



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:25 AM EDT

PDB ID : 7TTE
Title : Tubulin-RB3_SLD in complex with compound 12j
Authors : White, S.W.; Yun, M.
Deposited on : 2022-02-01
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

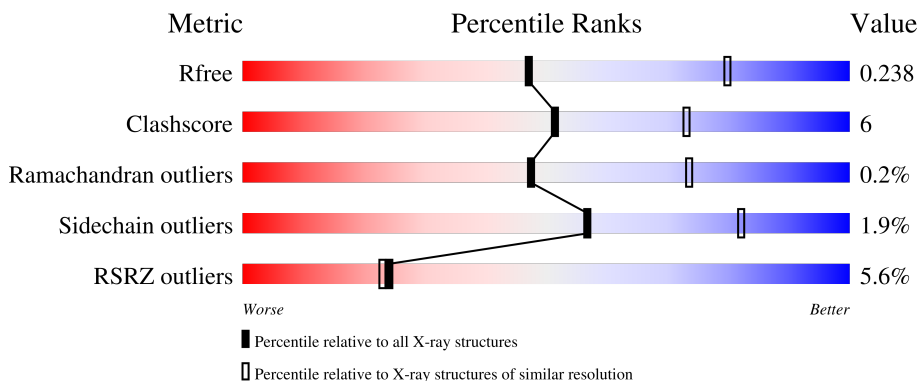
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


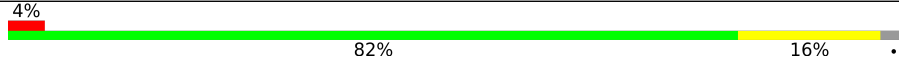
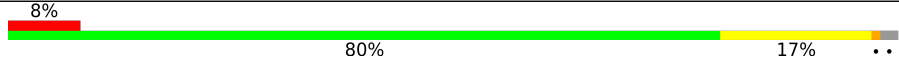
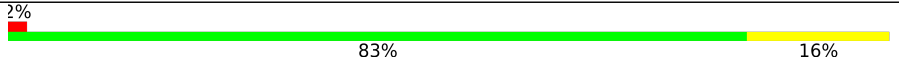
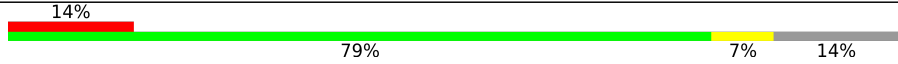
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	438	 5% 81% 15% ..
1	C	438	 4% 82% 16% .
2	B	433	 8% 80% 17% ..
2	D	433	 2% 83% 16%
3	E	143	 14% 79% 7% 14%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 14586 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
			Total	C	N	O	S			
1	A	424	3319	2103	564	630	22	0	0	0
1	C	427	3343	2118	568	635	22	0	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3329	2088	569	645	27	0	0	0
2	D	431	3379	2121	576	655	27	0	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1010	626	184	197	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

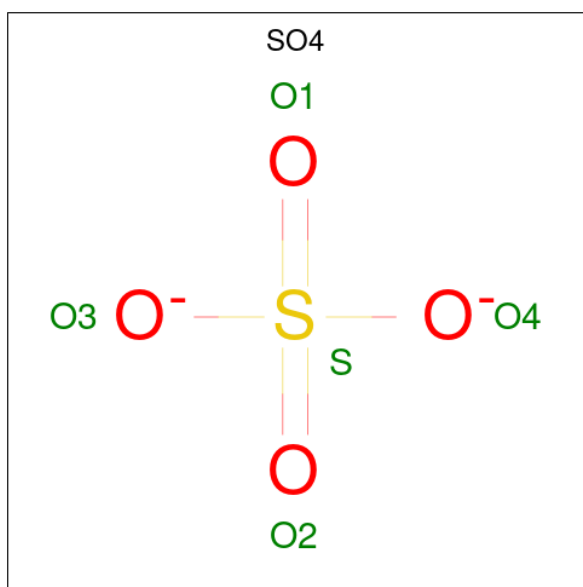
Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



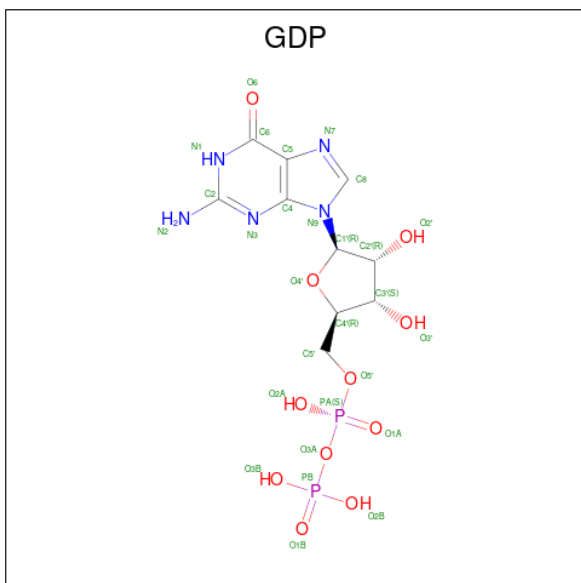
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

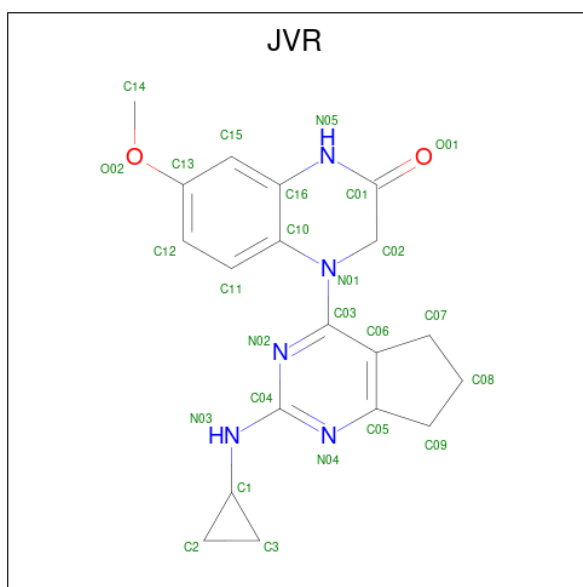
Continued on next page...

Continued from previous page...

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

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





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	23	16	5	2	0	0
7	D	1	26	19	5	2	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	C	1	1	1	0	0

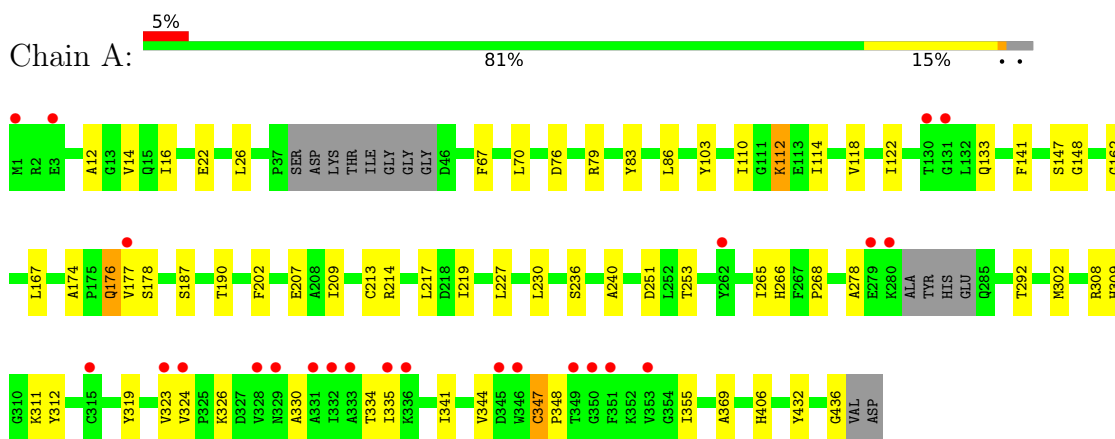
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	1	1	1	0	0
9	B	2	2	2	0	0
9	C	6	6	6	0	0
9	D	3	3	3	0	0

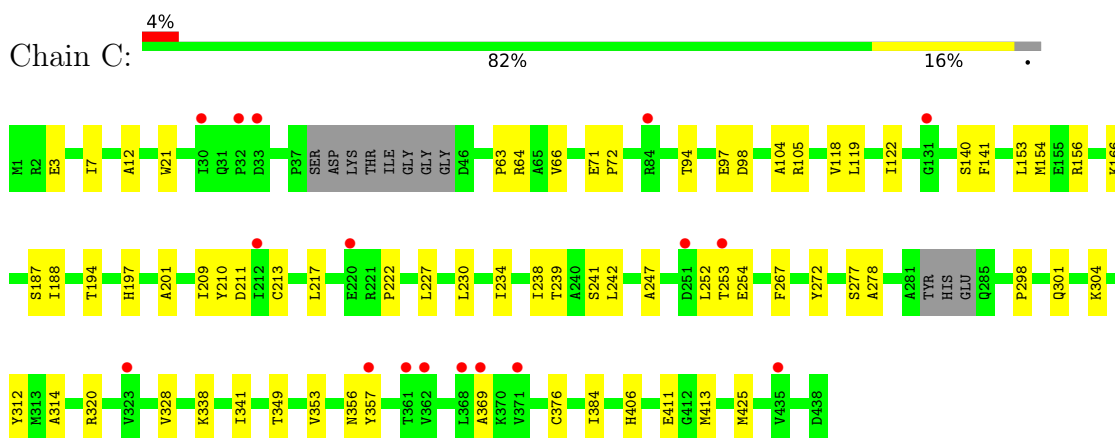
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

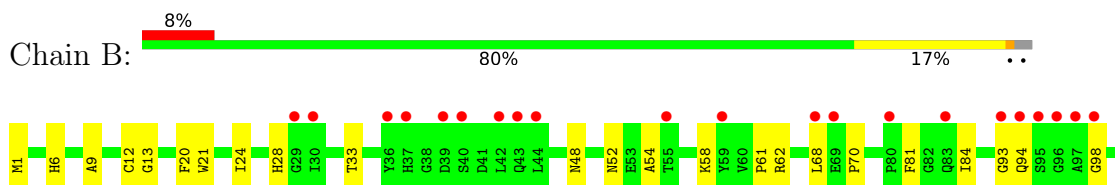
- Molecule 1: Tubulin alpha-1B chain

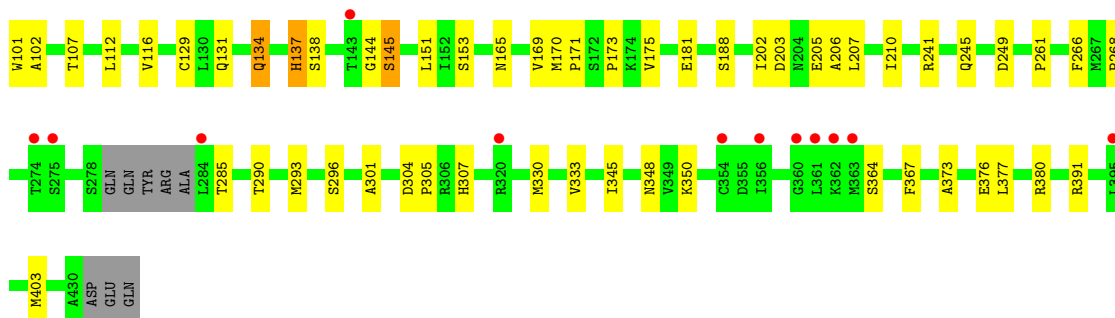


- Molecule 1: Tubulin alpha-1B chain

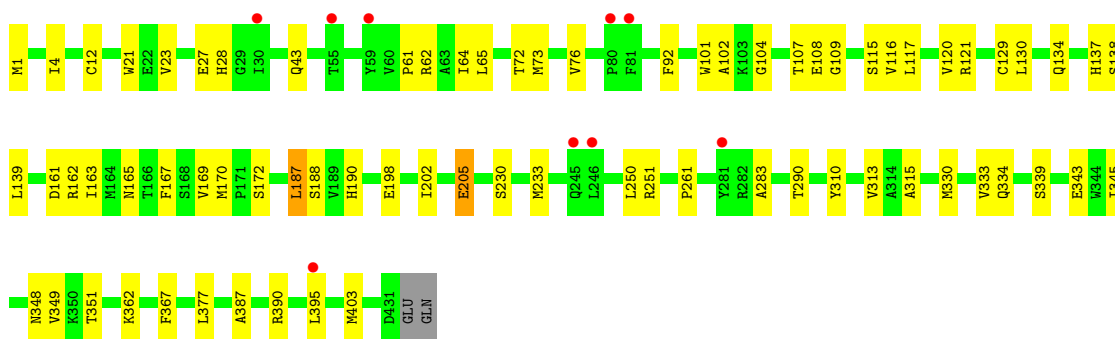
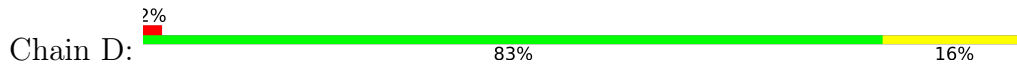


- Molecule 2: Tubulin beta chain

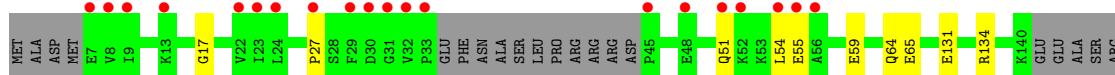
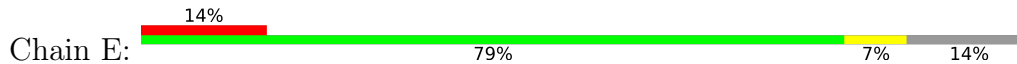




● Molecule 2: Tubulin beta chain



● Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.06Å 127.42Å 251.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.12 – 2.70 46.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (45.12-2.70) 87.6 (46.81-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.171 , 0.239 0.173 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtrriage
Anisotropy	0.642	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14586	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/3393	0.56	0/4605
1	C	0.41	0/3417	0.54	0/4637
2	B	0.41	0/3401	0.57	0/4606
2	D	0.46	0/3454	0.59	0/4680
3	E	0.37	0/1021	0.47	0/1357
All	All	0.42	0/14686	0.56	0/19885

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3319	0	3233	42	0
1	C	3343	0	3262	38	0
2	B	3329	0	3211	43	0
2	D	3379	0	3249	39	0
3	E	1010	0	1019	6	0
4	A	32	0	12	0	0
4	C	32	0	12	1	0
4	D	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	A	5	0	0	0	0
5	B	5	0	0	0	0
5	D	10	0	0	0	0
6	B	28	0	12	1	0
7	B	23	0	0	0	0
7	D	26	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	C	6	0	0	0	0
9	D	3	0	0	0	0
All	All	14586	0	14022	160	0

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

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.64	0.79
2:B:170:MET:HG2	2:B:377:LEU:HD11	1.64	0.77
2:B:52:ASN:OD1	2:B:62:ARG:NH1	2.22	0.73
1:A:319:TYR:HB3	1:A:323:VAL:HG11	1.70	0.72
1:A:308:ARG:HG3	1:A:309:HIS:HD2	1.55	0.71
2:B:54:ALA:HB3	2:B:58:LYS:HB2	1.73	0.70
2:B:48:ASN:O	2:B:62:ARG:NH2	2.26	0.68
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.77	0.67
1:C:105:ARG:HG3	1:C:411:GLU:HG3	1.78	0.66
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.81	0.63
2:B:1:MET:N	2:B:129:CYS:SG	2.72	0.61
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.81	0.61
1:C:166:LYS:HE2	1:C:197:HIS:O	2.00	0.61
1:A:76:ASP:HA	1:A:79:ARG:HG2	1.83	0.60
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.83	0.60
2:D:64:ILE:HD13	2:D:120:VAL:HG22	1.83	0.60
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.85	0.59
1:C:320:ARG:HA	1:C:356:ASN:O	2.04	0.58
1:C:298:PRO:HA	1:C:301:GLN:HG2	1.86	0.58
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.85	0.57
1:A:112:LYS:HG3	3:E:54:LEU:HB3	1.87	0.57
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.88	0.56
2:D:161:ASP:O	2:D:251:ARG:NH2	2.38	0.56
1:A:174:ALA:O	1:A:178:SER:HB3	2.06	0.55
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.39	0.55
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.88	0.55
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.42	0.55
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.88	0.55
2:B:293:MET:HB2	2:B:367:PHE:CE1	2.42	0.55
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.42	0.55
1:A:311:LYS:NZ	1:A:436:GLY:O	2.40	0.55
2:D:169:VAL:HA	2:D:202:ILE:O	2.07	0.54
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.89	0.54
2:D:134:GLN:HA	2:D:165:ASN:O	2.08	0.54
2:D:313:VAL:HB	2:D:349:VAL:HG22	1.90	0.53
1:C:312:TYR:CE2	1:C:341:ILE:HG23	2.44	0.53
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.44	0.52
2:B:296:SER:OG	2:B:305:PRO:HD2	2.09	0.52
1:A:118:VAL:O	1:A:122:ILE:HG13	2.09	0.52
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.45	0.52
1:C:213:CYS:HA	1:C:217:LEU:HD12	1.92	0.51
1:A:266:HIS:O	1:A:268:PRO:HD3	2.10	0.51
2:D:139:LEU:HD22	2:D:188:SER:HB3	1.92	0.51
2:B:70:PRO:HD3	2:B:94:GLN:HA	1.93	0.51
1:C:154:MET:HG3	1:C:194:THR:HG23	1.91	0.51
1:C:98:ASP:HB2	4:C:501:GTP:O2G	2.10	0.51
1:C:72:PRO:HA	1:C:94:THR:HG21	1.92	0.51
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.46	0.50
2:B:290:THR:HG22	2:B:333:VAL:HG21	1.93	0.50
2:D:172:SER:HB2	2:D:205:GLU:HB2	1.94	0.50
1:A:70:LEU:HD13	1:A:110:ILE:HD13	1.93	0.50
2:B:203:ASP:HB2	2:B:301:ALA:HA	1.94	0.50
2:B:206:ALA:O	2:B:210:ILE:HG13	2.12	0.50
1:A:167:LEU:HD23	1:A:202:PHE:HE2	1.77	0.49
1:C:272:TYR:HD1	1:C:376:CYS:HB2	1.77	0.49
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.49
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.44	0.48
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.49	0.48
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.94	0.48
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.96	0.48
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.96	0.48
2:B:131:GLN:OE1	2:B:249:ASP:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:VAL:O	1:C:122:ILE:HG13	2.15	0.47
1:A:70:LEU:HD21	1:A:114:ILE:HD13	1.97	0.47
1:A:213:CYS:O	1:A:217:LEU:HB2	2.13	0.47
2:B:68:LEU:HD23	2:B:112:LEU:HD22	1.96	0.47
2:B:373:ALA:O	2:B:376:GLU:HG3	2.14	0.47
2:D:283:ALA:HB2	2:D:362:LYS:HB2	1.97	0.47
2:D:23:VAL:O	2:D:27:GLU:HG3	2.15	0.46
2:B:81:PHE:O	2:B:84:ILE:HG22	2.16	0.46
2:B:391:ARG:HA	2:B:391:ARG:HD2	1.85	0.46
1:C:141:PHE:HB3	1:C:187:SER:OG	2.16	0.46
2:B:290:THR:HG23	2:B:330:MET:SD	2.56	0.46
1:A:355:ILE:O	3:E:17:GLY:HA2	2.16	0.46
1:C:97:GLU:HG3	2:D:1:MET:HG2	1.98	0.46
1:C:234:ILE:O	1:C:238:ILE:HG12	2.16	0.46
1:C:338:LYS:HB2	1:C:341:ILE:HD12	1.98	0.46
1:A:12:ALA:O	1:A:16:ILE:HG13	2.15	0.45
3:E:131:GLU:CD	3:E:134:ARG:HH12	2.19	0.45
1:A:292:THR:HG22	1:A:335:ILE:HD11	1.97	0.45
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.98	0.45
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.99	0.45
2:D:102:ALA:HB2	2:D:403:MET:SD	2.57	0.45
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.99	0.45
1:A:83:TYR:HB3	1:A:86:LEU:HD12	1.99	0.45
1:A:133:GLN:HE22	1:A:251:ASP:HA	1.82	0.45
2:B:12:CYS:HB3	2:B:138:SER:HB3	1.99	0.45
2:B:102:ALA:HB2	2:B:403:MET:SD	2.57	0.45
2:B:203:ASP:OD2	2:B:380:ARG:NH2	2.49	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.45
2:D:101:TRP:CE2	2:D:187:LEU:HB3	2.51	0.45
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.99	0.44
2:D:104:GLY:O	2:D:109:GLY:HA3	2.17	0.44
1:C:104:ALA:HB2	1:C:413:MET:SD	2.57	0.44
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.00	0.44
2:B:350:LYS:HA	2:B:350:LYS:HD2	1.74	0.44
1:A:312:TYR:CE2	1:A:341:ILE:HG23	2.52	0.44
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.83	0.43
2:B:151:LEU:HA	2:B:151:LEU:HD23	1.67	0.43
2:D:330:MET:O	2:D:334:GLN:HG3	2.17	0.43
1:A:22:GLU:O	1:A:26:LEU:HG	2.17	0.43
2:D:116:VAL:O	2:D:120:VAL:HG23	2.18	0.43
1:A:176:GLN:OE1	1:A:207:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.52	0.43
3:E:55:GLU:O	3:E:59:GLU:HG2	2.17	0.43
2:B:173:PRO:HA	1:C:349:THR:HG22	2.00	0.43
2:B:266:PHE:O	2:B:268:PRO:HD3	2.18	0.43
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.54	0.43
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.83	0.42
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.49	0.42
3:E:64:GLN:HG3	3:E:65:GLU:N	2.34	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.19	0.42
1:C:201:ALA:HB3	1:C:267:PHE:CD1	2.55	0.42
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.42
1:A:324:VAL:HG12	1:A:326:LYS:HG2	2.00	0.42
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.01	0.42
2:B:93:GLY:O	2:B:94:GLN:HG2	2.20	0.42
1:A:177:VAL:HG13	1:A:177:VAL:O	2.20	0.42
2:B:98:GLY:HA2	1:C:254:GLU:HG3	2.02	0.42
2:D:65:LEU:HD12	2:D:65:LEU:N	2.35	0.42
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.54	0.42
1:C:239:THR:HA	1:C:242:LEU:HD13	2.02	0.41
1:A:308:ARG:HG3	1:A:309:HIS:CD2	2.45	0.41
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.56	0.41
1:A:330:ALA:O	1:A:334:THR:HG23	2.19	0.41
1:A:209:ILE:HD11	1:A:302:MET:SD	2.61	0.41
1:A:214:ARG:HA	1:A:219:ILE:O	2.21	0.41
1:A:344:VAL:CG2	1:A:347:CYS:HB2	2.49	0.41
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.02	0.41
2:B:304:ASP:O	2:B:307:HIS:HB2	2.21	0.41
2:B:28:HIS:CE1	2:B:241:ARG:HB3	2.56	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.41
1:C:247:ALA:HB2	1:C:357:TYR:HE1	1.85	0.41
2:D:130:LEU:O	2:D:162:ARG:HD2	2.20	0.41
2:B:9:ALA:O	2:B:13:GLY:HA3	2.21	0.41
2:D:107:THR:OG1	2:D:108:GLU:N	2.51	0.41
1:A:141:PHE:HB3	1:A:187:SER:OG	2.21	0.41
1:A:236:SER:O	1:A:240:ALA:N	2.54	0.41
2:D:72:THR:O	2:D:76:VAL:HG23	2.20	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.21	0.41
2:D:315:ALA:HB3	2:D:351:THR:HG22	2.03	0.41
1:A:176:GLN:HE21	1:A:176:GLN:HB3	1.58	0.41
2:B:101:TRP:HD1	2:B:145:SER:OG	2.04	0.41
2:D:1:MET:N	2:D:129:CYS:SG	2.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:LEU:HD22	2:D:188:SER:CB	2.49	0.41
2:D:165:ASN:HA	2:D:198:GLU:O	2.20	0.41
2:D:395:LEU:HD23	2:D:395:LEU:HA	1.91	0.41
2:B:345:ILE:HG22	2:B:348:ASN:HB3	2.02	0.41
2:D:387:ALA:HA	2:D:390:ARG:NH1	2.35	0.41
2:B:137:HIS:ND1	2:B:144:GLY:O	2.45	0.40
1:C:238:ILE:HG12	1:C:238:ILE:H	1.71	0.40
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.55	0.40
2:B:171:PRO:HB2	2:B:181:GLU:OE1	2.21	0.40
2:D:28:HIS:HA	2:D:43:GLN:HB3	2.03	0.40
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.57	0.40
2:B:207:LEU:HD23	2:B:207:LEU:HA	1.93	0.40
2:D:4:ILE:O	2:D:62:ARG:HD2	2.20	0.40
2:D:117:LEU:O	2:D:121:ARG:HG3	2.22	0.40
1:A:406:HIS:CD2	2:B:261:PRO:HD3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	418/438 (95%)	401 (96%)	16 (4%)	1 (0%)	47 73
1	C	421/438 (96%)	408 (97%)	12 (3%)	1 (0%)	47 73
2	B	421/433 (97%)	405 (96%)	15 (4%)	1 (0%)	47 73
2	D	429/433 (99%)	416 (97%)	13 (3%)	0	100 100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100 100
All	All	1808/1885 (96%)	1748 (97%)	57 (3%)	3 (0%)	47 73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
1	C	314	ALA
2	B	175	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	358/369 (97%)	354 (99%)	4 (1%)	73	90
1	C	361/369 (98%)	356 (99%)	5 (1%)	67	86
2	B	366/374 (98%)	355 (97%)	11 (3%)	41	70
2	D	370/374 (99%)	362 (98%)	8 (2%)	52	79
3	E	107/126 (85%)	106 (99%)	1 (1%)	78	92
All	All	1562/1612 (97%)	1533 (98%)	29 (2%)	57	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
1	A	176	GLN
1	A	253	THR
1	A	347	CYS
2	B	33	THR
2	B	107	THR
2	B	134	GLN
2	B	137	HIS
2	B	145	SER
2	B	153	SER
2	B	188	SER
2	B	205	GLU
2	B	245	GLN
2	B	285	THR
2	B	364	SER
1	C	66	VAL
1	C	241	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	253	THR
1	C	277	SER
1	C	384	ILE
2	D	115	SER
2	D	137	HIS
2	D	187	LEU
2	D	190	HIS
2	D	205	GLU
2	D	230	SER
2	D	339	SER
2	D	343	GLU
3	E	51	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	GLN
1	A	406	HIS
1	C	61	HIS
2	D	15	GLN
2	D	195	ASN
2	D	375	GLN
3	E	108	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	SO4	A	502	-	4,4,4	0.16	0	6,6,6	0.72	0
4	GTP	C	501	8	26,34,34	1.25	2 (7%)	32,54,54	1.40	3 (9%)
4	GTP	D	501	-	26,34,34	1.22	3 (11%)	32,54,54	1.33	4 (12%)
4	GTP	A	501	-	26,34,34	1.22	2 (7%)	32,54,54	1.29	4 (12%)
5	SO4	D	503	-	4,4,4	0.12	0	6,6,6	0.51	0
7	JVR	B	502	-	26,26,30	1.39	5 (19%)	33,38,44	1.89	5 (15%)
7	JVR	D	502	-	30,30,30	1.25	3 (10%)	38,44,44	1.88	12 (31%)
6	GDP	B	501	-	24,30,30	1.45	5 (20%)	30,47,47	1.42	4 (13%)
5	SO4	D	504	-	4,4,4	0.19	0	6,6,6	0.50	0
5	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	D	501	-	-	9/18/38/38	0/3/3/3
4	GTP	C	501	8	-	6/18/38/38	0/3/3/3
4	GTP	A	501	-	-	3/18/38/38	0/3/3/3
7	JVR	B	502	-	-	2/5/24/30	0/4/4/5
7	JVR	D	502	-	-	4/9/30/30	0/5/5/5
6	GDP	B	501	-	-	4/12/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	502	JVR	C04-N03	3.54	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	JVR	C03-N01	3.35	1.42	1.37
7	B	502	JVR	C04-N03	3.34	1.40	1.33
6	B	501	GDP	PB-O1B	3.19	1.60	1.50
4	A	501	GTP	O4'-C1'	3.11	1.45	1.41
7	D	502	JVR	C01-N05	2.92	1.38	1.35
4	A	501	GTP	C8-N7	-2.74	1.30	1.35
4	C	501	GTP	C8-N7	-2.72	1.30	1.35
4	D	501	GTP	C8-N7	-2.65	1.30	1.35
7	B	502	JVR	C10-N01	2.63	1.44	1.40
6	B	501	GDP	C5-C6	-2.52	1.42	1.47
6	B	501	GDP	C8-N7	-2.51	1.30	1.35
7	D	502	JVR	C03-N01	2.49	1.40	1.37
4	D	501	GTP	O4'-C1'	2.47	1.44	1.41
6	B	501	GDP	PA-O1A	2.46	1.59	1.50
4	C	501	GTP	C5-C6	-2.38	1.42	1.47
6	B	501	GDP	O4'-C1'	2.13	1.44	1.41
7	B	502	JVR	C02-C01	2.10	1.53	1.51
4	D	501	GTP	C6-N1	-2.02	1.34	1.37
7	B	502	JVR	C02-N01	2.02	1.49	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	502	JVR	C08-C09-C05	-5.20	100.14	103.93
7	B	502	JVR	O01-C01-N05	-5.07	116.96	121.43
7	B	502	JVR	C08-C09-C05	-4.46	100.67	103.93
4	D	501	GTP	C8-N7-C5	4.32	111.21	102.99
4	A	501	GTP	C8-N7-C5	4.03	110.67	102.99
6	B	501	GDP	C8-N7-C5	4.00	110.61	102.99
4	C	501	GTP	C8-N7-C5	3.81	110.26	102.99
7	D	502	JVR	C09-C05-C06	3.69	113.74	111.09
7	D	502	JVR	O01-C01-N05	-3.66	118.20	121.43
7	B	502	JVR	C14-O02-C13	3.45	124.99	117.51
7	B	502	JVR	C06-C05-N04	-3.07	122.44	125.80
7	D	502	JVR	C14-O02-C13	3.06	124.16	117.51
7	D	502	JVR	C06-C05-N04	-3.03	122.48	125.80
4	C	501	GTP	C5-C6-N1	3.02	119.29	113.95
7	D	502	JVR	C3-C1-N03	-2.77	113.81	118.52
4	D	501	GTP	O4'-C1'-C2'	-2.77	102.88	106.93
4	C	501	GTP	C2-N1-C6	-2.73	120.08	125.10
7	D	502	JVR	C01-C02-N01	-2.71	107.52	113.13
7	D	502	JVR	N02-C03-N01	-2.62	113.50	116.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	502	JVR	C2-C1-N03	-2.61	114.08	118.52
6	B	501	GDP	C2-N1-C6	-2.60	120.31	125.10
4	A	501	GTP	C5-C6-N1	2.57	118.50	113.95
4	D	501	GTP	O6-C6-N1	-2.49	117.70	120.65
4	A	501	GTP	O3G-PG-O3B	2.45	112.85	104.64
4	A	501	GTP	C2-N1-C6	-2.43	120.63	125.10
6	B	501	GDP	C5-C6-N1	2.39	118.18	113.95
7	D	502	JVR	C02-C01-N05	2.37	119.08	116.13
7	D	502	JVR	C16-N05-C01	-2.31	121.63	124.49
7	D	502	JVR	C06-C03-N02	-2.30	119.06	122.61
7	B	502	JVR	N03-C04-N02	2.08	120.48	117.25
4	D	501	GTP	O2G-PG-O3B	2.03	111.45	104.64
6	B	501	GDP	O5'-C5'-C4'	-2.02	102.03	108.99

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
7	B	502	JVR	C06-C03-N01-C02
7	B	502	JVR	N02-C03-N01-C02
4	A	501	GTP	C3'-C4'-C5'-O5'
4	D	501	GTP	C3'-C4'-C5'-O5'
4	C	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O2A
7	D	502	JVR	N02-C03-N01-C02
7	D	502	JVR	C06-C03-N01-C02
6	B	501	GDP	PB-O3A-PA-O2A
4	A	501	GTP	O4'-C4'-C5'-O5'
4	D	501	GTP	O4'-C4'-C5'-O5'
7	D	502	JVR	C15-C13-O02-C14
4	C	501	GTP	PB-O3B-PG-O1G
4	D	501	GTP	PB-O3B-PG-O1G
7	D	502	JVR	C12-C13-O02-C14

Continued on next page...

Continued from previous page...

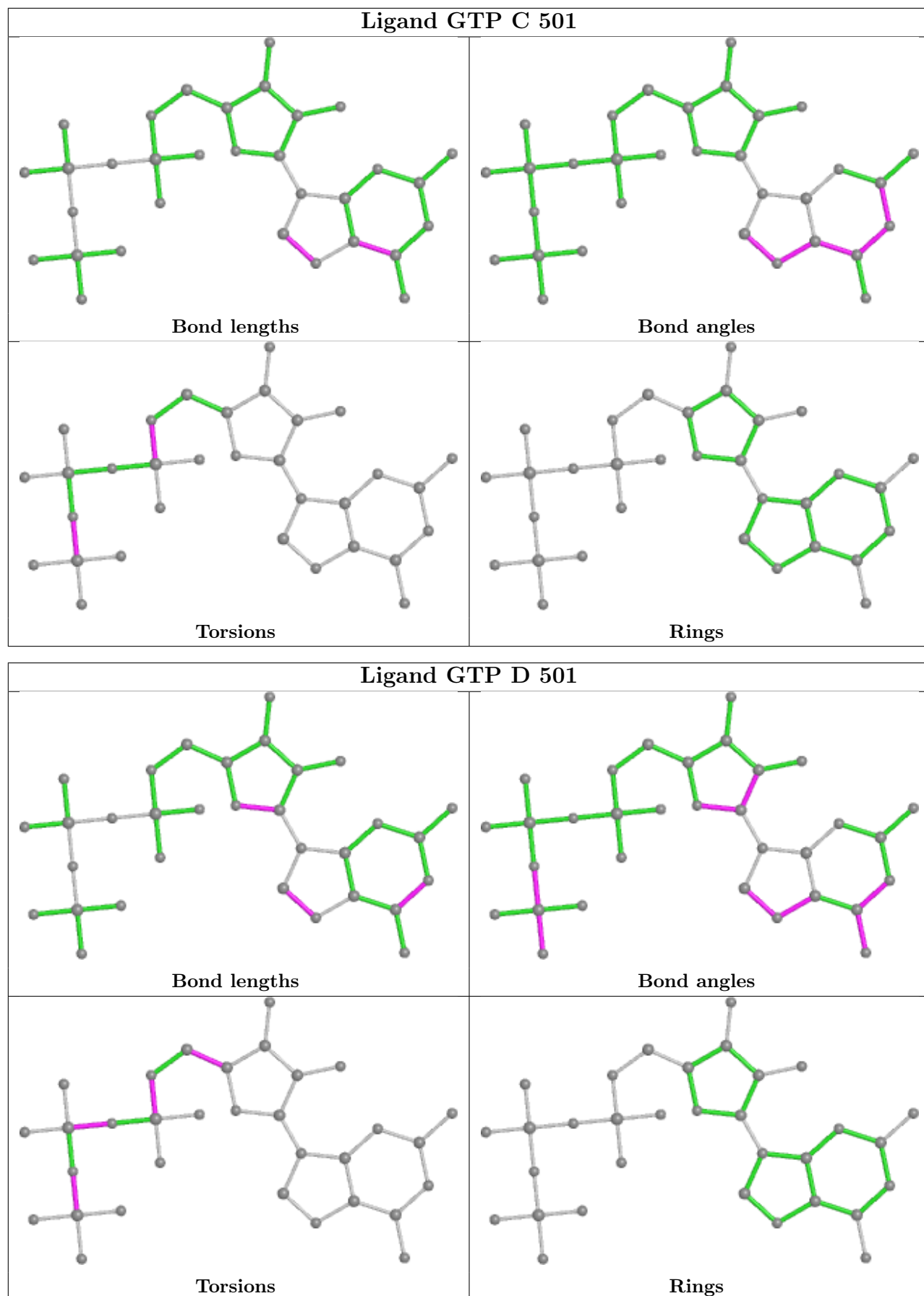
Mol	Chain	Res	Type	Atoms
4	C	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	PG-O3B-PB-O2B
4	D	501	GTP	PA-O3A-PB-O2B

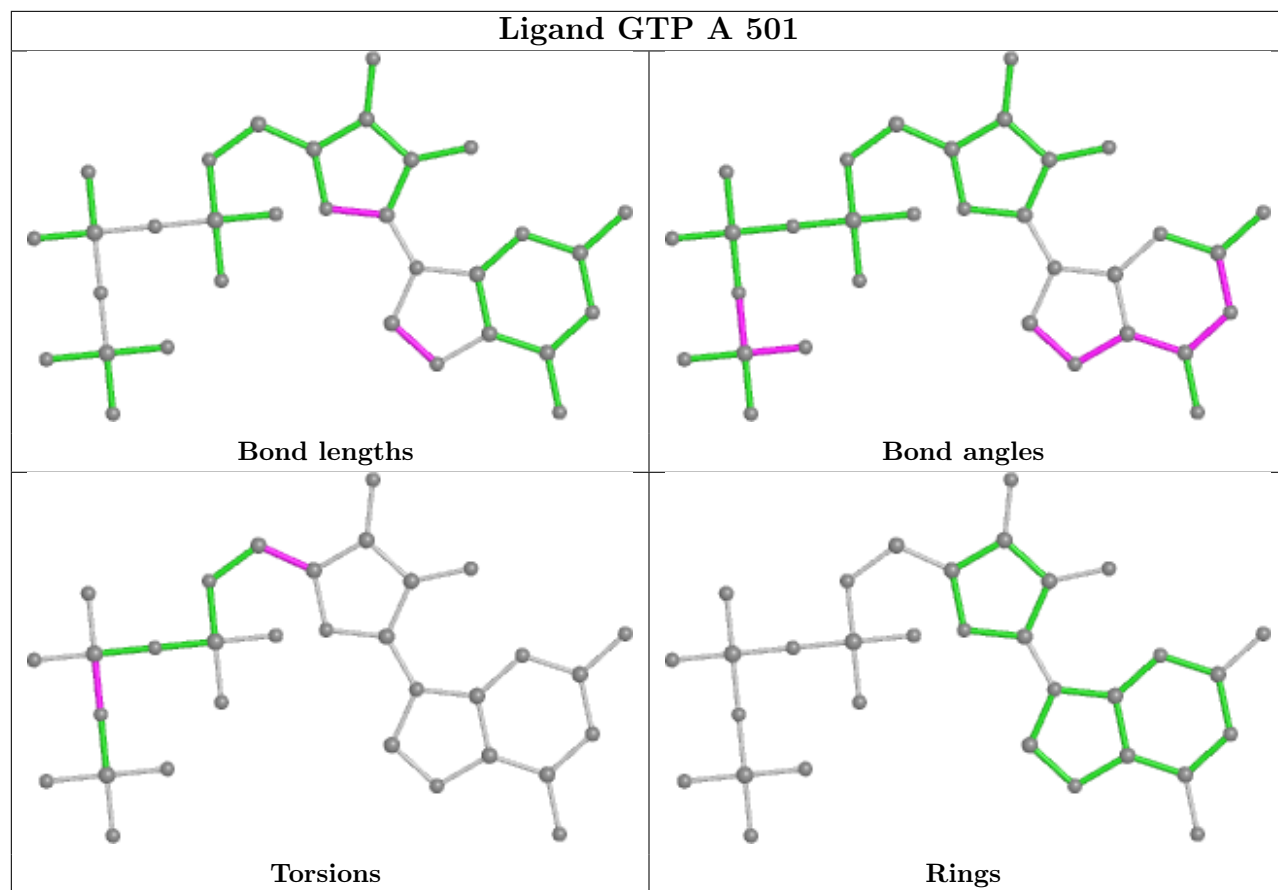
There are no ring outliers.

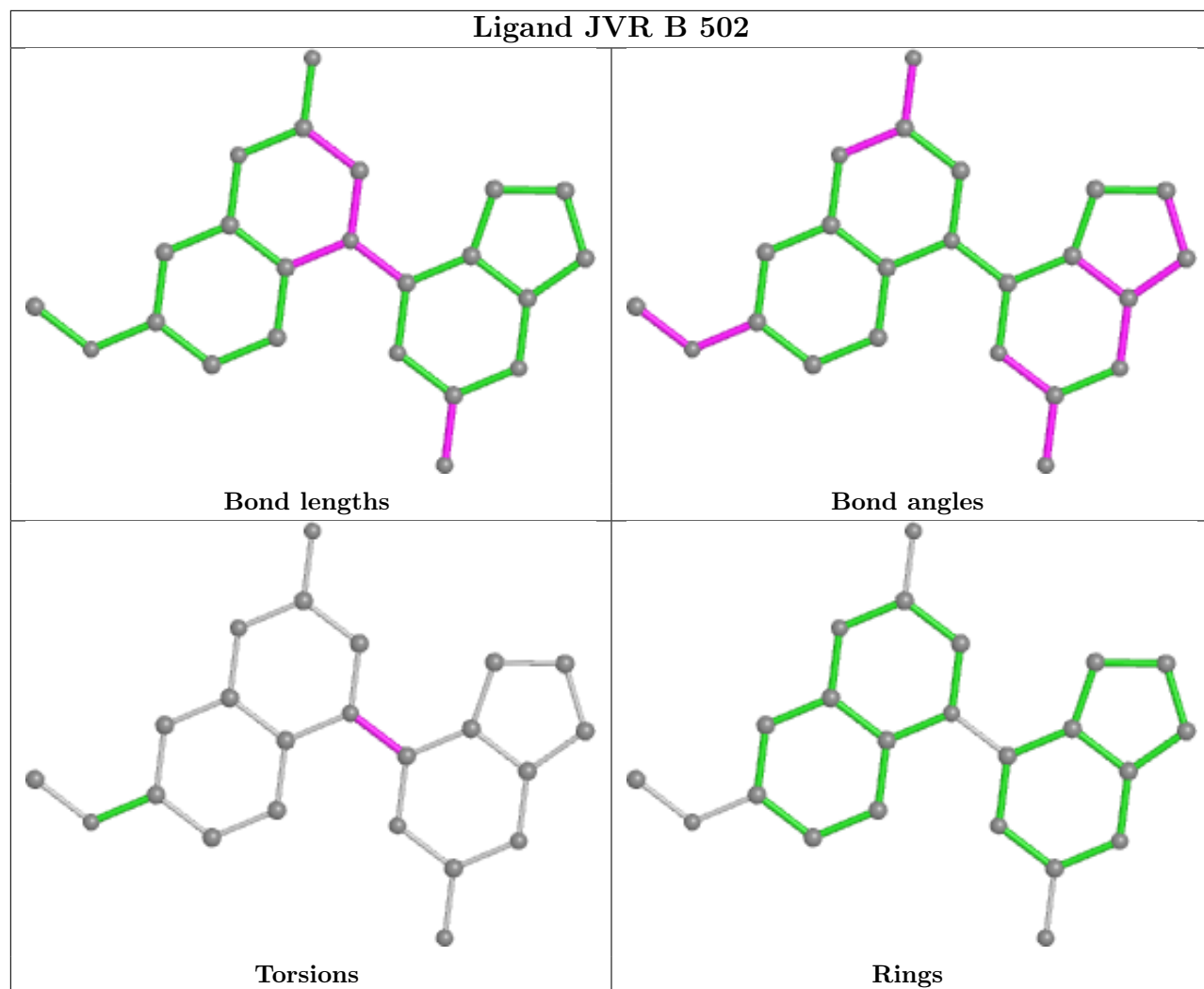
2 monomers are involved in 2 short contacts:

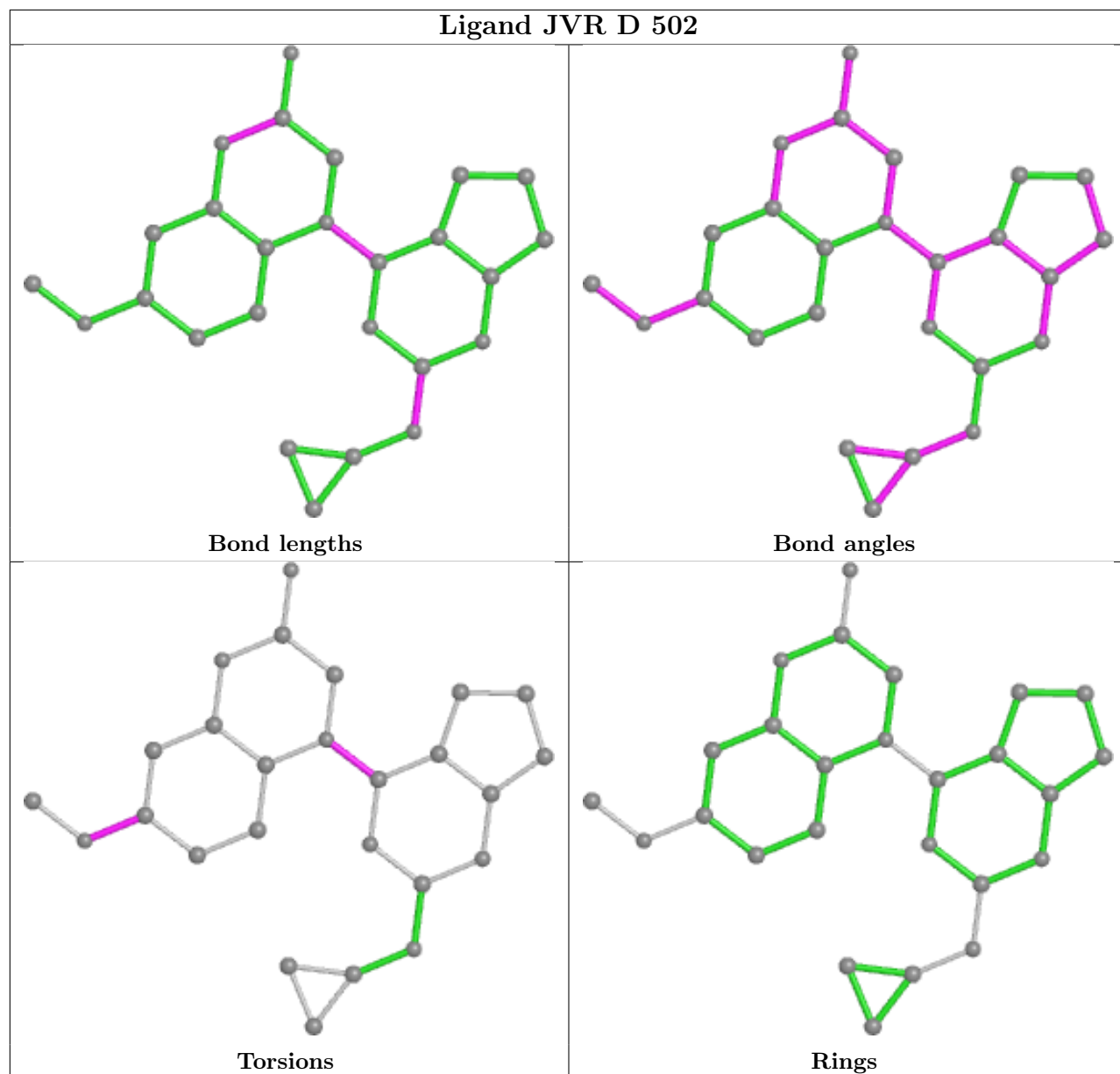
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	GTP	1	0
6	B	501	GDP	1	0

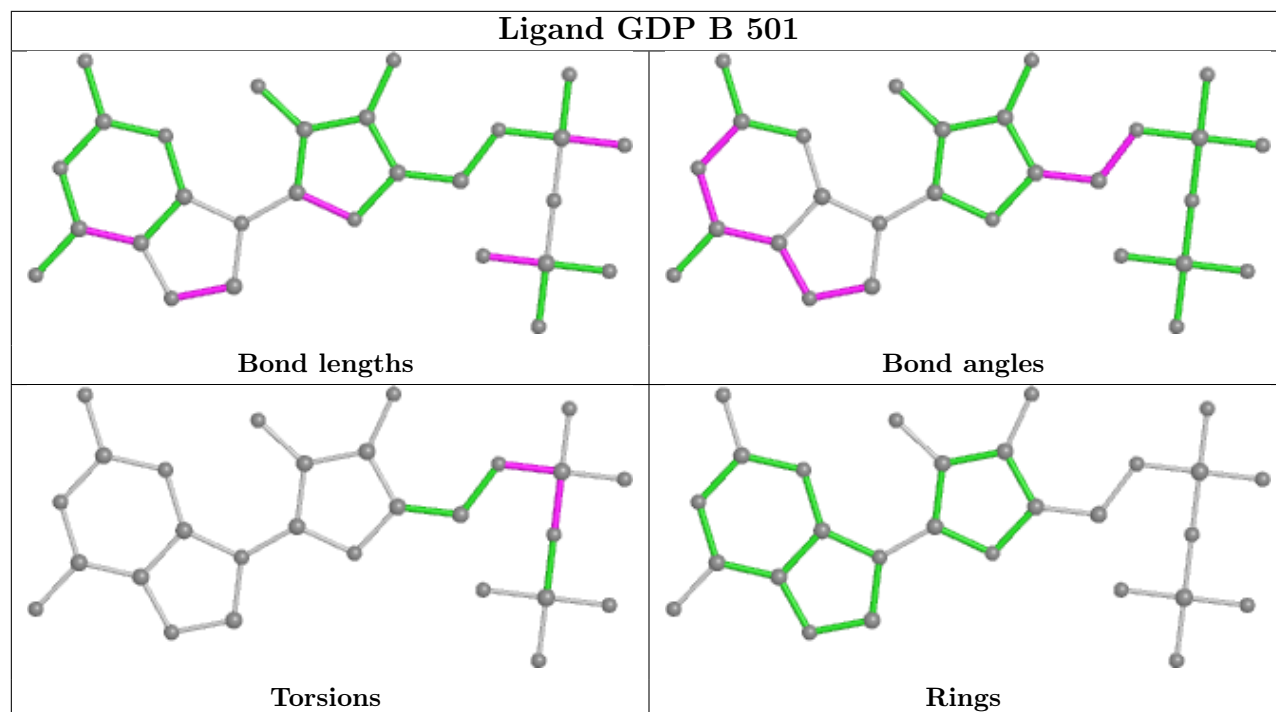
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	424/438 (96%)	0.25	24 (5%) 23 22	62, 100, 145, 181	0
1	C	427/438 (97%)	0.20	17 (3%) 38 37	61, 92, 136, 162	0
2	B	425/433 (98%)	0.38	33 (7%) 13 11	61, 90, 144, 183	0
2	D	431/433 (99%)	0.13	9 (2%) 63 65	54, 81, 134, 179	0
3	E	123/143 (86%)	0.66	20 (16%) 1 1	84, 109, 150, 173	0
All	All	1830/1885 (97%)	0.27	103 (5%) 24 23	54, 94, 143, 183	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.8
2	B	95	SER	5.3
2	B	42	LEU	5.0
3	E	9	ILE	4.4
2	B	363	MET	4.4
3	E	29	PHE	4.2
1	A	346	TRP	4.1
3	E	52	LYS	4.0
3	E	30	ASP	3.9
3	E	22	VAL	3.8
3	E	33	PRO	3.8
2	B	69	GLU	3.7
2	B	36	TYR	3.7
2	B	360	GLY	3.7
2	B	30	ILE	3.6
3	E	8	VAL	3.5
2	B	361	LEU	3.5
2	D	281	TYR	3.5
2	B	55	THR	3.5
3	E	24	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	37	HIS	3.5
3	E	23	ILE	3.5
1	A	351	PHE	3.4
2	D	81	PHE	3.4
3	E	32	VAL	3.4
2	B	59	TYR	3.2
3	E	31	GLY	3.1
1	A	349	THR	3.1
1	C	368	LEU	3.1
1	C	323	VAL	3.0
1	A	353	VAL	3.0
1	C	371	VAL	2.9
3	E	27	PRO	2.9
2	B	356	ILE	2.9
1	C	362	VAL	2.9
1	C	32	PRO	2.8
1	A	350	GLY	2.8
3	E	45	PRO	2.8
2	D	55	THR	2.8
1	A	130	THR	2.8
2	B	96	GLY	2.7
2	B	320	ARG	2.7
1	A	331	ALA	2.7
3	E	7	GLU	2.7
2	B	43	GLN	2.7
1	A	279	GLU	2.7
3	E	54	LEU	2.7
2	B	94	GLN	2.6
3	E	51	GLN	2.6
2	B	275	SER	2.6
1	C	251	ASP	2.6
1	A	315	CYS	2.6
2	B	68	LEU	2.6
1	A	335	ILE	2.5
2	B	39	ASP	2.5
2	B	83	GLN	2.5
1	A	332	ILE	2.5
1	A	280	LYS	2.5
1	C	369	ALA	2.4
2	B	395	LEU	2.4
2	B	40	SER	2.4
1	C	361	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.4
2	B	354	CYS	2.4
3	E	48	GLU	2.4
2	B	80	PRO	2.4
1	C	435	VAL	2.4
1	C	253	THR	2.3
1	A	131	GLY	2.3
2	D	245	GLN	2.3
1	C	33	ASP	2.3
1	A	333	ALA	2.3
3	E	13	LYS	2.3
1	A	324	VAL	2.3
1	C	84	ARG	2.3
2	B	98	GLY	2.3
1	A	3	GLU	2.3
2	B	143	THR	2.3
1	C	220	GLU	2.2
1	A	345	ASP	2.2
2	B	284	LEU	2.2
2	B	97	ALA	2.2
3	E	56	ALA	2.2
2	D	30	ILE	2.2
2	D	395	LEU	2.2
1	A	328	VAL	2.2
2	D	80	PRO	2.2
2	B	274	THR	2.2
1	A	177	VAL	2.1
2	B	362	LYS	2.1
1	A	323	VAL	2.1
1	C	212	ILE	2.1
3	E	55	GLU	2.1
1	C	357	TYR	2.1
2	B	93	GLY	2.1
1	C	30	ILE	2.1
1	A	336	LYS	2.1
2	D	246	LEU	2.0
2	D	59	TYR	2.0
1	C	131	GLY	2.0
1	A	329	ASN	2.0
2	B	44	LEU	2.0
2	B	29	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

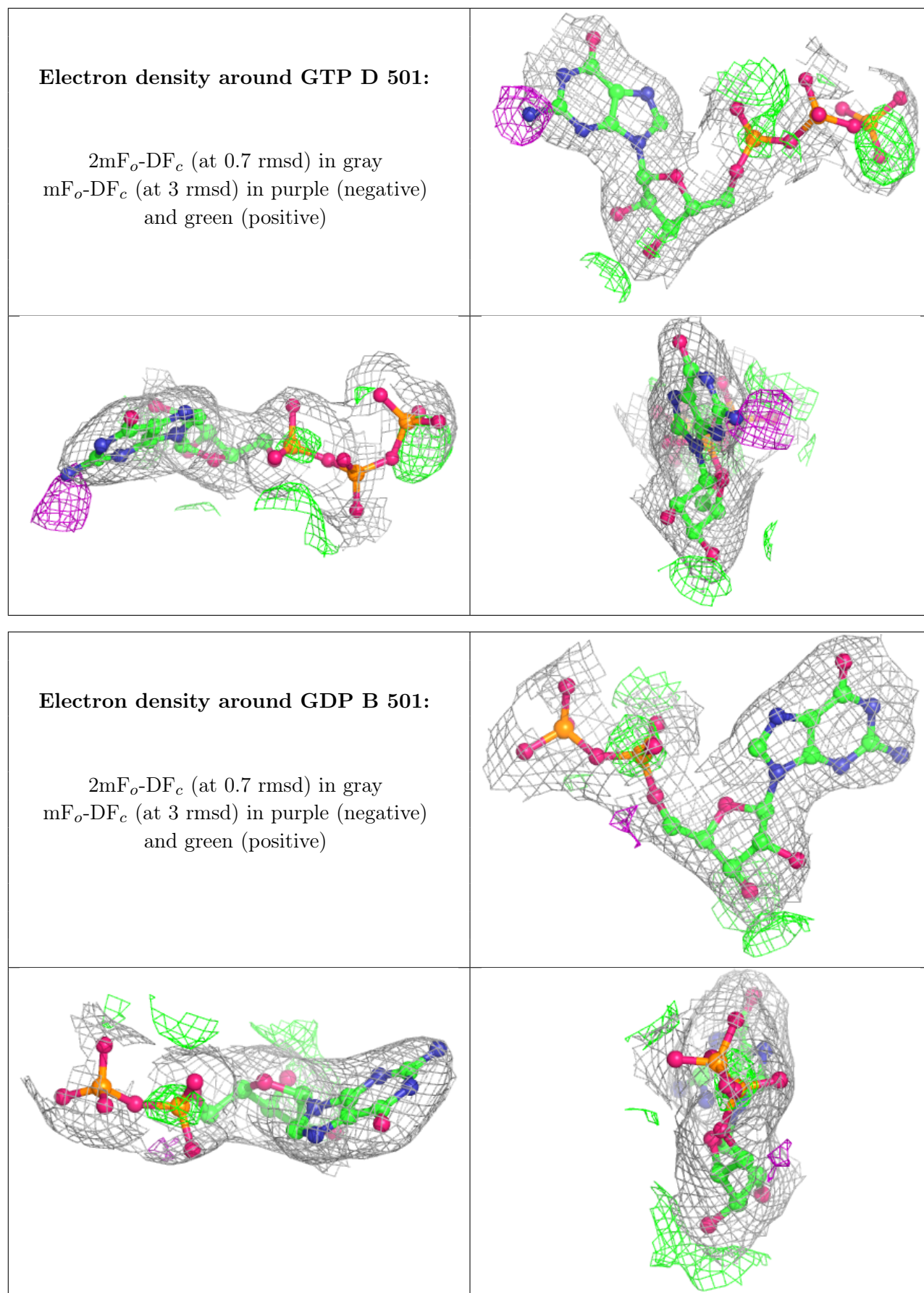
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

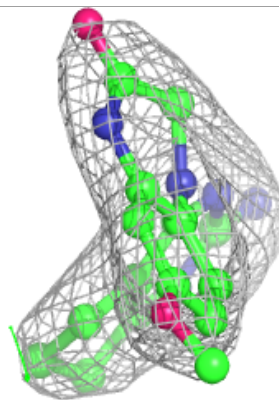
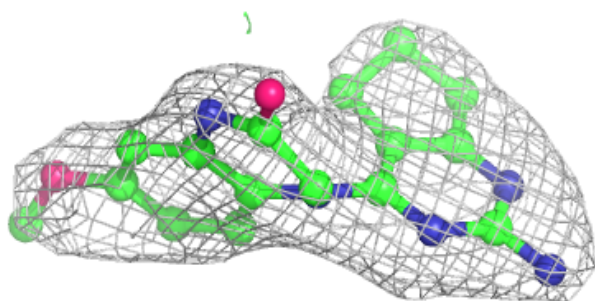
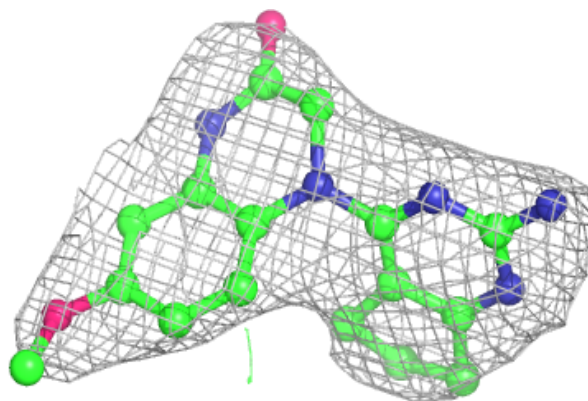
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	502	5/5	0.90	0.25	163,168,174,175	0
4	GTP	D	501	32/32	0.93	0.17	56,71,156,170	0
5	SO4	D	503	5/5	0.93	0.10	122,139,140,141	0
6	GDP	B	501	28/28	0.93	0.27	65,77,107,129	0
5	SO4	D	504	5/5	0.94	0.12	96,116,127,137	0
5	SO4	B	503	5/5	0.95	0.16	153,153,155,156	0
7	JVR	B	502	23/26	0.95	0.23	79,94,103,109	0
4	GTP	C	501	32/32	0.97	0.23	69,78,89,102	0
4	GTP	A	501	32/32	0.98	0.22	64,76,88,100	0
7	JVR	D	502	26/26	0.98	0.28	66,83,116,119	0
8	MG	C	502	1/1	0.98	0.19	87,87,87,87	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.

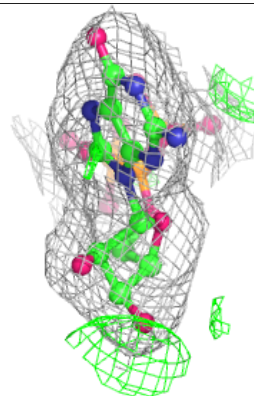
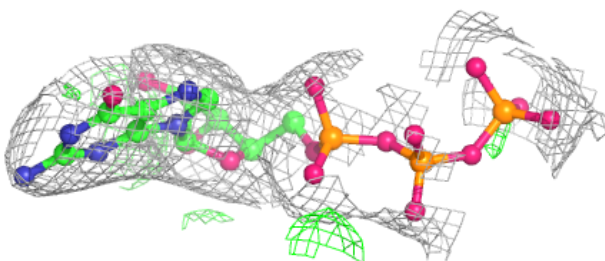
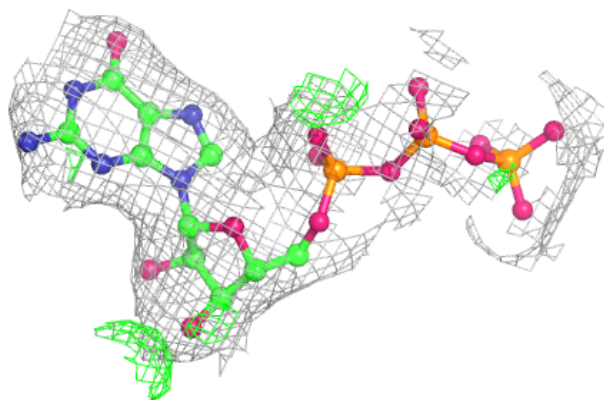


Electron density around JVR B 502:

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

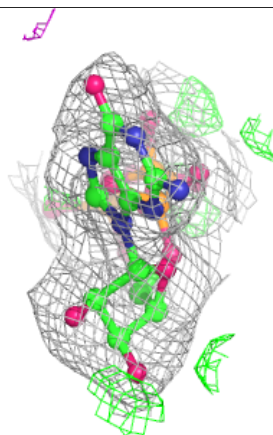
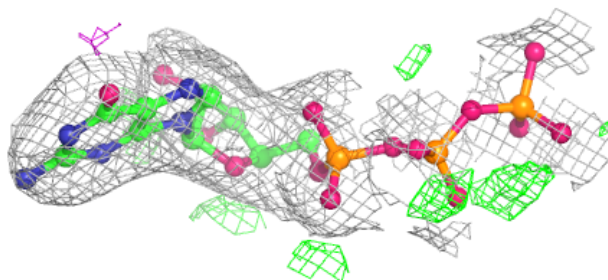
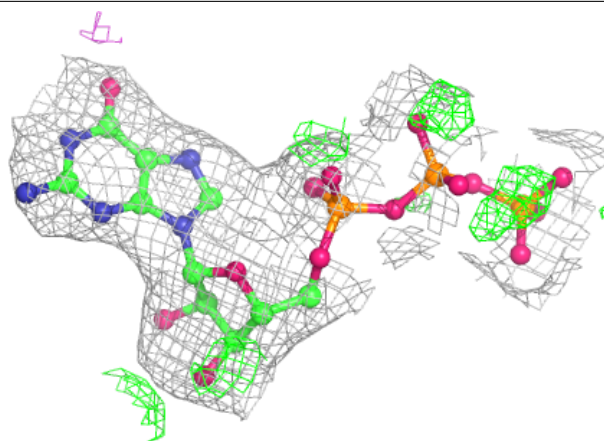
**Electron density around GTP C 501:**

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

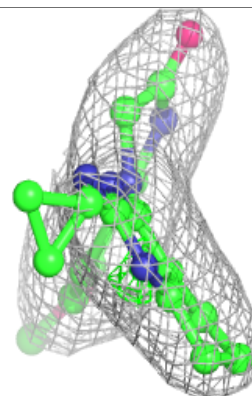
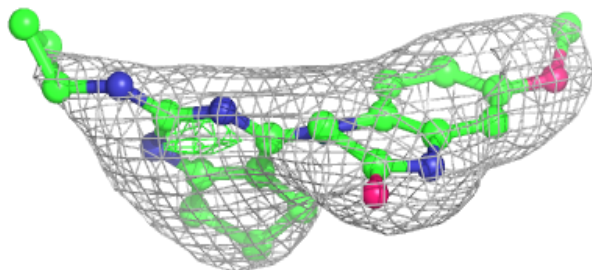
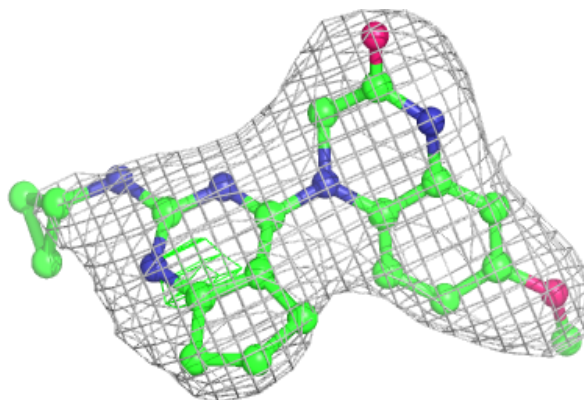


Electron density around GTP A 501:

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

**Electron density around JVR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.