Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2024 – 01:18 PM JST

PDB ID	:	8WD0
Title	:	Crystal structure of T2R-TTL-Erianin complex
Authors	:	Yang, J.
Deposited on	:	2023-09-14
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

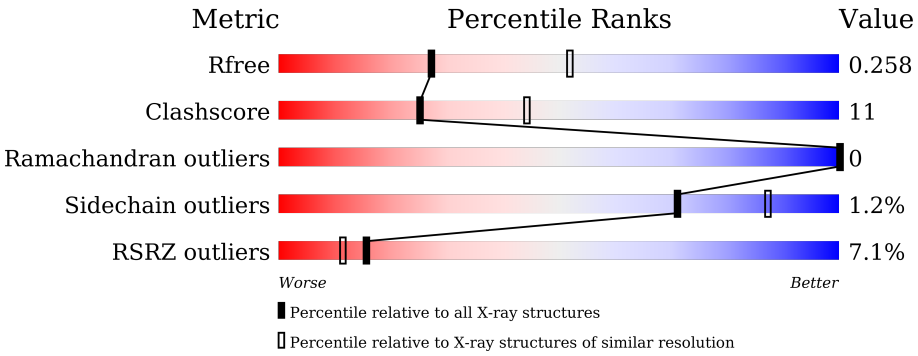
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	3% 78% 18% ·
1	C	451	% 77% 20% ·
2	B	445	4% 74% 22% ·
2	D	445	8% 70% 24% · 5%
3	E	189	6% 54% 10% 36%
4	F	380	19% 65% 22% · 12%

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
10	W4F	B	503	-	X	-	-
10	W4F	D	503	-	X	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17492 atoms, of which 44 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
			3402	2156	577	647	22			
1	C	440	Total	C	N	O	S	0	0	0
			3427	2169	580	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3334	2095	566	647	26			
2	D	421	Total	C	N	O	S	0	0	0
			3280	2066	554	634	26			

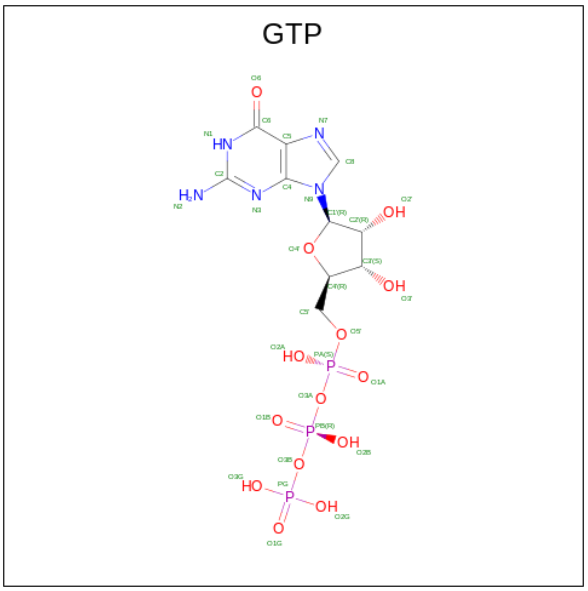
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			996	614	180	197	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2717	1747	460	496	14			

- 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 32 10 5 14 3	32	0
5	C	1	Total C N O P 32 10 5 14 3	32	0
5	D	1	Total C N O P 32 10 5 14 3	32	0

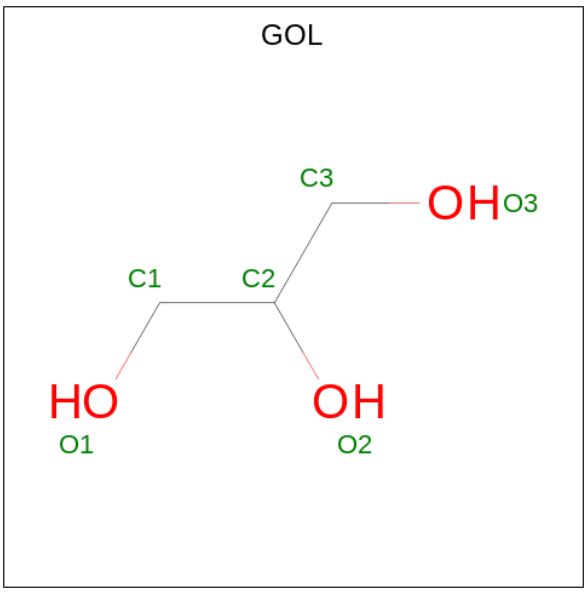
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

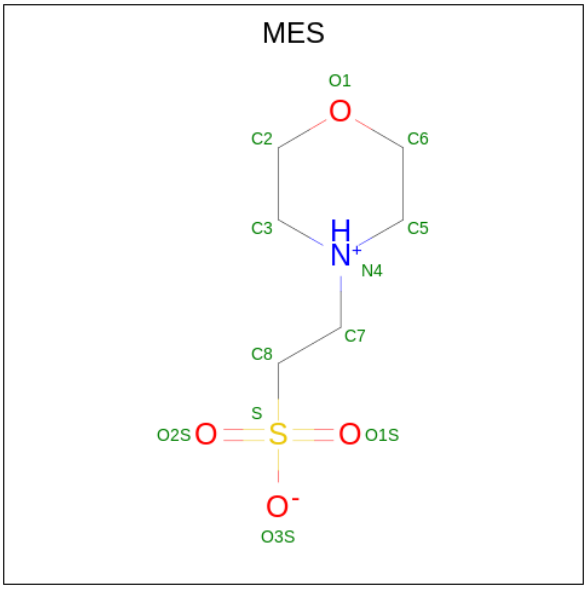
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	1	0
7	C	1	Total Ca 1 1	1	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



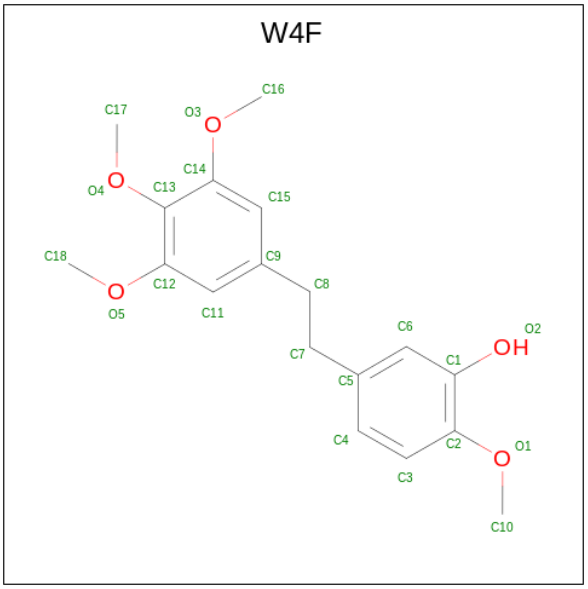
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	6	0

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



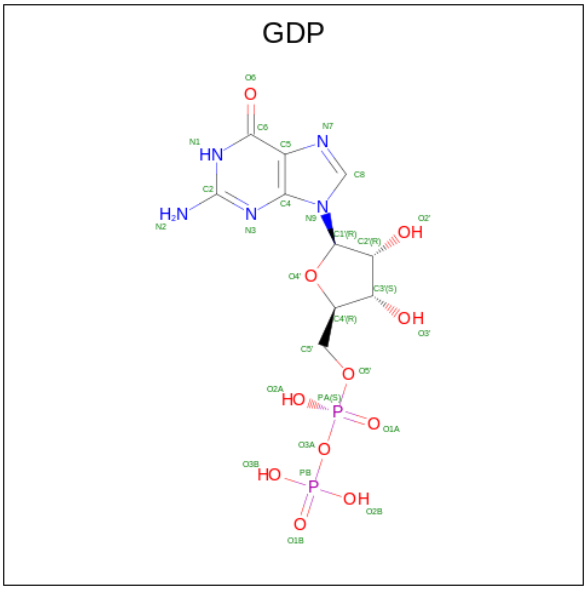
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	12	0

- Molecule 10 is 2-methoxy-5-[2-(3,4,5-trimethoxyphenyl)ethyl]phenol (three-letter code: W4F) (formula: $C_{18}H_{22}O_5$) (labeled as "Ligand of Interest" by depositor).



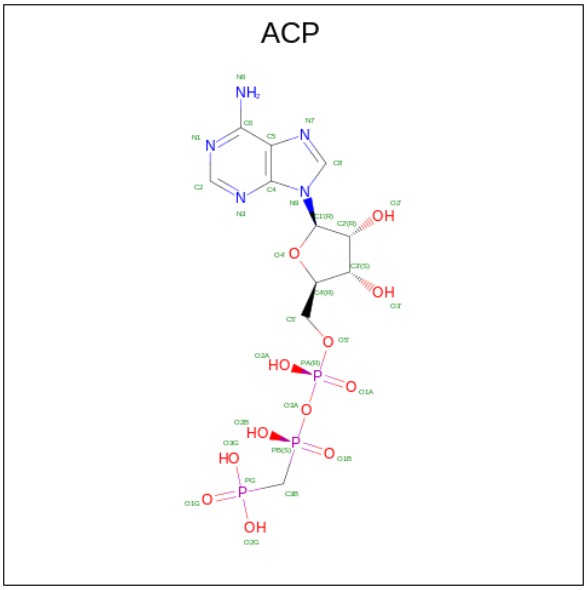
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			45	18	22	5		
10	D	1	Total	C	H	O	0	0
			45	18	22	5		

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



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	31	0
			31	11	5	12	3		

- Molecule 13 is water.

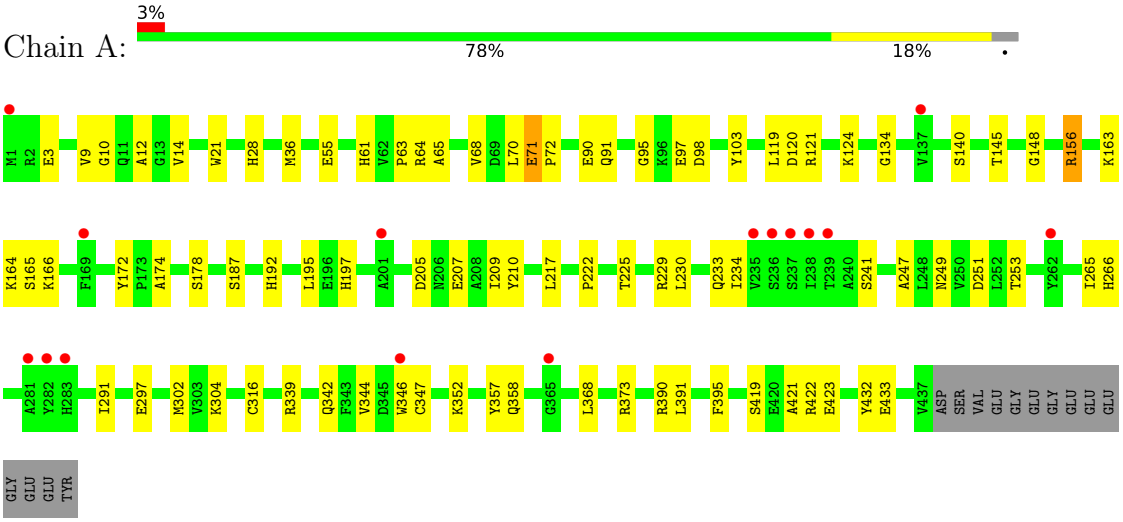
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	11	Total	O	0	0
			11	11		
13	B	15	Total	O	0	0
			15	15		
13	C	28	Total	O	0	0
			28	28		
13	D	4	Total	O	0	0
			4	4		
13	E	4	Total	O	0	0
			4	4		
13	F	5	Total	O	0	0
			5	5		

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.

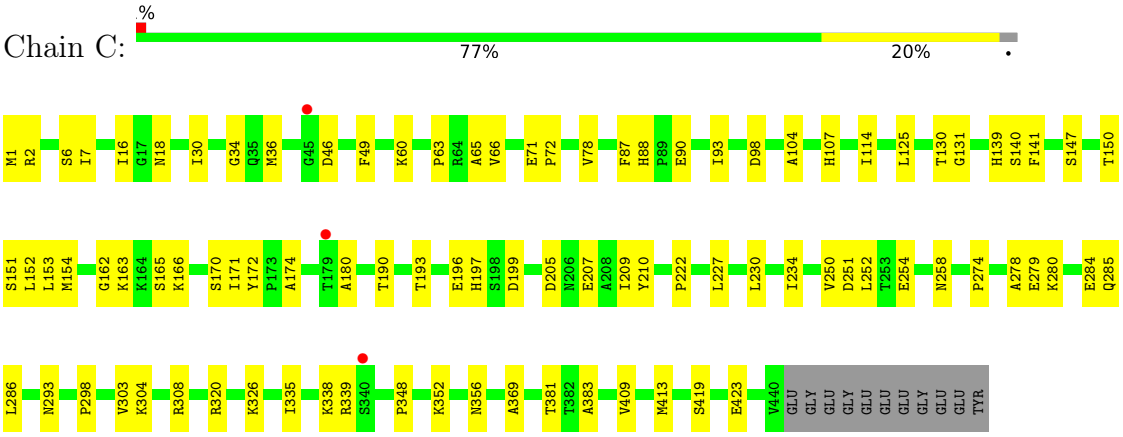
• Molecule 1: Tubulin alpha-1B chain

Chain A:



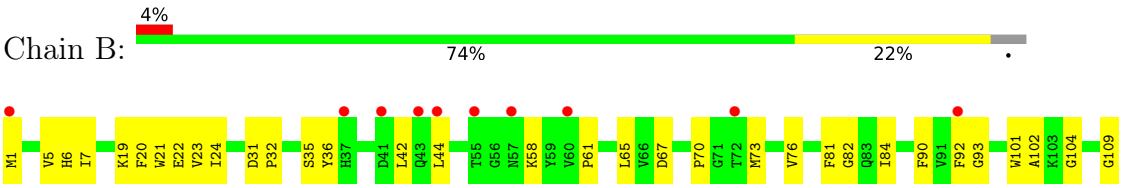
• Molecule 1: Tubulin alpha-1B chain

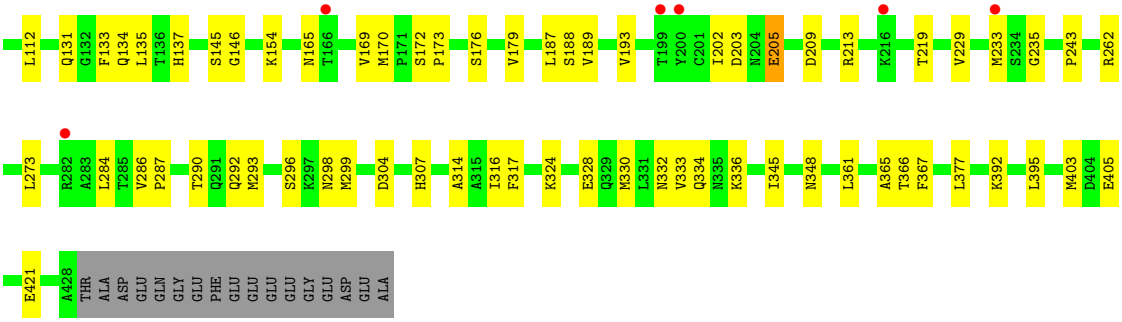
Chain C:



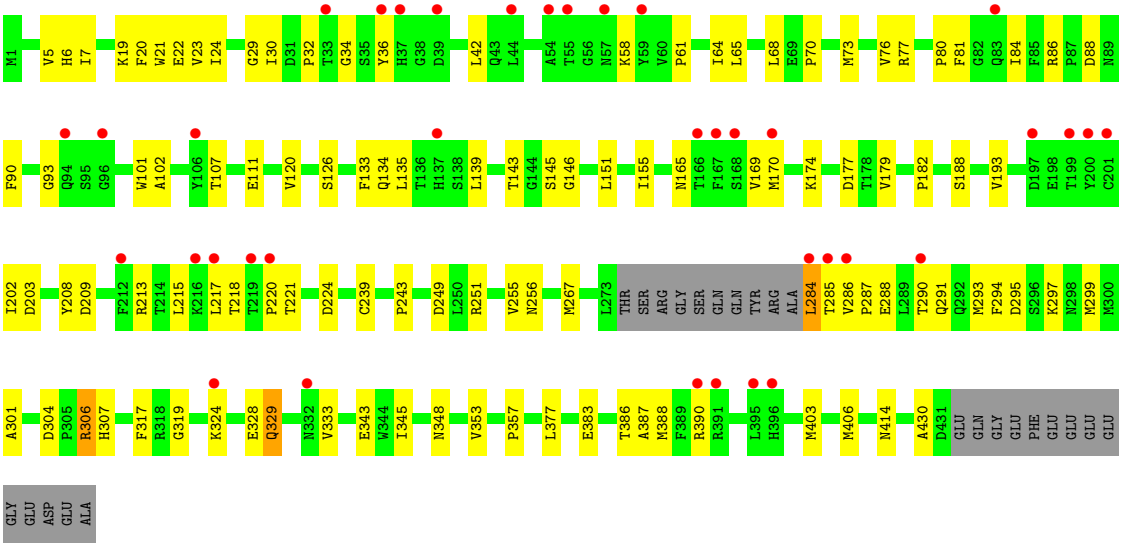
• Molecule 2: Tubulin beta chain

Chain B:

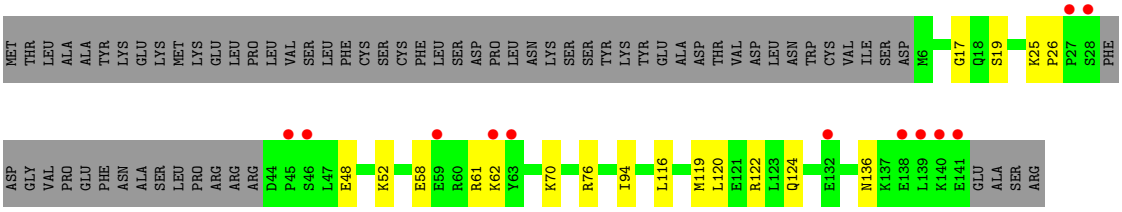




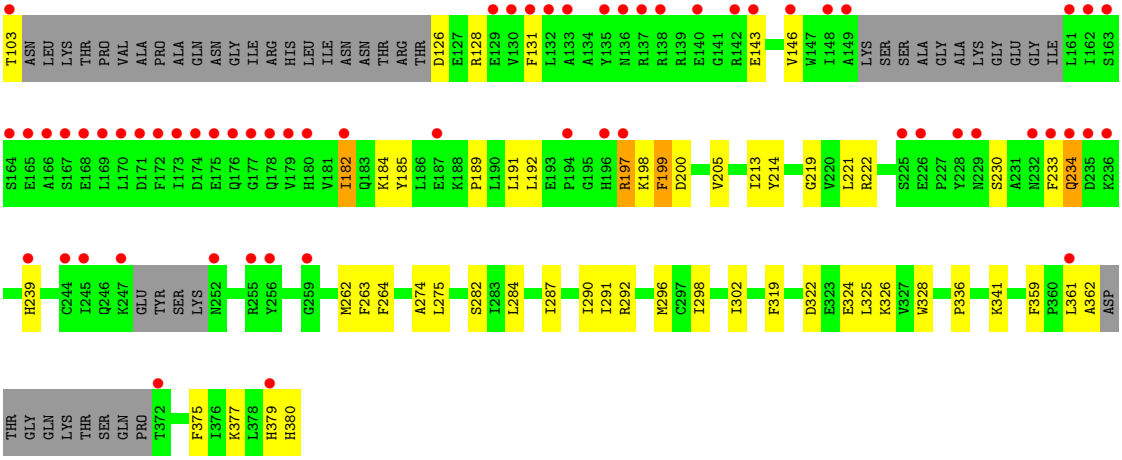
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase


T103 ASN LEU LYS THR PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG THR D126 E127 R128 E129 V130 F131 L132 A133 A134 Y135 N136 R137 R138 R139 E140 G141 R142 E143 V146 W147 I148 A149 LYS SER SER ALA GLY ALA LYS GLY GLU GLY ILE L161 I162 S163
S164 E165 A166 S167 E168 L169 L170 D171 F172 I173 D174 E175 Q176 G177 Q178 V179 H180 V181 I182 Q183 K184 Y185 L186 E187 K188 P189 L190 L191 L192 E193 P194 G195 H196 R197 K198 F199 D200 V205 I213 Y214 G219 V220 L221 R222 S225 E226 P227 Y228 N229 S230 A231 N232 F233 Q234 D235 K236
H239 C244 I245 Q246 K247 GLU TYR SER LYS M252 R255 Y256 G259 M262 F263 F264 A274 L275 S282 I283 L284 I287 I290 I291 R292 M296 C297 I298 I302 F319 D322 E323 E324 L325 K326 V327 W328 P336 K341 F359 P360 L361 A362 ASP
THR GLY GLN LYS THR SER GLN PRO T372 F375 Y376 K377 L378 H379 H380

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	156.56Å 181.54Å 104.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.26 – 2.60 38.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.26-2.60) 98.8 (38.26-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.227 , 0.258 0.227 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17492	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, W4F, GOL, CA, MES, GDP, GTP, ACP

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	0.36	0/3480	0.51	0/4726
1	C	0.42	0/3505	0.53	0/4761
2	B	0.40	0/3409	0.53	0/4624
2	D	0.37	0/3353	0.52	0/4546
3	E	0.32	0/1004	0.41	0/1333
4	F	0.33	0/2778	0.49	0/3756
All	All	0.38	0/17529	0.51	0/23746

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

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	3402	0	3309	62	0
1	C	3427	0	3326	68	0
2	B	3334	0	3181	73	0
2	D	3280	0	3144	74	2
3	E	996	0	1007	19	0
4	F	2717	0	2662	78	2
5	A	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	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
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	12	0	12	0	0
10	B	23	22	0	2	0
10	D	23	22	0	1	0
11	B	28	0	12	0	0
12	F	31	0	14	0	0
13	A	11	0	0	1	0
13	B	15	0	0	0	0
13	C	28	0	0	1	0
13	D	4	0	0	0	0
13	E	4	0	0	0	0
13	F	5	0	0	0	0
All	All	17448	44	16711	362	2

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 11.

All (362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HB3	2:B:131:GLN:HB3	1.36	1.06
3:E:48:GLU:HG2	3:E:52:LYS:HE2	1.44	0.98
2:D:73:MET:HB3	2:D:77:ARG:HH21	1.31	0.94
4:F:200:ASP:OD1	4:F:222:ARG:HD3	1.68	0.94
1:A:119:LEU:HD11	1:A:156:ARG:HG2	1.52	0.91
4:F:199:PHE:CE1	4:F:221:LEU:HG	2.06	0.90
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.13	0.83
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.59	0.82
4:F:263:PHE:HE2	4:F:341:LYS:HD3	1.44	0.82
1:A:166:LYS:HE2	1:A:197:HIS:O	1.80	0.81
2:B:332:ASN:OD1	2:B:336:LYS:HE3	1.81	0.81
2:D:134:GLN:HA	2:D:165:ASN:O	1.80	0.80
4:F:199:PHE:CD1	4:F:221:LEU:HG	2.16	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:HB2	2:B:1:MET:HG3	1.65	0.79
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.67	0.77
1:C:147:SER:HB2	1:C:190:THR:OG1	1.85	0.77
1:C:381:THR:HG22	1:C:383:ALA:H	1.49	0.77
2:B:1:MET:HB3	2:B:131:GLN:CB	2.14	0.76
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.67	0.76
3:E:120:LEU:O	3:E:124:GLN:HG2	1.86	0.75
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.68	0.75
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.67	0.74
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.70	0.74
4:F:13:VAL:O	4:F:17:VAL:HG23	1.89	0.73
1:C:1:MET:HB3	1:C:130:THR:OG1	1.89	0.72
1:A:163:LYS:HE2	1:A:164:LYS:HZ3	1.55	0.71
4:F:199:PHE:CE1	4:F:221:LEU:CD2	2.74	0.70
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.72	0.70
1:C:230:LEU:O	1:C:234:ILE:HD12	1.91	0.70
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.73	0.70
2:D:239:CYS:HB2	10:D:503:W4F:C18	2.22	0.69
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.75	0.69
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.58	0.69
4:F:31:ARG:HH21	4:F:32:LYS:HG3	1.57	0.69
2:B:42:LEU:CD2	2:B:243:PRO:HG2	2.23	0.68
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.74	0.68
4:F:199:PHE:CE1	4:F:221:LEU:CG	2.77	0.68
2:D:73:MET:HB3	2:D:77:ARG:NH2	2.08	0.68
4:F:16:GLU:O	4:F:20:LEU:HG	1.92	0.68
4:F:100:ILE:HD11	4:F:128:ARG:HA	1.76	0.68
2:D:65:LEU:HD22	2:D:90:PHE:CE2	2.31	0.66
1:A:247:ALA:HB3	3:E:19:SER:OG	1.95	0.66
2:D:284:LEU:HD23	2:D:288:GLU:HB2	1.78	0.66
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.77	0.66
4:F:82:LYS:NZ	4:F:97:SER:O	2.28	0.66
2:B:395:LEU:HD21	2:B:405:GLU:HG2	1.78	0.66
2:B:134:GLN:HA	2:B:165:ASN:O	1.94	0.65
4:F:16:GLU:OE2	4:F:20:LEU:HD21	1.98	0.64
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.80	0.64
4:F:199:PHE:CD1	4:F:221:LEU:CG	2.80	0.64
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.33	0.64
2:B:392:LYS:HD3	2:B:405:GLU:OE2	1.98	0.64
1:A:230:LEU:O	1:A:234:ILE:HD12	1.99	0.63
2:D:30:ILE:HG13	2:D:30:ILE:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:ARG:HB2	4:F:76:SER:OG	1.98	0.63
4:F:191:LEU:HA	4:F:197:ARG:O	1.99	0.63
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.35	0.62
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.81	0.62
4:F:78:VAL:HG13	4:F:82:LYS:HZ2	1.63	0.62
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.36	0.61
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.35	0.61
4:F:8:ASP:OD2	4:F:11:SER:HB2	2.01	0.61
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.31	0.60
4:F:199:PHE:HE1	4:F:221:LEU:CD2	2.14	0.60
2:D:32:PRO:HA	2:D:81:PHE:CD2	2.36	0.60
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.36	0.60
2:B:324:LYS:O	2:B:328:GLU:HG3	2.02	0.60
1:C:252:LEU:HD12	1:C:252:LEU:O	2.02	0.60
4:F:292:ARG:O	4:F:296:MET:HG2	2.02	0.60
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.02	0.59
4:F:199:PHE:CD1	4:F:221:LEU:CD2	2.86	0.59
2:B:36:TYR:CD2	2:B:44:LEU:HD21	2.37	0.58
1:A:156:ARG:CG	1:A:156:ARG:HH21	2.16	0.58
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.37	0.58
2:D:29:GLY:O	2:D:36:TYR:CD1	2.56	0.58
1:A:187:SER:CB	1:A:391:LEU:HD21	2.33	0.58
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.85	0.58
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.85	0.58
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.19	0.57
1:A:251:ASP:OD2	1:A:253:THR:HB	2.05	0.57
2:D:81:PHE:O	2:D:84:ILE:HG22	2.05	0.57
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.87	0.57
1:A:28:HIS:HB3	1:A:36:MET:HE3	1.85	0.57
2:B:73:MET:HE3	2:B:90:PHE:CD2	2.40	0.56
2:D:221:THR:HG23	2:D:224:ASP:H	1.69	0.56
4:F:192:LEU:HD22	4:F:262:MET:CE	2.35	0.56
2:B:67:ASP:O	2:B:92:PHE:HA	2.06	0.56
2:B:324:LYS:HE2	2:B:328:GLU:OE2	2.06	0.56
2:D:295:ASP:OD2	2:D:297:LYS:HE3	2.06	0.56
2:B:345:ILE:HG22	2:B:348:ASN:HB3	1.87	0.56
2:D:406:MET:HA	2:D:406:MET:CE	2.35	0.56
1:C:280:LYS:O	1:C:284:GLU:HG3	2.06	0.56
2:D:22:GLU:OE2	2:D:80:PRO:HG2	2.05	0.56
2:D:294:PHE:O	2:D:306:ARG:NH2	2.37	0.56
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:PHE:HB2	2:B:233:MET:HE3	1.88	0.56
2:B:229:VAL:HG12	2:B:233:MET:HE2	1.87	0.55
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.71	0.55
2:B:172:SER:OG	2:B:205:GLU:CG	2.55	0.55
2:D:406:MET:HA	2:D:406:MET:HE2	1.87	0.55
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.37	0.55
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.41	0.55
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.89	0.55
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.89	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
2:B:170:MET:HB2	2:B:203:ASP:HA	1.90	0.54
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.71	0.54
2:D:208:TYR:HE2	2:D:220:PRO:HD3	1.72	0.54
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.38	0.54
1:A:419:SER:O	1:A:423:GLU:HG3	2.08	0.54
1:C:207:GLU:OE1	1:C:304:LYS:HE2	2.08	0.54
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.43	0.54
2:D:287:PRO:HA	2:D:329:GLN:HG3	1.90	0.54
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.91	0.53
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.89	0.53
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.89	0.53
2:B:316:ILE:CG2	2:B:366:THR:HB	2.38	0.53
2:D:284:LEU:HD23	2:D:288:GLU:CB	2.38	0.53
4:F:14:TYR:HA	4:F:17:VAL:HG23	1.90	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.53
2:D:7:ILE:O	2:D:135:LEU:HA	2.08	0.53
1:A:119:LEU:CD1	1:A:156:ARG:HG2	2.34	0.53
1:A:163:LYS:HE2	1:A:164:LYS:NZ	2.22	0.53
2:B:145:SER:HG	2:B:188:SER:HG	1.54	0.53
1:C:30:ILE:HD11	1:C:36:MET:HE2	1.90	0.53
4:F:191:LEU:HD22	4:F:197:ARG:O	2.08	0.53
2:D:267:MET:HB2	2:D:301:ALA:HB3	1.91	0.53
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.89	0.52
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.90	0.52
3:E:116:LEU:HD23	3:E:119:MET:CE	2.40	0.52
2:B:20:PHE:HB2	2:B:233:MET:CE	2.40	0.52
1:A:207:GLU:OE2	1:A:304:LYS:HD2	2.09	0.52
2:D:42:LEU:HD22	2:D:243:PRO:HG2	1.92	0.52
1:C:1:MET:O	1:C:2:ARG:HB2	2.09	0.52
2:D:343:GLU:HG2	2:D:430:ALA:HB2	1.92	0.52
4:F:324:GLU:O	4:F:324:GLU:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:VAL:HA	2:B:202:ILE:O	2.10	0.52
4:F:199:PHE:HE1	4:F:221:LEU:CG	2.23	0.51
1:C:147:SER:HB2	1:C:190:THR:HG1	1.72	0.51
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.39	0.51
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.93	0.51
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.46	0.51
2:D:68:LEU:H	2:D:143:THR:HG21	1.76	0.51
2:D:174:LYS:HB3	2:D:208:TYR:CD1	2.45	0.51
2:B:81:PHE:O	2:B:84:ILE:HG22	2.10	0.51
2:B:314:ALA:HB1	10:B:503:W4F:C16	2.40	0.51
4:F:69:ASP:OD1	4:F:69:ASP:N	2.44	0.51
4:F:199:PHE:HE1	4:F:221:LEU:HD21	1.75	0.51
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.46	0.51
2:D:61:PRO:HD3	2:D:84:ILE:HG12	1.93	0.50
2:D:299:MET:HA	2:D:299:MET:HE2	1.93	0.50
4:F:24:THR:HG21	4:F:361:LEU:HD13	1.92	0.50
1:A:10:GLY:O	1:A:14:VAL:HG23	2.12	0.50
4:F:326:LYS:HD3	4:F:328:TRP:CZ2	2.47	0.50
2:B:209:ASP:HB3	2:B:213:ARG:HD2	1.94	0.50
2:B:330:MET:O	2:B:334:GLN:HG3	2.11	0.50
2:D:169:VAL:HA	2:D:202:ILE:O	2.11	0.50
3:E:58:GLU:HG2	3:E:62:LYS:HE2	1.92	0.50
4:F:213:ILE:HD12	4:F:296:MET:CE	2.42	0.50
1:A:120:ASP:O	1:A:124:LYS:HG2	2.11	0.50
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.47	0.50
1:A:174:ALA:O	1:A:178:SER:HB3	2.12	0.49
2:D:304:ASP:HB3	2:D:307:HIS:ND1	2.27	0.49
4:F:199:PHE:C	4:F:199:PHE:CD2	2.85	0.49
2:D:7:ILE:O	2:D:135:LEU:HD12	2.12	0.49
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.93	0.49
1:C:285:GLN:OE1	1:C:285:GLN:HA	2.11	0.49
2:D:32:PRO:HA	2:D:81:PHE:CE2	2.47	0.49
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.28	0.49
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.49
2:D:73:MET:CB	2:D:77:ARG:HH21	2.16	0.49
2:D:290:THR:CG2	2:D:333:VAL:HG21	2.40	0.49
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.48	0.49
2:B:76:VAL:O	2:B:82:GLY:HA3	2.13	0.49
2:D:65:LEU:N	2:D:65:LEU:HD12	2.28	0.49
2:B:7:ILE:O	2:B:135:LEU:HA	2.13	0.49
2:B:172:SER:OG	2:B:205:GLU:HG2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.48	0.49
2:D:70:PRO:HG3	2:D:93:GLY:O	2.13	0.48
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.94	0.48
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.49	0.48
2:D:64:ILE:HD13	2:D:120:VAL:HG22	1.96	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.48
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.48	0.48
4:F:274:ALA:C	4:F:275:LEU:HD12	2.34	0.48
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.48	0.48
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.94	0.48
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.29	0.48
4:F:40:MET:HE2	4:F:47:LEU:HG	1.96	0.48
2:B:104:GLY:O	2:B:109:GLY:HA3	2.14	0.48
2:D:285:THR:OG1	2:D:288:GLU:HG3	2.13	0.48
2:D:386:THR:O	2:D:390:ARG:HG2	2.14	0.48
1:A:12:ALA:CB	1:A:140:SER:HB3	2.44	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.49	0.47
2:B:73:MET:SD	2:B:92:PHE:HB3	2.54	0.47
2:B:172:SER:OG	2:B:205:GLU:HG3	2.14	0.47
1:C:180:ALA:HB1	2:D:256:ASN:OD1	2.14	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.47
2:D:29:GLY:O	2:D:36:TYR:HD1	1.98	0.47
1:C:71:GLU:CB	1:C:98:ASP:HB3	2.40	0.47
4:F:14:TYR:HA	4:F:17:VAL:CG2	2.44	0.47
1:A:90:GLU:O	1:A:121:ARG:HD2	2.13	0.47
1:A:156:ARG:CG	1:A:156:ARG:NH2	2.73	0.47
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.49	0.47
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.45	0.47
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.97	0.47
2:D:139:LEU:HD12	2:D:170:MET:SD	2.54	0.47
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.45	0.47
4:F:131:PHE:CD1	4:F:182:ILE:HG21	2.50	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.47
2:D:182:PRO:HG2	2:D:388:MET:HE2	1.96	0.47
4:F:185:TYR:OH	4:F:239:HIS:CD2	2.68	0.47
1:A:70:LEU:HG	1:A:145:THR:HG23	1.96	0.47
2:D:170:MET:HB2	2:D:203:ASP:HA	1.98	0.46
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.50	0.46
4:F:31:ARG:HE	4:F:32:LYS:H	1.63	0.46
2:B:235:GLY:HA3	2:B:366:THR:OG1	2.16	0.46
4:F:189:PRO:HA	4:F:322:ASP:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HD3	1:A:95:GLY:O	2.14	0.46
2:B:296:SER:HA	2:B:299:MET:HG2	1.97	0.46
2:D:145:SER:OG	2:D:188:SER:OG	2.24	0.46
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.50	0.46
1:C:274:PRO:HG3	1:C:286:LEU:HD13	1.97	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.46
4:F:24:THR:HG21	4:F:361:LEU:CD1	2.46	0.46
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.51	0.46
4:F:199:PHE:HD1	4:F:221:LEU:CG	2.29	0.46
1:C:162:GLY:CA	3:E:94:ILE:HD11	2.44	0.46
2:D:218:THR:O	2:D:218:THR:HG23	2.16	0.46
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.81	0.45
4:F:3:THR:HB	4:F:30:LEU:HD11	1.98	0.45
2:B:102:ALA:HB2	2:B:403:MET:SD	2.56	0.45
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.98	0.45
2:B:154:LYS:HE3	3:E:76:ARG:CZ	2.46	0.45
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.98	0.45
2:B:73:MET:CE	2:B:90:PHE:HB3	2.47	0.45
2:B:173:PRO:HA	2:B:176:SER:HB2	1.97	0.45
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.52	0.45
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.10	0.45
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.52	0.45
2:D:221:THR:HG22	2:D:224:ASP:OD2	2.16	0.45
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.52	0.45
2:B:316:ILE:HG23	2:B:366:THR:HB	1.98	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
1:A:134:GLY:HA3	1:A:165:SER:O	2.16	0.45
2:B:219:THR:HG21	1:C:326:LYS:HA	1.99	0.45
1:C:163:LYS:HA	1:C:163:LYS:HD3	1.57	0.45
1:C:165:SER:HA	1:C:199:ASP:OD2	2.16	0.45
3:E:58:GLU:O	3:E:62:LYS:HG2	2.17	0.45
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.46	0.44
1:A:358:GLN:NE2	13:A:601:HOH:O	2.50	0.44
1:C:419:SER:O	1:C:423:GLU:HG3	2.16	0.44
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.51	0.44
1:C:409:VAL:HA	1:C:413:MET:O	2.18	0.44
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.35	0.44
1:C:1:MET:O	13:C:601:HOH:O	2.21	0.44
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.52	0.44
4:F:93:TRP:HB2	4:F:290:ILE:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:377:LYS:HD3	4:F:379:HIS:NE2	2.32	0.44
2:B:317:PHE:HE1	2:B:330:MET:HE2	1.82	0.44
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.46	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.53	0.44
1:C:6:SER:O	1:C:65:ALA:HA	2.18	0.44
2:D:19:LYS:O	2:D:23:VAL:HG23	2.18	0.44
2:B:189:VAL:O	2:B:193:VAL:HG23	2.17	0.44
2:D:324:LYS:HG2	2:D:328:GLU:OE2	2.18	0.44
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.00	0.44
2:D:126:SER:O	2:D:126:SER:OG	2.21	0.44
1:C:107:HIS:O	1:C:152:LEU:HD22	2.18	0.43
4:F:4:PHE:HA	4:F:39:LEU:O	2.18	0.43
1:A:65:ALA:O	1:A:91:GLN:NE2	2.39	0.43
2:B:284:LEU:HD21	2:B:292:GLN:OE1	2.18	0.43
2:B:19:LYS:O	2:B:23:VAL:HG23	2.19	0.43
2:B:65:LEU:N	2:B:65:LEU:HD12	2.33	0.43
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.53	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
3:E:70:LYS:HE3	3:E:70:LYS:HB2	1.79	0.43
4:F:182:ILE:HD13	4:F:182:ILE:HA	1.65	0.43
2:B:317:PHE:CZ	2:B:330:MET:HE1	2.53	0.43
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.47	0.43
4:F:324:GLU:OE1	4:F:324:GLU:HA	2.19	0.43
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.01	0.43
2:B:70:PRO:HG3	2:B:93:GLY:O	2.19	0.43
2:D:383:GLU:O	2:D:386:THR:HG22	2.19	0.43
2:D:387:ALA:HA	2:D:390:ARG:NE	2.34	0.43
4:F:146:VAL:HG11	4:F:233:PHE:CZ	2.54	0.43
2:B:7:ILE:O	2:B:135:LEU:HD12	2.19	0.42
1:C:104:ALA:HB2	1:C:413:MET:SD	2.59	0.42
2:D:32:PRO:O	2:D:84:ILE:HB	2.18	0.42
4:F:18:SER:HA	4:F:21:LEU:HD12	2.01	0.42
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.54	0.42
1:C:151:SER:HB2	1:C:193:THR:CG2	2.50	0.42
1:A:156:ARG:HG2	1:A:156:ARG:NH2	2.33	0.42
2:B:101:TRP:NE1	2:B:146:GLY:HA2	2.35	0.42
1:C:196:GLU:HG2	1:C:197:HIS:CD2	2.55	0.42
3:E:116:LEU:O	3:E:120:LEU:HG	2.19	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.42
2:B:293:MET:HE2	2:B:367:PHE:HB2	2.00	0.42
1:C:1:MET:HB2	1:C:131:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ARG:NH2	2:D:88:ASP:OD2	2.51	0.42
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.01	0.42
4:F:146:VAL:O	4:F:184:LYS:HD2	2.20	0.42
2:B:35:SER:OG	2:B:58:LYS:HE2	2.20	0.42
1:C:293:ASN:CG	1:C:339:ARG:HH21	2.23	0.42
2:D:107:THR:O	2:D:111:GLU:HG3	2.19	0.42
4:F:296:MET:CE	4:F:380:HIS:CG	3.03	0.42
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.01	0.42
3:E:116:LEU:HD23	3:E:119:MET:HE3	2.02	0.42
1:A:225:THR:O	1:A:229:ARG:HG3	2.18	0.42
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.35	0.42
1:C:150:THR:O	1:C:154:MET:HG2	2.20	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.55	0.42
1:A:316:CYS:HA	1:A:352:LYS:O	2.20	0.42
2:B:154:LYS:HE3	3:E:76:ARG:NE	2.35	0.42
4:F:213:ILE:HD12	4:F:296:MET:HE1	2.01	0.42
4:F:361:LEU:O	4:F:362:ALA:C	2.58	0.42
2:B:5:VAL:HB	2:B:133:PHE:CD1	2.56	0.41
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.41
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.50	0.41
2:D:317:PHE:O	2:D:353:VAL:HA	2.20	0.41
2:D:209:ASP:HB3	2:D:213:ARG:HD3	2.02	0.41
2:D:102:ALA:HB2	2:D:403:MET:SD	2.60	0.41
1:C:16:ILE:HD13	1:C:171:ILE:HD11	2.01	0.41
4:F:284:LEU:HA	4:F:284:LEU:HD12	1.78	0.41
2:B:286:VAL:HB	2:B:287:PRO:HD3	2.03	0.41
3:E:25:LYS:HG3	3:E:26:PRO:HD2	2.03	0.41
2:B:262:ARG:HE	2:B:421:GLU:CD	2.24	0.41
10:B:503:W4F:O2	10:B:503:W4F:C10	2.68	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.41
4:F:199:PHE:HD1	4:F:221:LEU:HD23	1.81	0.41
1:C:174:ALA:HB2	1:C:207:GLU:N	2.36	0.41
2:D:193:VAL:HG11	2:D:414:ASN:ND2	2.36	0.41
2:D:215:LEU:C	2:D:217:LEU:HD12	2.41	0.41
4:F:143:GLU:OE1	4:F:143:GLU:HA	2.20	0.41
2:B:290:THR:HG22	2:B:333:VAL:HG21	2.02	0.41
2:D:251:ARG:O	2:D:255:VAL:HG23	2.21	0.41
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.54	0.41
2:B:112:LEU:HG	2:B:112:LEU:O	2.20	0.41
2:D:151:LEU:O	2:D:155:ILE:HG13	2.21	0.41
3:E:119:MET:HA	3:E:122:ARG:CZ	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:191:LEU:CD2	4:F:197:ARG:O	2.68	0.41
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.41
3:E:119:MET:HA	3:E:122:ARG:NH2	2.36	0.41
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.56	0.40
2:B:293:MET:CE	2:B:365:ALA:HB1	2.50	0.40
1:C:7:ILE:HG21	1:C:153:LEU:CD2	2.51	0.40
2:D:249:ASP:OD1	2:D:251:ARG:N	2.54	0.40
4:F:13:VAL:HG21	4:F:336:PRO:O	2.21	0.40
4:F:234:GLN:OE1	4:F:234:GLN:CA	2.69	0.40
1:A:344:VAL:HG21	1:A:346:TRP:CE2	2.56	0.40
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.56	0.40
1:A:9:VAL:HA	1:A:68:VAL:HG13	2.02	0.40
2:D:34:GLY:O	2:D:58:LYS:HA	2.22	0.40
1:A:9:VAL:HG22	1:A:68:VAL:HG11	2.03	0.40
1:A:241:SER:HB2	1:A:249:ASN:O	2.21	0.40
1:C:338:LYS:HE2	1:C:338:LYS:HB2	1.94	0.40
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.03	0.40
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.03	0.40
1:C:46:ASP:OD1	1:C:46:ASP:N	2.55	0.40
1:C:209:ILE:CG2	1:C:227:LEU:HD22	2.43	0.40
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:GLN:NE2	4:F:90:SER:OG[4_455]	2.02	0.18
2:D:291:GLN:OE1	4:F:90:SER:OG[4_455]	2.13	0.07

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	435/451 (96%)	426 (98%)	9 (2%)	0	100	100
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	426/445 (96%)	415 (97%)	11 (3%)	0	100	100
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	117/189 (62%)	114 (97%)	3 (3%)	0	100	100
4	F	324/380 (85%)	316 (98%)	8 (2%)	0	100	100
All	All	2157/2361 (91%)	2107 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/379 (96%)	361 (99%)	4 (1%)	73	88
1	C	369/379 (97%)	367 (100%)	2 (0%)	88	96
2	B	362/383 (94%)	359 (99%)	3 (1%)	81	92
2	D	357/383 (93%)	351 (98%)	6 (2%)	60	81
3	E	108/171 (63%)	107 (99%)	1 (1%)	78	91
4	F	294/338 (87%)	288 (98%)	6 (2%)	55	78
All	All	1855/2033 (91%)	1833 (99%)	22 (1%)	71	87

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	156	ARG
1	A	342	GLN
1	A	433	GLU
2	B	137	HIS
2	B	205	GLU
2	B	361	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	251	ASP
1	C	279	GLU
2	D	177	ASP
2	D	179	VAL
2	D	284	LEU
2	D	293	MET
2	D	306	ARG
2	D	329	GLN
3	E	136	ASN
4	F	103	THR
4	F	182	ILE
4	F	197	ARG
4	F	199	PHE
4	F	230	SER
4	F	234	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.58	7 (21%)
10	W4F	B	503	-	24,24,24	3.31	21 (87%)	32,32,32	2.34	10 (31%)
12	ACP	F	401	-	27,33,33	1.36	5 (18%)	32,52,52	1.41	4 (12%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.56	6 (18%)
9	MES	B	502	-	12,12,12	2.28	1 (8%)	14,16,16	1.86	5 (35%)
5	GTP	D	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.60	7 (21%)
11	GDP	B	504	6	24,30,30	0.94	1 (4%)	30,47,47	1.20	4 (13%)
8	GOL	A	504	-	5,5,5	0.91	0	5,5,5	1.01	0
10	W4F	D	503	-	24,24,24	2.97	19 (79%)	32,32,32	2.35	11 (34%)

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
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	W4F	B	503	-	-	8/13/13/13	0/2/2/2
12	ACP	F	401	-	-	6/15/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
9	MES	B	502	-	-	2/6/14/14	0/1/1/1
5	GTP	D	501	6	-	8/18/38/38	0/3/3/3
11	GDP	B	504	6	-	3/12/32/32	0/3/3/3
8	GOL	A	504	-	-	0/4/4/4	-
10	W4F	D	503	-	-	5/13/13/13	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.64	1.66	1.77
10	B	503	W4F	O4-C13	-5.53	1.28	1.38
10	D	503	W4F	O4-C13	-4.92	1.29	1.38
10	B	503	W4F	C6-C1	-4.49	1.32	1.38
10	D	503	W4F	O4-C17	-4.41	1.29	1.42
10	B	503	W4F	O3-C16	-4.41	1.29	1.42
10	D	503	W4F	O5-C12	-4.32	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	W4F	O2-C1	-4.29	1.27	1.36
10	B	503	W4F	C14-C13	-4.17	1.32	1.41
10	B	503	W4F	O4-C17	-4.12	1.30	1.42
5	D	501	GTP	C5-C6	-4.00	1.39	1.47
5	A	501	GTP	C5-C6	-3.98	1.39	1.47
10	B	503	W4F	C8-C9	-3.95	1.40	1.51
5	C	501	GTP	C5-C6	-3.94	1.39	1.47
10	B	503	W4F	O1-C2	-3.83	1.31	1.37
10	D	503	W4F	O1-C2	-3.79	1.31	1.37
10	D	503	W4F	O5-C18	-3.79	1.31	1.42
10	D	503	W4F	O3-C16	-3.65	1.31	1.42
10	B	503	W4F	C11-C9	-3.63	1.33	1.39
10	D	503	W4F	O1-C10	-3.62	1.31	1.42
10	D	503	W4F	C14-C13	-3.55	1.33	1.41
10	B	503	W4F	O1-C10	-3.51	1.32	1.42
10	B	503	W4F	C7-C5	-3.48	1.41	1.51
10	B	503	W4F	C12-C13	-3.47	1.33	1.41
10	B	503	W4F	C15-C9	-3.20	1.33	1.39
10	D	503	W4F	C12-C13	-3.11	1.34	1.41
10	D	503	W4F	O3-C14	-3.07	1.32	1.37
10	D	503	W4F	O2-C1	-3.04	1.30	1.36
10	D	503	W4F	C11-C9	-2.96	1.34	1.39
12	F	401	ACP	PG-O3G	2.85	1.61	1.54
12	F	401	ACP	PG-O2G	2.83	1.61	1.54
10	D	503	W4F	C11-C12	-2.66	1.33	1.38
10	D	503	W4F	C4-C5	-2.66	1.33	1.38
10	B	503	W4F	C11-C12	-2.58	1.34	1.38
12	F	401	ACP	PB-O3A	2.57	1.61	1.58
10	B	503	W4F	O3-C14	-2.51	1.33	1.37
12	F	401	ACP	C5-C4	2.50	1.47	1.40
10	D	503	W4F	C3-C4	-2.49	1.34	1.38
10	D	503	W4F	C7-C5	-2.46	1.44	1.51
10	B	503	W4F	C4-C5	-2.44	1.33	1.38
10	B	503	W4F	C3-C2	-2.36	1.34	1.39
11	B	504	GDP	C6-N1	-2.34	1.34	1.37
10	B	503	W4F	C15-C14	-2.31	1.34	1.38
10	D	503	W4F	C3-C2	-2.30	1.34	1.39
5	A	501	GTP	C2-N3	2.22	1.38	1.33
5	D	501	GTP	C2-N3	2.20	1.38	1.33
10	D	503	W4F	C6-C1	-2.20	1.35	1.38
5	C	501	GTP	C2-N3	2.17	1.38	1.33
12	F	401	ACP	PB-O2B	2.17	1.61	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	W4F	C6-C5	-2.12	1.35	1.39
10	B	503	W4F	C3-C4	-2.12	1.34	1.38
10	B	503	W4F	O5-C18	-2.10	1.36	1.42
10	D	503	W4F	C6-C5	-2.08	1.35	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	503	W4F	O1-C2-C1	8.64	127.08	114.57
10	D	503	W4F	C18-O5-C12	-6.78	107.29	117.53
10	D	503	W4F	O1-C2-C1	5.34	122.31	114.57
10	B	503	W4F	O1-C2-C3	-4.91	115.95	124.37
9	B	502	MES	C5-N4-C3	3.97	117.78	108.83
10	D	503	W4F	O5-C12-C11	-3.96	117.30	124.12
5	D	501	GTP	PB-O3B-PG	-3.86	119.59	132.83
12	F	401	ACP	PB-O3A-PA	-3.74	120.70	132.56
10	D	503	W4F	C11-C12-C13	3.66	124.36	120.22
5	A	501	GTP	PB-O3B-PG	-3.59	120.51	132.83
5	C	501	GTP	PB-O3B-PG	-3.54	120.66	132.83
5	A	501	GTP	PA-O3A-PB	-3.53	120.70	132.83
5	C	501	GTP	PA-O3A-PB	-3.51	120.78	132.83
10	D	503	W4F	C7-C5-C6	3.48	126.25	120.54
5	D	501	GTP	PA-O3A-PB	-3.42	121.10	132.83
12	F	401	ACP	C3'-C2'-C1'	3.36	106.04	100.98
10	B	503	W4F	C10-O1-C2	3.32	122.53	117.53
11	B	504	GDP	PA-O3A-PB	-3.30	121.49	132.83
5	D	501	GTP	C5-C6-N1	3.23	119.65	113.95
5	A	501	GTP	C5-C6-N1	3.22	119.63	113.95
5	C	501	GTP	C5-C6-N1	3.18	119.57	113.95
12	F	401	ACP	N3-C2-N1	-3.15	123.75	128.68
10	B	503	W4F	C8-C9-C15	3.14	125.69	120.54
5	A	501	GTP	C8-N7-C5	3.04	108.78	102.99
5	D	501	GTP	C8-N7-C5	3.04	108.78	102.99
5	C	501	GTP	C8-N7-C5	3.01	108.73	102.99
10	B	503	W4F	O3-C14-C15	-2.97	119.02	124.12
10	D	503	W4F	C14-C13-C12	-2.88	116.62	119.57
5	D	501	GTP	C2-N1-C6	-2.86	119.84	125.10
5	C	501	GTP	C2-N1-C6	-2.83	119.88	125.10
5	A	501	GTP	C2-N1-C6	-2.82	119.91	125.10
9	B	502	MES	O1S-S-C8	2.80	110.29	106.92
9	B	502	MES	C6-C5-N4	-2.70	106.01	110.10
5	D	501	GTP	C3'-C2'-C1'	2.70	105.04	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	503	W4F	O3-C14-C13	2.70	119.90	115.16
10	D	503	W4F	C8-C9-C15	2.68	124.94	120.54
12	F	401	ACP	C4-C5-N7	-2.61	106.68	109.40
10	B	503	W4F	C8-C9-C11	-2.41	116.58	120.54
11	B	504	GDP	C3'-C2'-C1'	2.41	104.61	100.98
11	B	504	GDP	C8-N7-C5	2.33	107.43	102.99
10	B	503	W4F	C3-C2-C1	-2.33	116.96	119.86
5	A	501	GTP	C3'-C2'-C1'	2.29	104.43	100.98
11	B	504	GDP	C5-C6-N1	2.28	117.98	113.95
10	D	503	W4F	C3-C2-C1	-2.25	117.05	119.86
5	C	501	GTP	O6-C6-C5	-2.22	120.03	124.37
10	B	503	W4F	C8-C7-C5	2.22	121.08	113.28
10	D	503	W4F	O1-C2-C3	-2.19	120.62	124.37
5	A	501	GTP	O6-C6-C5	-2.15	120.18	124.37
5	D	501	GTP	O6-C6-C5	-2.14	120.19	124.37
10	D	503	W4F	C7-C8-C9	2.13	120.76	113.28
9	B	502	MES	O2S-S-C8	2.12	109.47	106.92
10	B	503	W4F	C7-C8-C9	2.10	120.64	113.28
10	D	503	W4F	C11-C9-C15	-2.09	116.11	118.98
9	B	502	MES	C7-N4-C5	2.04	116.44	111.23

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	502	MES	C8-C7-N4-C5
11	B	504	GDP	C5'-O5'-PA-O1A
11	B	504	GDP	C5'-O5'-PA-O2A
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O2G
12	F	401	ACP	PB-C3B-PG-O3G
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O3A
10	B	503	W4F	C1-C2-O1-C10
10	B	503	W4F	C3-C2-O1-C10
10	D	503	W4F	C3-C2-O1-C10
10	B	503	W4F	C15-C14-O3-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	503	W4F	C13-C14-O3-C16
10	D	503	W4F	C1-C2-O1-C10
10	D	503	W4F	C11-C12-O5-C18
10	D	503	W4F	C13-C12-O5-C18
9	B	502	MES	C8-C7-N4-C3
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O2A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	503	W4F	C7-C8-C9-C15
10	B	503	W4F	C7-C8-C9-C11
5	D	501	GTP	O4'-C4'-C5'-O5'
10	B	503	W4F	C4-C5-C7-C8
10	B	503	W4F	C6-C5-C7-C8
10	D	503	W4F	C5-C7-C8-C9
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
11	B	504	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

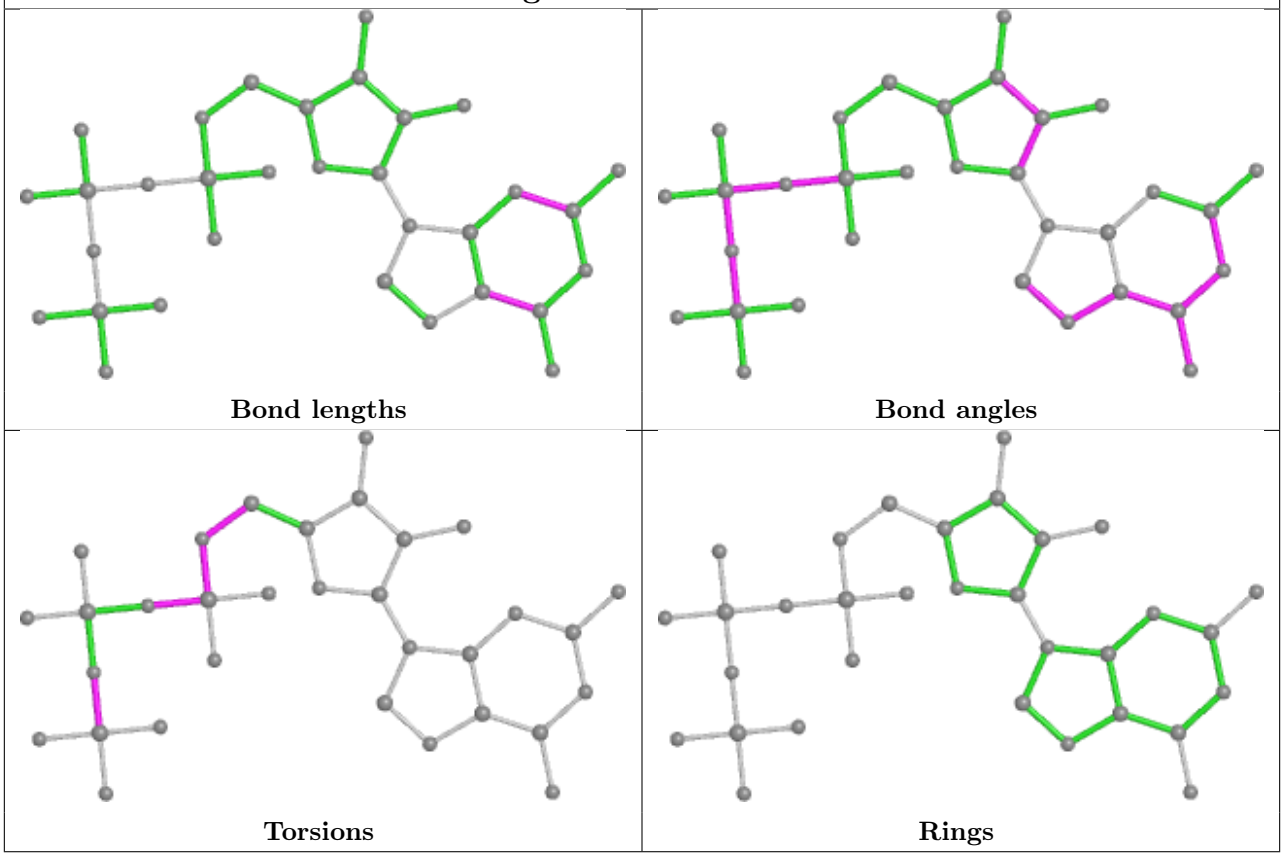
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	W4F	2	0
10	D	503	W4F	1	0

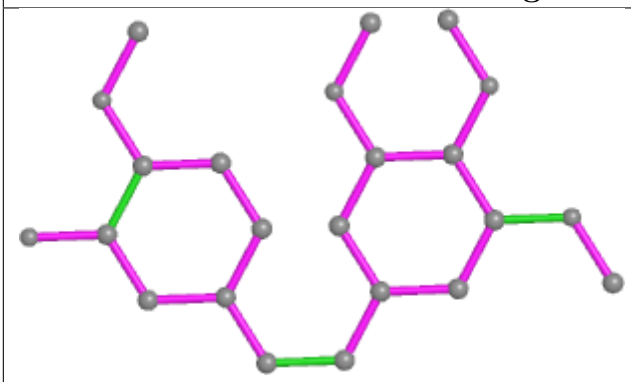
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

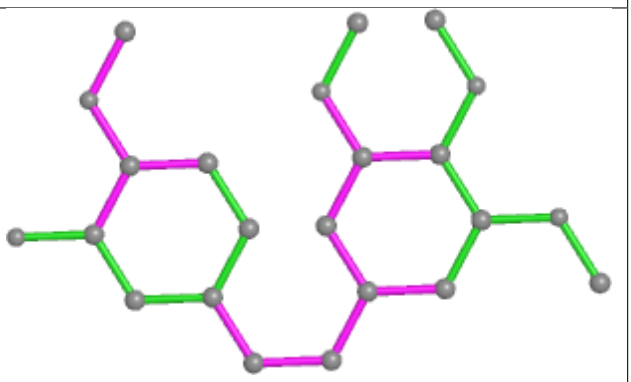
Ligand GTP A 501



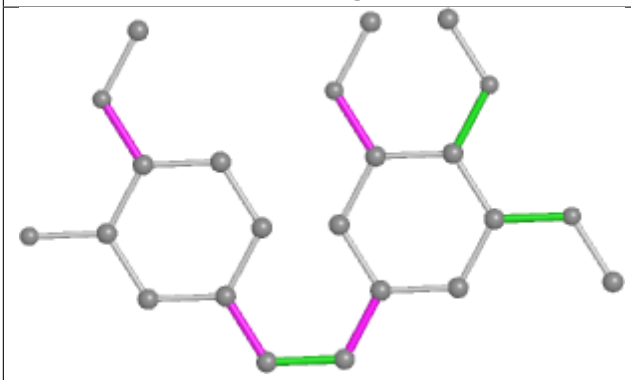
Ligand W4F B 503



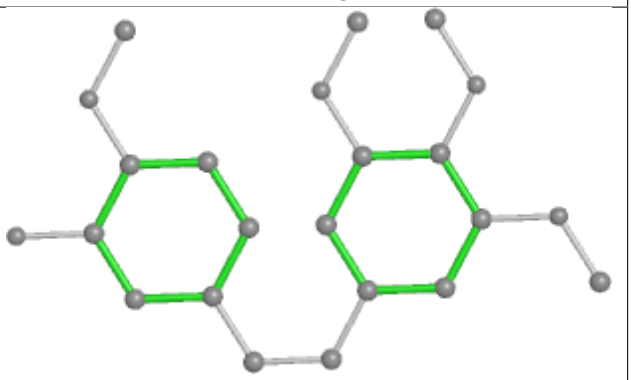
Bond lengths



Bond angles

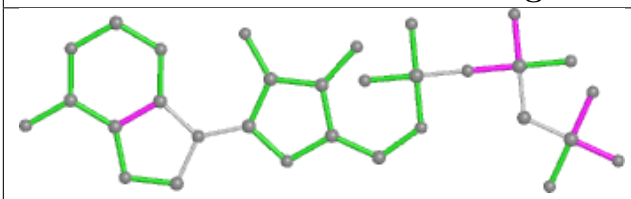


Torsions

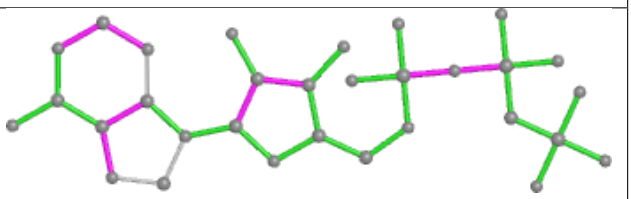


Rings

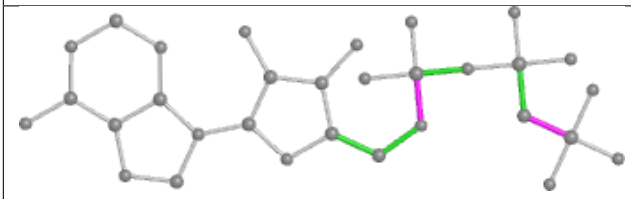
Ligand ACP F 401



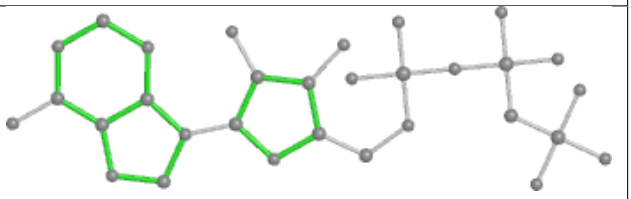
Bond lengths



Bond angles

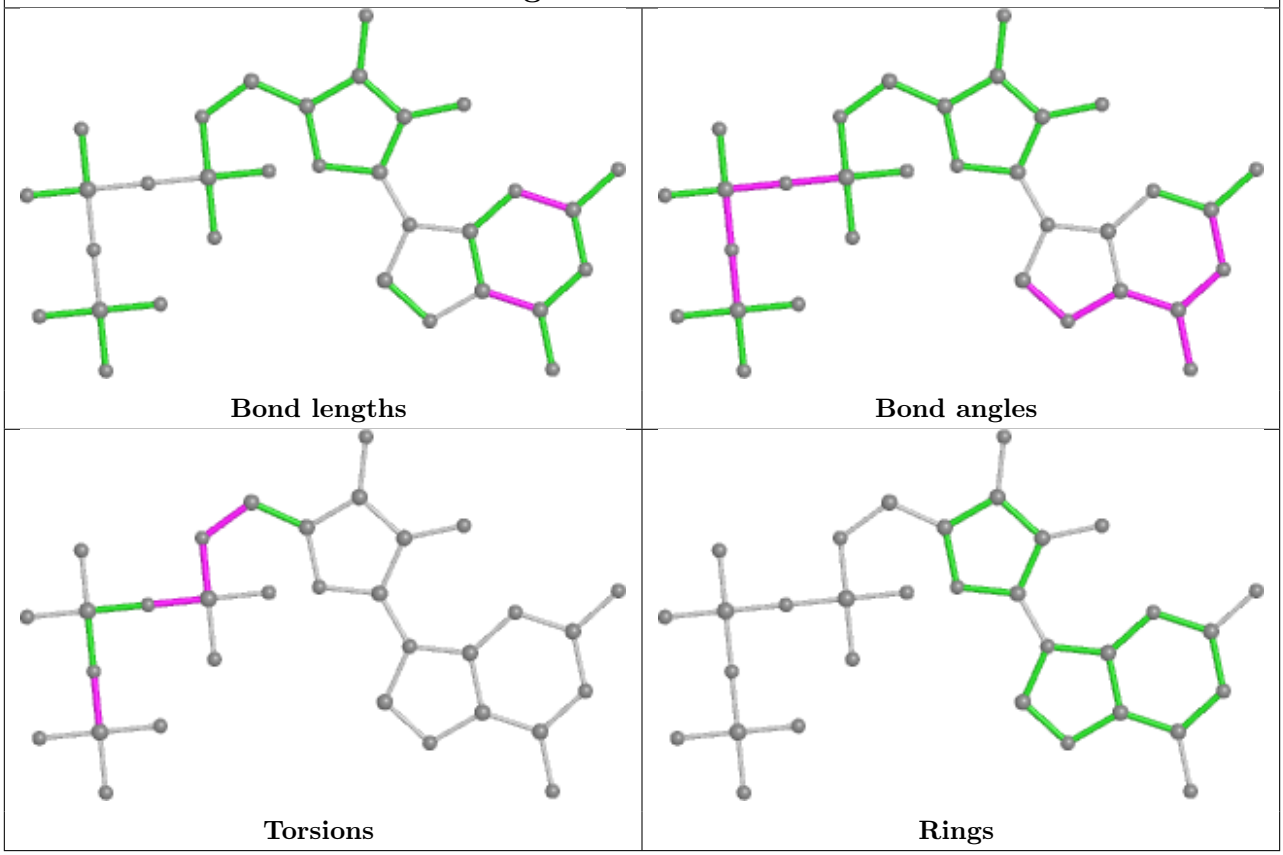


Torsions

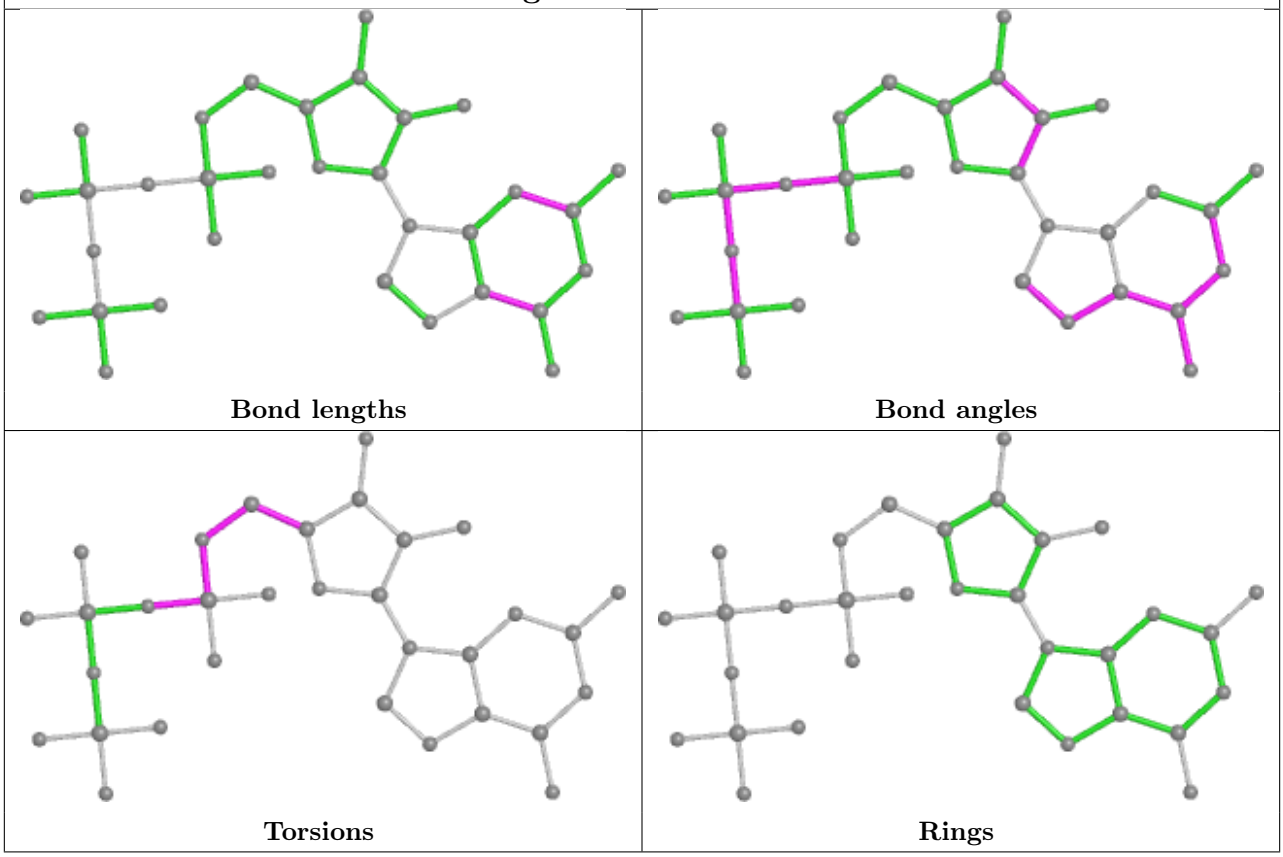


Rings

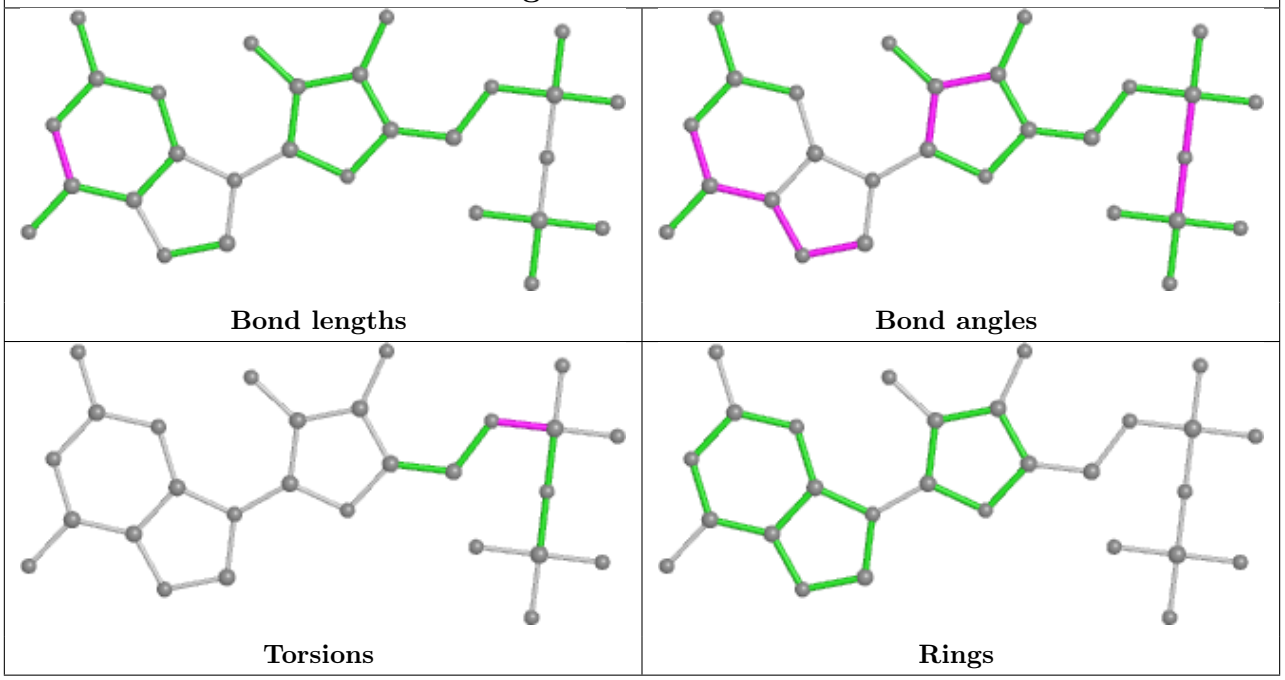
Ligand GTP C 501



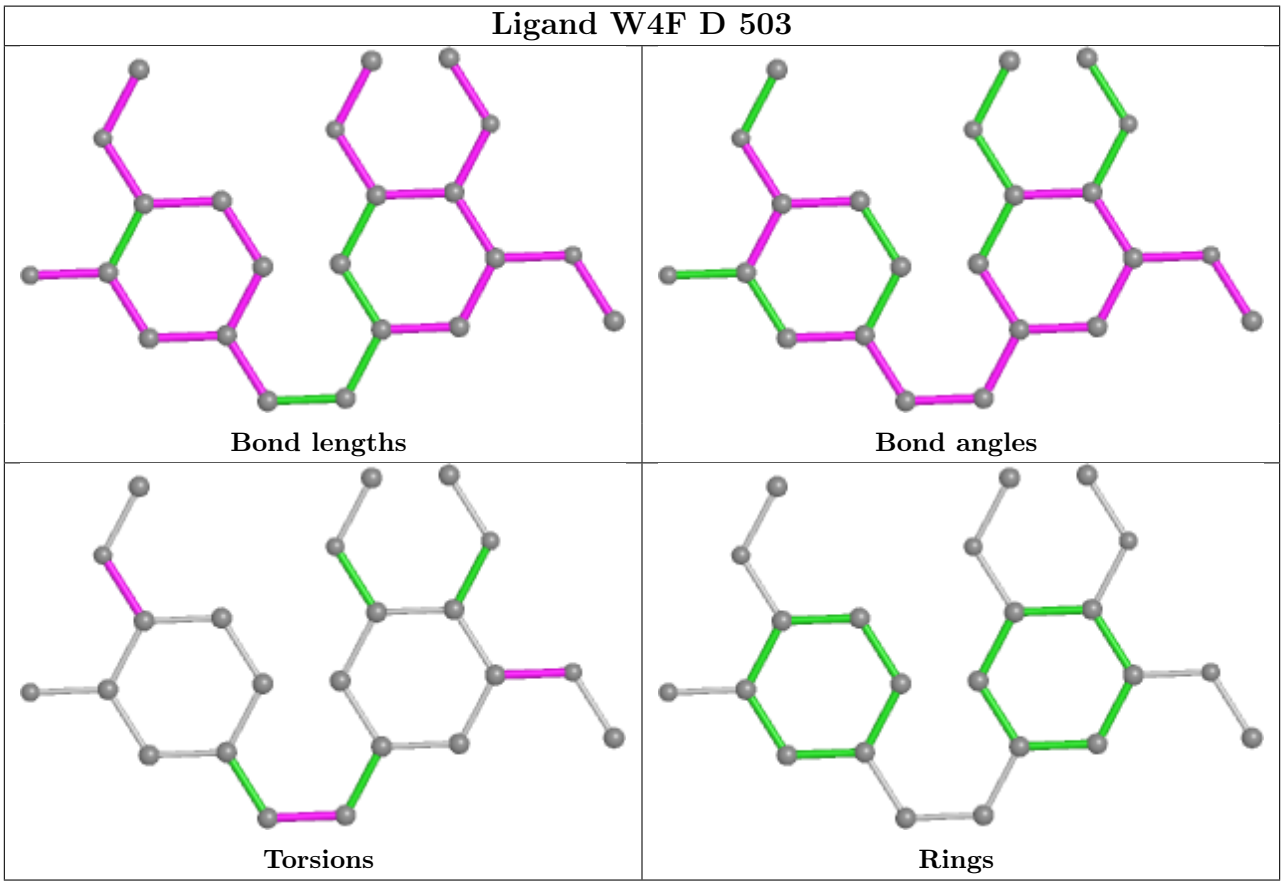
Ligand GTP D 501



Ligand GDP B 504



Ligand W4F D 503



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, 95^{th} 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%)	0.15	15 (3%) 45 38	42, 60, 78, 92	0
1	C	440/451 (97%)	-0.06	3 (0%) 87 86	36, 51, 71, 85	0
2	B	428/445 (96%)	0.27	16 (3%) 41 34	39, 61, 87, 118	0
2	D	421/445 (94%)	0.57	37 (8%) 10 7	46, 76, 99, 118	0
3	E	121/189 (64%)	0.53	12 (9%) 7 5	52, 73, 102, 122	0
4	F	334/380 (87%)	0.96	71 (21%) 0 0	54, 86, 137, 152	0
All	All	2181/2361 (92%)	0.36	154 (7%) 16 11	36, 65, 105, 152	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	7.5
4	F	132	LEU	7.4
4	F	161	LEU	7.3
4	F	172	PHE	6.9
4	F	100	ILE	5.9
4	F	169	LEU	5.9
4	F	233	PHE	5.8
4	F	177	GLY	5.6
4	F	166	ALA	5.2
2	B	1	MET	5.2
2	D	216	LYS	4.8
3	E	139	LEU	4.8
2	D	219	THR	4.8
1	C	179	THR	4.7
4	F	101	TYR	4.5
4	F	179	VAL	4.5
4	F	130	VAL	4.4
4	F	252	ASN	4.4
2	D	390	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	55	THR	4.2
4	F	361	LEU	4.2
2	B	57	ASN	4.2
4	F	129	GLU	4.1
4	F	133	ALA	4.1
4	F	21	LEU	4.1
4	F	234	GLN	4.1
4	F	143	GLU	4.0
2	D	37	HIS	4.0
4	F	229	ASN	4.0
4	F	175	GLU	3.9
4	F	182	ILE	3.9
4	F	140	GLU	3.9
4	F	256	TYR	3.8
4	F	180	HIS	3.8
2	D	96	GLY	3.8
1	A	281	ALA	3.8
1	A	262	TYR	3.8
1	A	282	TYR	3.7
4	F	162	ILE	3.7
4	F	194	PRO	3.7
3	E	141	GLU	3.7
3	E	27	PRO	3.7
2	B	216	LYS	3.7
2	D	391	ARG	3.7
4	F	142	ARG	3.6
2	D	284	LEU	3.6
4	F	372	THR	3.6
2	B	55	THR	3.6
4	F	239	HIS	3.6
2	D	54	ALA	3.6
4	F	103	THR	3.6
4	F	135	TYR	3.5
4	F	149	ALA	3.4
4	F	102	PRO	3.4
2	D	217	LEU	3.4
4	F	232	ASN	3.3
4	F	171	ASP	3.3
4	F	245	ILE	3.3
2	B	37	HIS	3.3
1	C	45	GLY	3.2
2	B	166	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	236	LYS	3.2
4	F	170	LEU	3.2
4	F	225	SER	3.2
4	F	379	HIS	3.2
4	F	178	GLN	3.2
1	A	346	TRP	3.2
2	B	72	THR	3.1
2	D	290	THR	3.1
4	F	9	GLU	3.1
4	F	146	VAL	3.1
2	D	324	LYS	3.0
2	D	137	HIS	3.0
2	D	44	LEU	3.0
2	D	166	THR	3.0
4	F	138	ARG	2.9
4	F	255	ARG	2.9
2	B	92	PHE	2.9
2	D	220	PRO	2.9
3	E	59	GLU	2.9
4	F	235	ASP	2.9
2	D	332	ASN	2.9
2	D	168	SER	2.9
2	D	167	PHE	2.9
3	E	138	GLU	2.9
3	E	45	PRO	2.9
4	F	196	HIS	2.8
3	E	46	SER	2.8
1	A	201	ALA	2.7
4	F	176	GLN	2.7
4	F	131	PHE	2.7
2	D	396	HIS	2.7
4	F	164	SER	2.7
2	D	57	ASN	2.7
4	F	174	ASP	2.7
1	C	340	SER	2.6
2	D	285	THR	2.6
2	B	200	TYR	2.6
4	F	27	TRP	2.6
2	D	212	PHE	2.6
2	D	106	TYR	2.6
2	D	199	THR	2.6
1	A	235	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	237	SER	2.6
2	B	282	ARG	2.6
2	D	200	TYR	2.5
2	D	395	LEU	2.5
1	A	239	THR	2.5
4	F	137	ARG	2.5
1	A	365	GLY	2.5
3	E	132	GLU	2.5
4	F	165	GLU	2.5
2	B	233	MET	2.5
1	A	137	VAL	2.5
4	F	136	ASN	2.5
4	F	187	GLU	2.5
4	F	228	TYR	2.5
4	F	148	ILE	2.4
1	A	283	HIS	2.4
4	F	163	SER	2.4
4	F	197	ARG	2.4
2	B	43	GLN	2.4
4	F	168	GLU	2.4
1	A	238	ILE	2.4
2	D	286	VAL	2.4
4	F	20	LEU	2.4
4	F	25	GLY	2.4
2	B	199	THR	2.3
2	D	94	GLN	2.3
2	B	41	ASP	2.3
2	D	197	ASP	2.3
2	D	83	GLN	2.3
2	D	59	TYR	2.3
3	E	140	LYS	2.3
4	F	226	GLU	2.2
1	A	236	SER	2.2
4	F	244	CYS	2.2
2	B	60	VAL	2.2
3	E	62	LYS	2.2
2	D	170	MET	2.2
4	F	259	GLY	2.2
3	E	63	TYR	2.2
4	F	98	TYR	2.2
2	D	39	ASP	2.1
4	F	167	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	2.1
3	E	28	SER	2.1
2	B	44	LEU	2.1
2	D	201	CYS	2.1
2	D	36	TYR	2.0
4	F	22	LEU	2.0
4	F	247	LYS	2.0
2	D	33	THR	2.0
1	A	1	MET	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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.