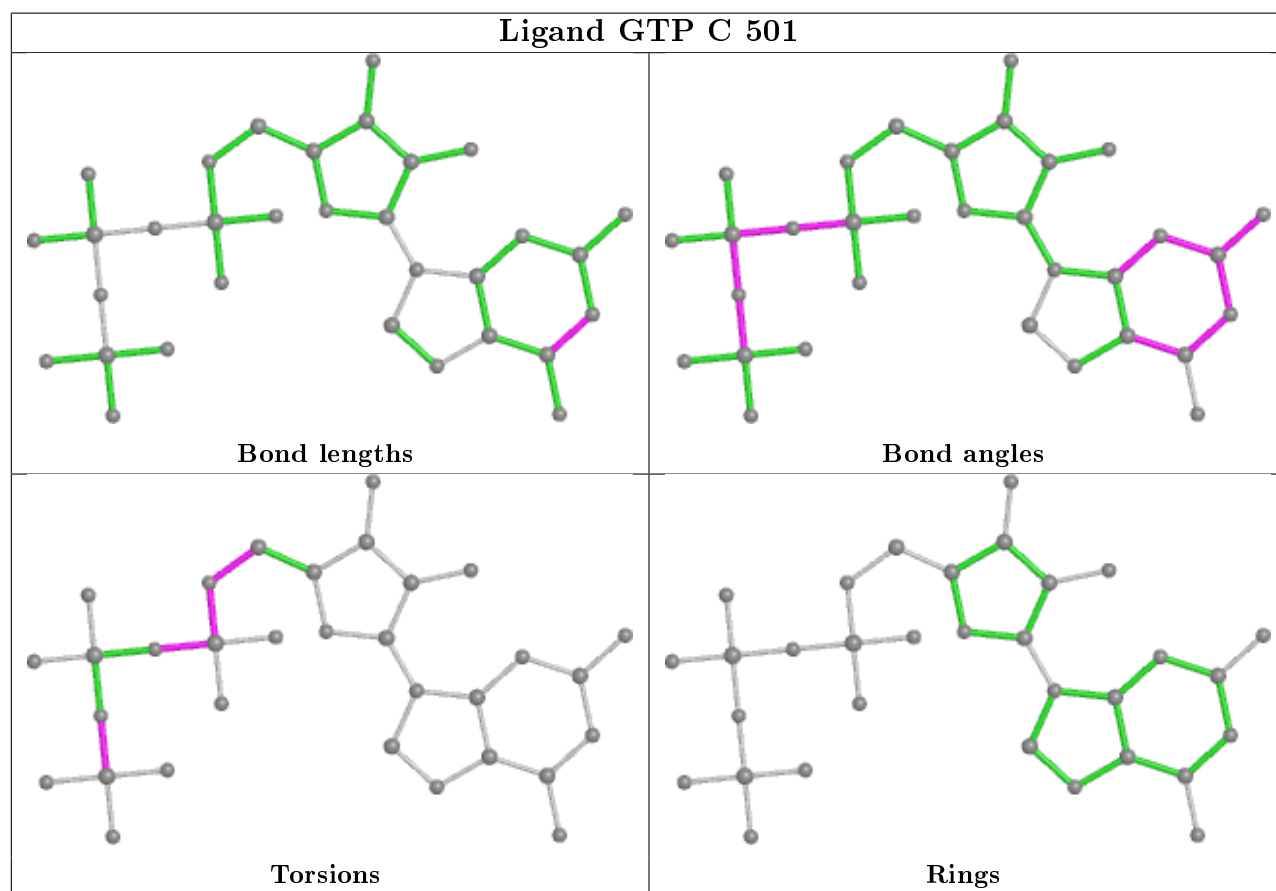
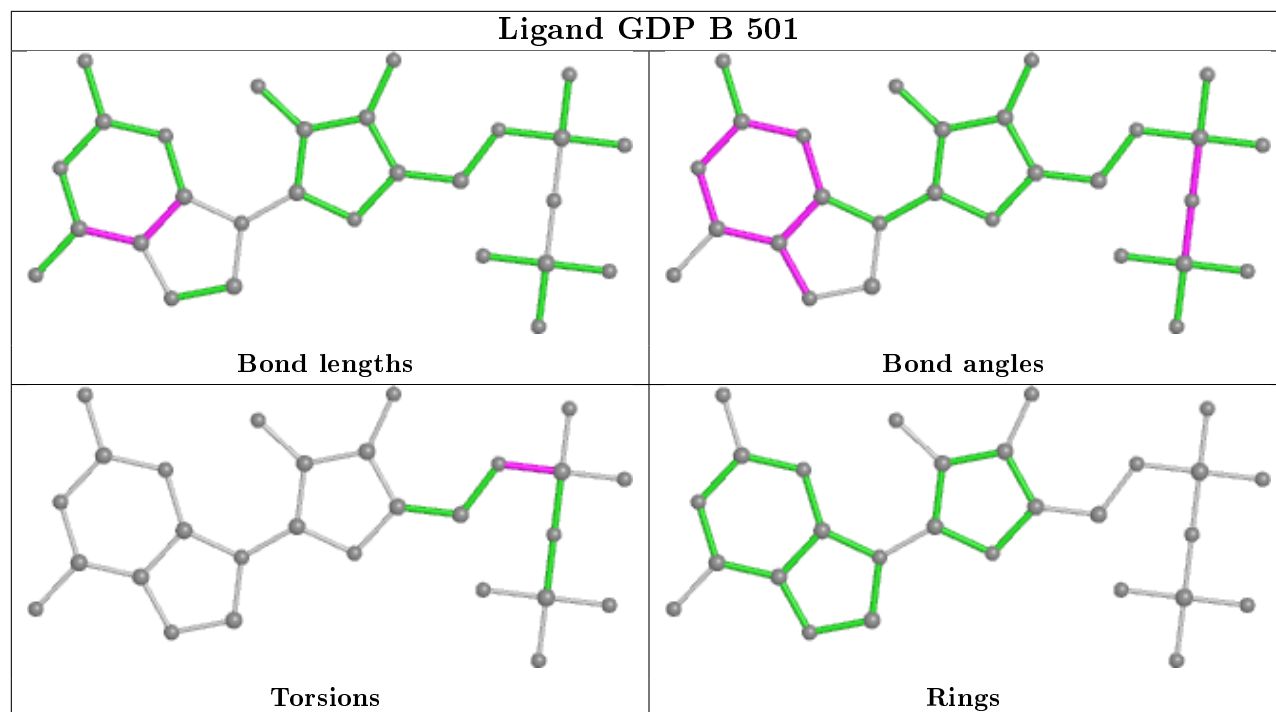
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	O91	3	0
9	B	504	MES	1	0
8	D	501	GDP	2	0
8	B	501	GDP	1	0
10	B	505	O91	1	0

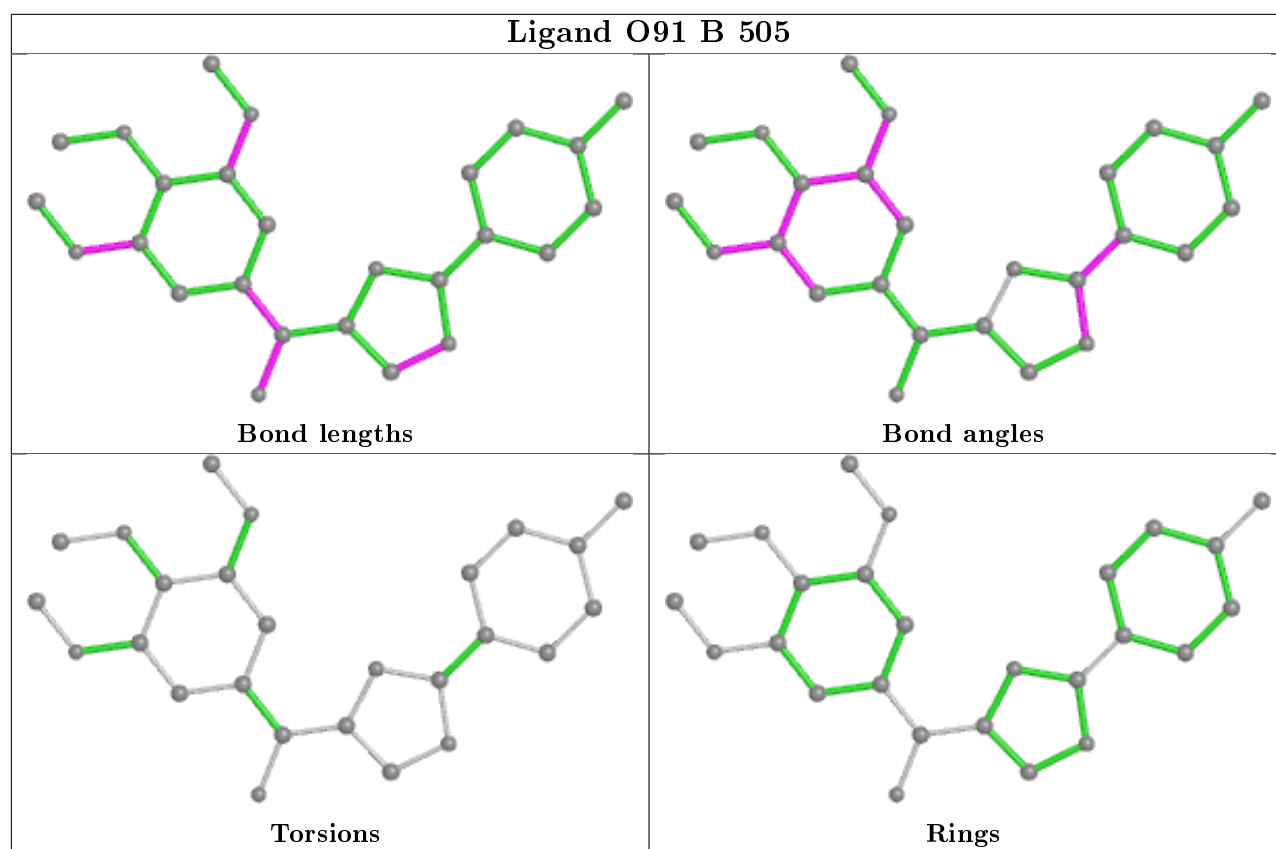
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	-0.25	2 (0%) 91 89	25, 41, 70, 85	0
1	C	440/450 (97%)	-0.38	1 (0%) 95 95	21, 32, 60, 91	0
2	B	427/445 (95%)	-0.24	10 (2%) 60 54	21, 39, 75, 128	0
2	D	421/445 (94%)	0.17	26 (6%) 20 15	28, 58, 100, 136	0
3	E	121/143 (84%)	0.12	2 (1%) 70 66	30, 57, 90, 125	0
4	F	332/384 (86%)	0.90	75 (22%) 0 0	30, 66, 138, 161	0
All	All	2178/2317 (94%)	0.00	116 (5%) 26 20	21, 47, 102, 161	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	6.4
4	F	177	GLY	6.1
4	F	244	CYS	6.0
4	F	256	TYR	6.0
4	F	239	HIS	5.7
4	F	130	VAL	5.5
2	D	55	THR	5.4
2	B	55	THR	4.8
4	F	253	TYR	4.7
2	B	57	ASN	4.6
4	F	132	LEU	4.6
4	F	101	TYR	4.6
4	F	259	GLY	4.5
4	F	100	ILE	4.5
4	F	182	ILE	4.5
4	F	131	PHE	4.5
3	E	27	PRO	4.4
4	F	225	SER	4.4
4	F	136	ASN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	103	THR	4.3
4	F	234	GLN	4.3
4	F	231	ALA	4.2
2	D	245	GLN	4.2
4	F	252	ASN	4.1
4	F	257	GLU	4.1
4	F	171	ASP	4.0
4	F	223	THR	4.0
4	F	163	SER	3.9
2	D	1	MET	3.8
4	F	255	ARG	3.5
4	F	232	ASN	3.4
4	F	243	HIS	3.4
4	F	133	ALA	3.4
2	D	390	ARG	3.3
2	D	219	THR	3.2
2	D	37	HIS	3.2
4	F	172	PHE	3.2
4	F	227	PRO	3.2
4	F	90	SER	3.2
4	F	194	PRO	3.2
4	F	238	CYS	3.2
2	D	56	GLY	3.1
4	F	144	GLY	3.1
4	F	143	GLU	3.1
4	F	242	ASN	3.1
4	F	254	GLY	3.0
4	F	240	LEU	3.0
4	F	162	ILE	3.0
4	F	148	ILE	3.0
4	F	181	VAL	3.0
4	F	235	ASP	3.0
2	D	95	SER	2.9
2	D	216	LYS	2.9
2	B	277	GLY	2.8
4	F	180	HIS	2.8
2	D	94	GLN	2.8
4	F	179	VAL	2.8
4	F	246	GLN	2.8
4	F	102	PRO	2.8
4	F	229	ASN	2.8
4	F	258	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	71	GLY	2.7
4	F	169	LEU	2.7
4	F	224	SER	2.7
4	F	237	THR	2.7
4	F	146	VAL	2.7
2	D	394	PHE	2.7
4	F	147	TRP	2.7
4	F	245	ILE	2.7
4	F	241	THR	2.6
4	F	166	ALA	2.6
4	F	247	LYS	2.6
2	B	279	GLN	2.6
1	C	1	MET	2.6
2	D	217	LEU	2.5
4	F	167	SER	2.5
4	F	183	GLN	2.5
3	E	48	GLU	2.5
2	B	428	ALA	2.5
1	A	262	TYR	2.5
4	F	134	ALA	2.4
2	B	37	HIS	2.4
4	F	196	HIS	2.4
4	F	20	LEU	2.4
4	F	149	ALA	2.4
2	D	41	ASP	2.4
2	B	58	LYS	2.4
4	F	228	TYR	2.4
2	D	405	GLU	2.3
4	F	135	TYR	2.3
1	A	59	GLY	2.3
2	D	246	LEU	2.3
4	F	129	GLU	2.3
2	B	54	ALA	2.2
2	D	247	ASN	2.2
4	F	361	LEU	2.2
2	D	54	ALA	2.2
2	D	177	ASP	2.2
4	F	192	LEU	2.2
2	D	92	PHE	2.2
4	F	263	PHE	2.2
4	F	98	TYR	2.1
4	F	178	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	78	SER	2.1
2	D	72	THR	2.1
2	B	245	GLN	2.1
4	F	164	SER	2.1
2	D	175	VAL	2.1
4	F	99	VAL	2.1
2	D	431	ASP	2.1
2	B	246	LEU	2.1
4	F	380	HIS	2.1
2	D	391	ARG	2.1
2	D	48	ASN	2.0
4	F	145	ASN	2.0
4	F	139	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
8	GDP	D	501	28/28	0.94	0.14	48,55,65,66	0
10	O91	D	502	26/26	0.94	0.18	44,52,60,65	0
9	MES	B	504	12/12	0.97	0.22	57,62,70,73	0
6	MG	B	502	1/1	0.97	0.27	35,35,35,35	0
10	O91	B	505	26/26	0.97	0.16	33,38,44,47	0
9	MES	B	503	12/12	0.98	0.12	32,46,61,64	0
7	CA	A	503	1/1	0.98	0.04	60,60,60,60	0
7	CA	C	503	1/1	0.98	0.09	45,45,45,45	0
5	GTP	A	501	32/32	0.99	0.18	22,28,34,39	0
8	GDP	B	501	28/28	0.99	0.16	18,25,33,35	0

Continued on next page...

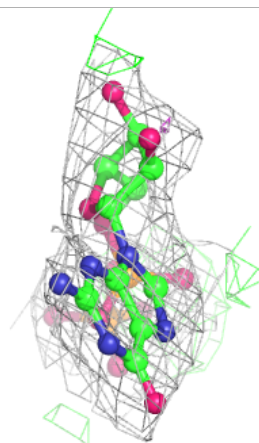
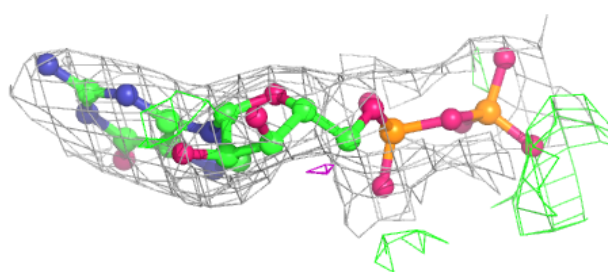
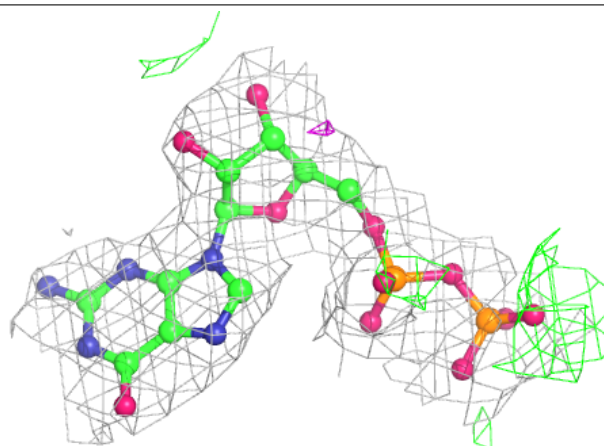
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	C	501	32/32	0.99	0.16	23,28,31,34	0
6	MG	A	502	1/1	0.99	0.17	24,24,24,24	0
6	MG	C	502	1/1	0.99	0.14	26,26,26,26	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.

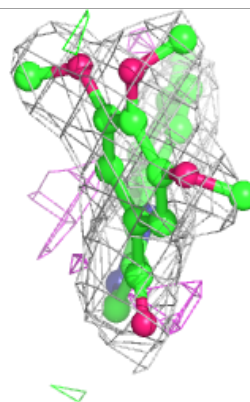
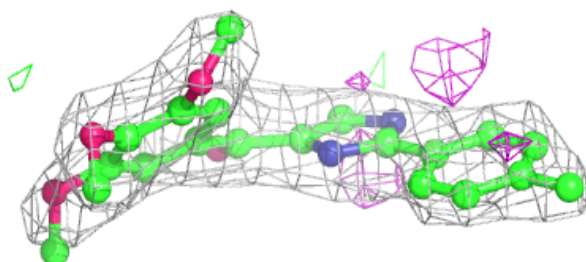
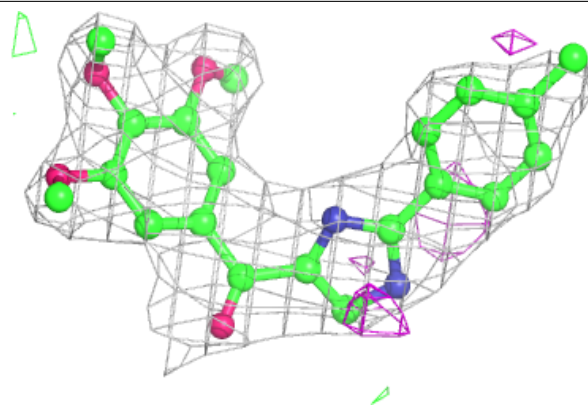
Electron density around GDP D 501:

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

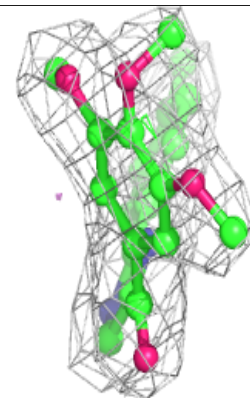
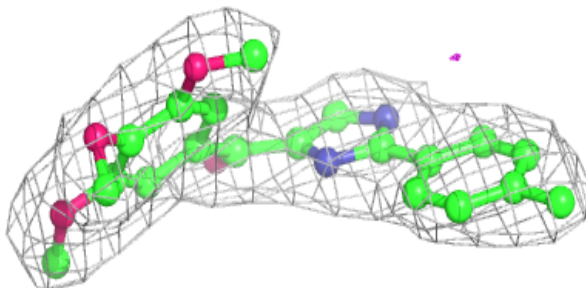
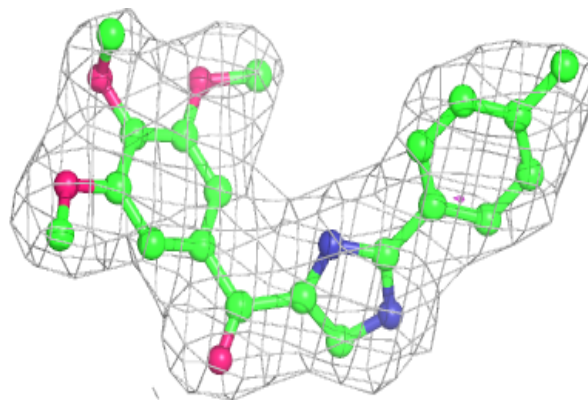


Electron density around O91 D 502:

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

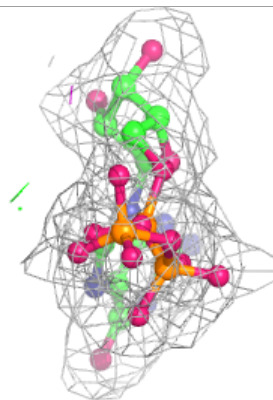
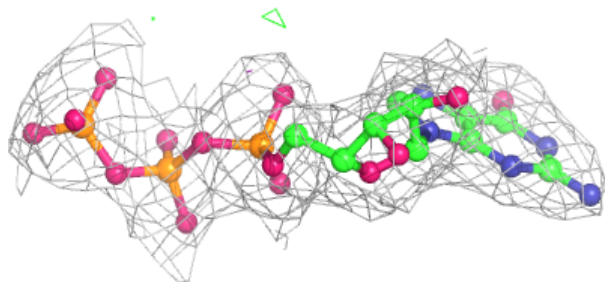
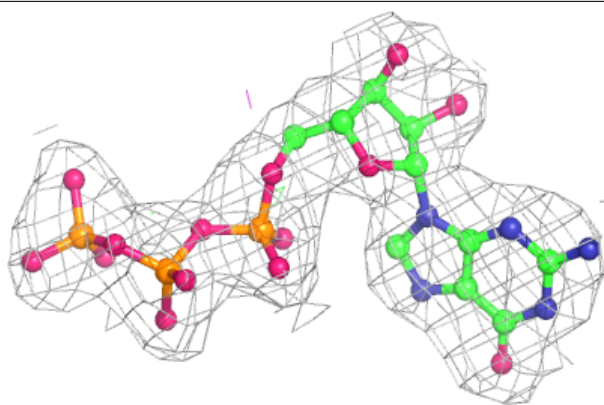
**Electron density around O91 B 505:**

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

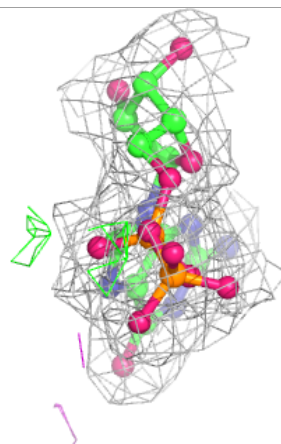
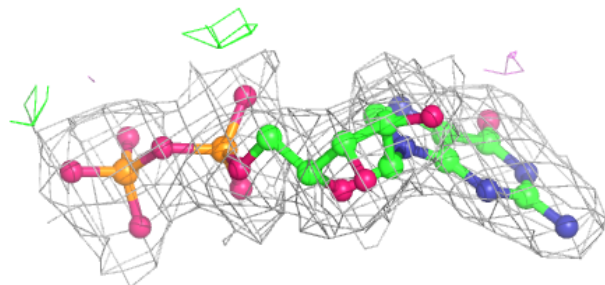
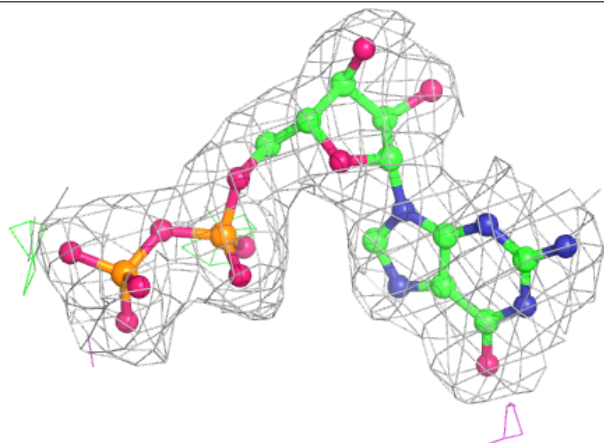


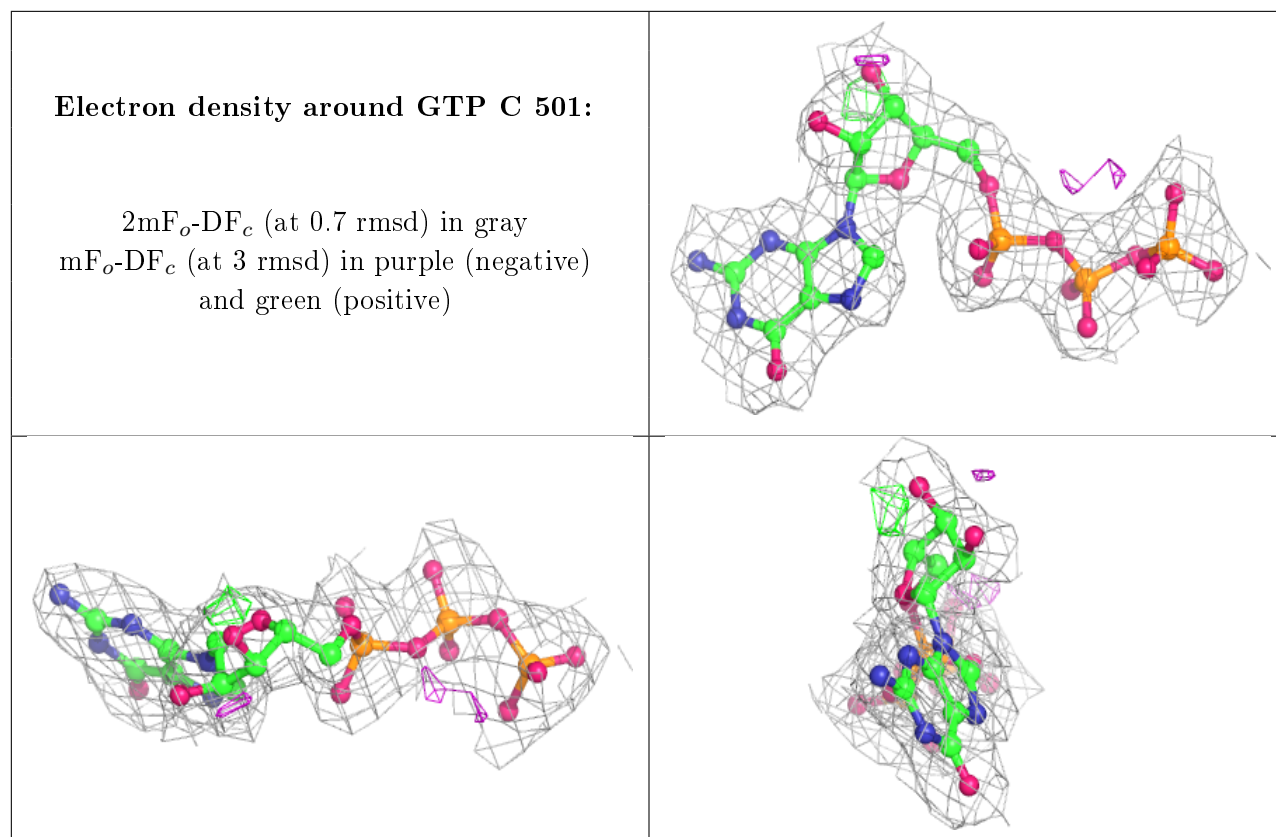
Electron density around GTP A 501:

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

**Electron density around GDP B 501:**

$2mF_o-DF_c$ (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.