



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2022 – 04:11 PM EDT

PDB ID : 5SB6
Title : Tubulin-todalam-10-complex
Authors : Muehlethaler, T.; Milanos, L.; Ortega, J.A.; Blum, T.B.; Gioia, D.; Prota, A.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2021-07-08
Resolution : 2.30 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 : 2.27
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) : 2.27

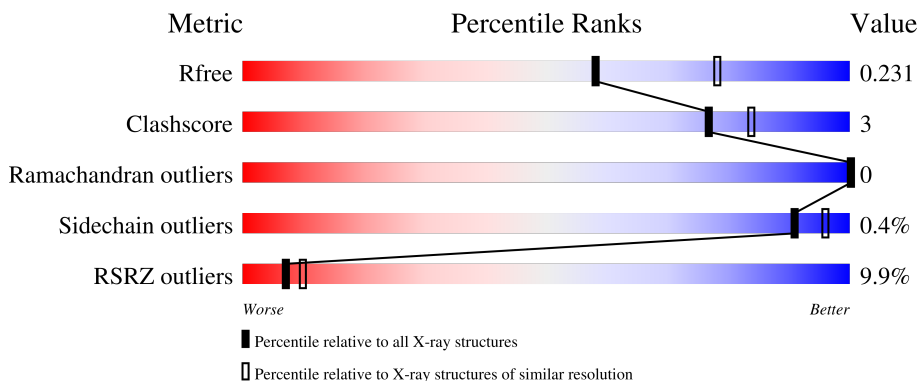
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	451	 5% 88% 9% .
1	C	451	 % 90% 7% .
2	B	445	 4% 87% 8% 5%
2	D	445	 11% 89% 6% .
3	E	143	 6% 81% . 15%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '30%', a green segment labeled '78%', a yellow segment labeled '8%', and a grey segment on the right labeled '14%'. The segments are stacked horizontally, with the red segment starting from the left and the grey segment ending at the right.</p>

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 17910 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	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
			Total	C	N	O	S			
2	B	423	Total	C	N	O	S	0	1	0
			3345	2102	572	644	27			
2	D	426	Total	C	N	O	S	1	0	0
			3342	2098	570	647	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 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

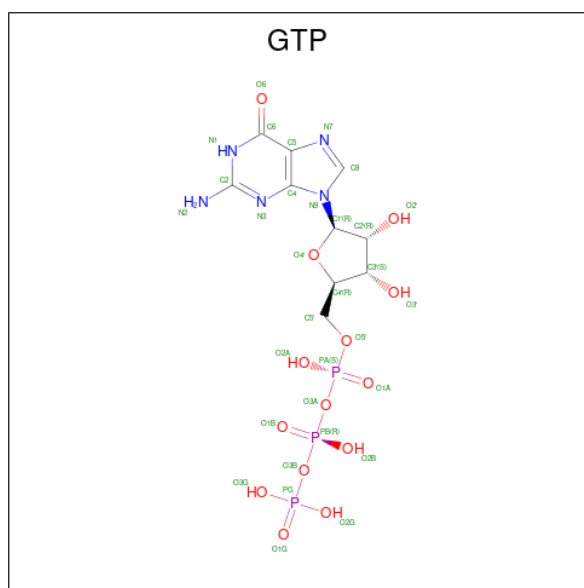
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	332	Total	C	N	O	S	0	0	0
			2714	1742	465	493	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	
			Total	C	N	O			P
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	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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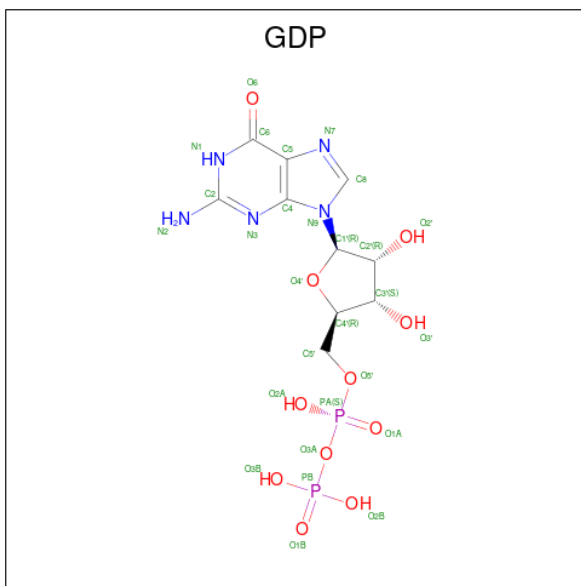
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



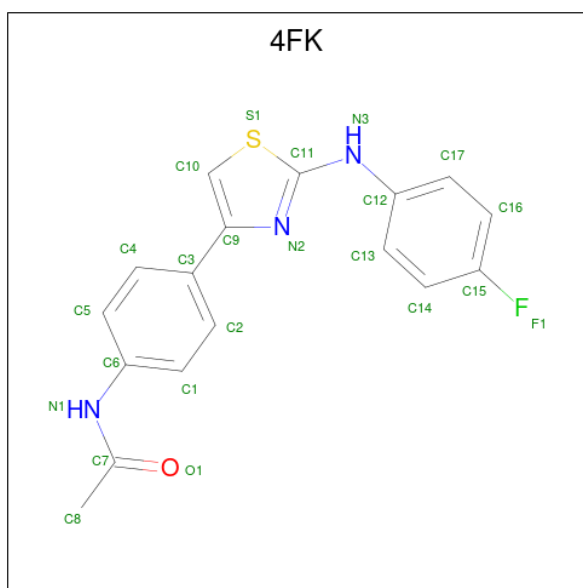
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



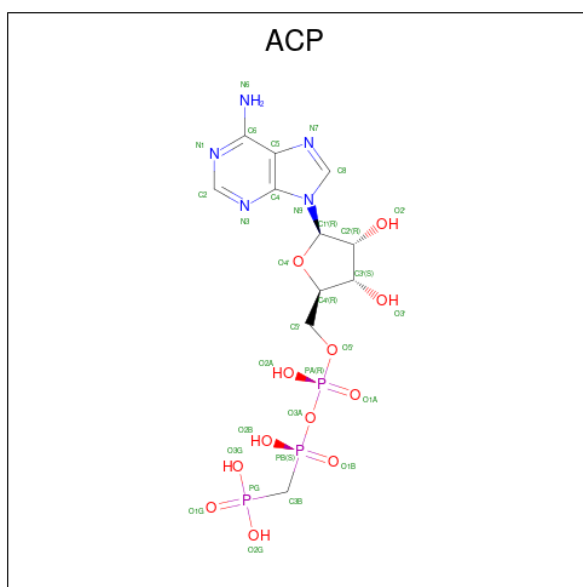
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is N-{4-[2-(4-fluoroanilino)-1,3-thiazol-4-yl]phenyl}acetamide (three-letter code: 4FK) (formula: $C_{17}H_{14}FN_3OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
10	C	1	23	17	1	3	1	1	0	0

- Molecule 11 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
			Total	C	N	O	P		
11	F	1	31	11	5	12	3	0	0

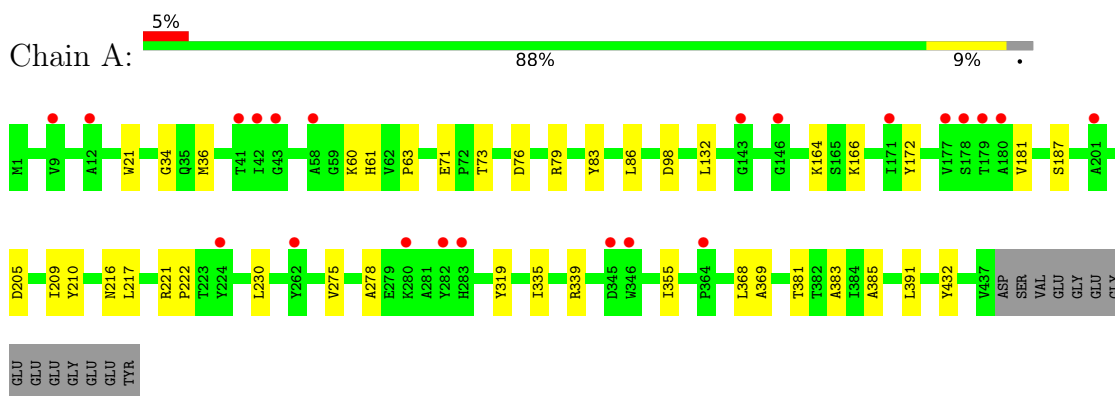
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	71	Total	O	0	0
			71	71		
12	B	92	Total	O	0	0
			92	92		
12	C	182	Total	O	0	0
			182	182		
12	D	60	Total	O	0	0
			60	60		
12	E	21	Total	O	0	0
			21	21		
12	F	35	Total	O	0	0
			35	35		

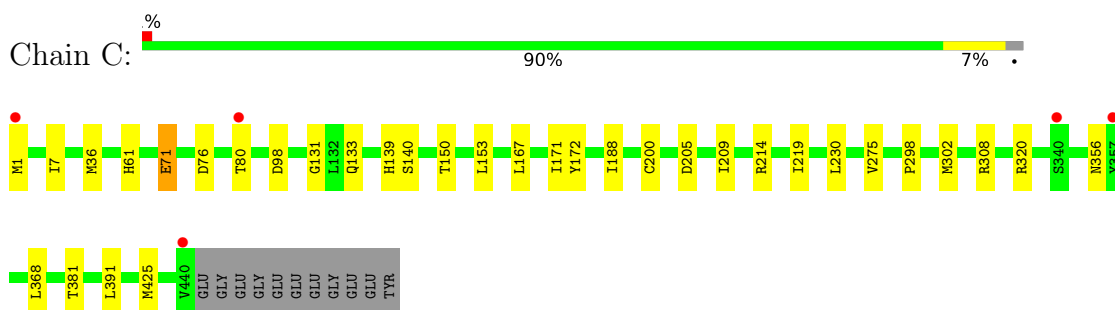
3 Residue-property plots [i](#)

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.

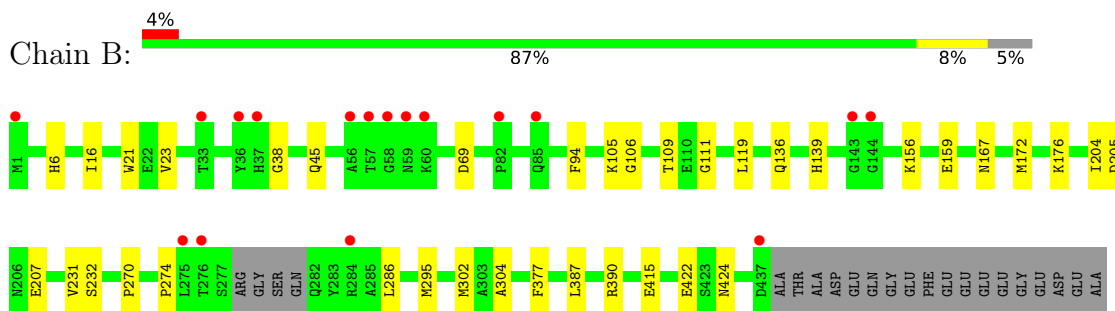
- Molecule 1: Tubulin alpha-1B chain



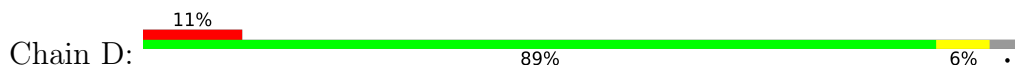
- Molecule 1: Tubulin alpha-1B chain

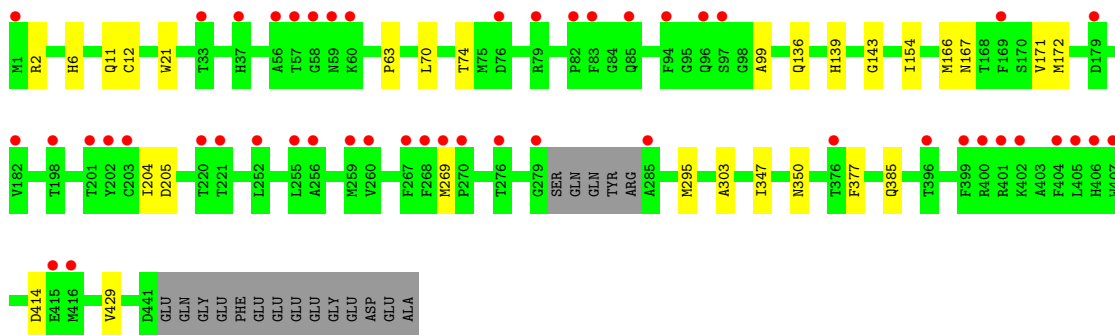


- Molecule 2: Tubulin beta-2B chain

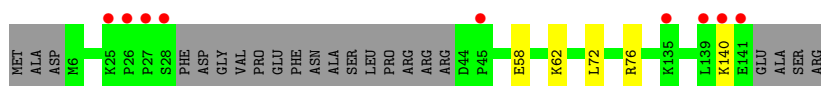
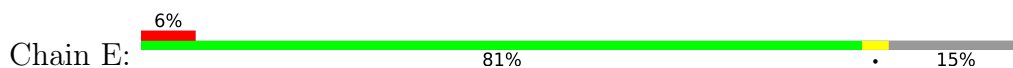


- Molecule 2: Tubulin beta-2B chain

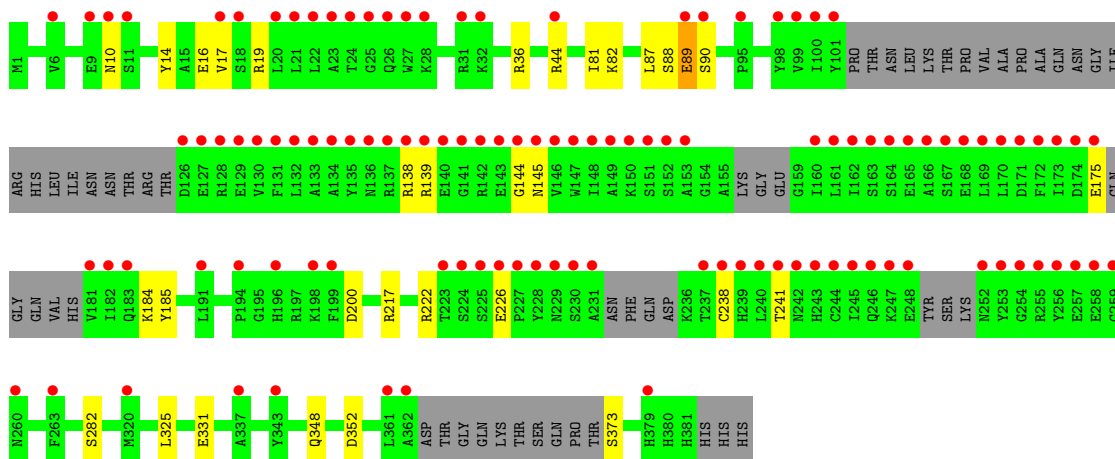
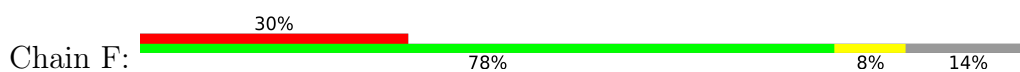




• Molecule 3: Stathmin-4



• 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	104.27Å 156.73Å 180.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 2.30 49.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.47-2.30) 100.0 (49.47-2.30)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.201 , 0.237 0.195 , 0.231	Depositor DCC
R_{free} test set	6562 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17910	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: MG, GTP, MES, CA, GDP, ACP, 4FK

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	0.26	0/3494	0.47	0/4743
1	C	0.27	0/3515	0.48	0/4772
2	B	0.26	0/3419	0.48	0/4629
2	D	0.25	0/3415	0.47	0/4625
3	E	0.24	0/1008	0.41	0/1337
4	F	0.24	0/2772	0.46	0/3738
All	All	0.25	0/17623	0.47	0/23844

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	3416	0	3330	20	0
1	C	3437	0	3348	20	0
2	B	3345	0	3227	22	0
2	D	3342	0	3222	16	0
3	E	1000	0	1018	3	0
4	F	2714	0	2687	20	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	12	0	0
10	C	23	0	0	2	0
11	F	31	0	14	3	0
12	A	71	0	0	1	0
12	B	92	0	0	5	0
12	C	182	0	0	0	0
12	D	60	0	0	1	0
12	E	21	0	0	0	0
12	F	35	0	0	3	0
All	All	17910	0	16906	102	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 3.

All (102) 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)
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.60	0.67
4:F:139:ARG:HB3	4:F:145:ASN:HD22	1.63	0.63
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.79	0.63
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.82	0.61
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.82	0.61
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.20	0.59
4:F:373:SER:N	12:F:504:HOH:O	2.36	0.58
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.83	0.58
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.86	0.58
4:F:82:LYS:HA	4:F:89:GLU:HB2	1.86	0.57
2:B:304:ALA:N	12:B:606:HOH:O	2.36	0.57
1:A:132:LEU:O	1:A:164:LYS:NZ	2.38	0.57
1:A:166:LYS:NZ	12:A:603:HOH:O	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.88	0.56
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.86	0.56
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.87	0.55
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.24	0.55
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.88	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.54
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.89	0.54
2:B:415:GLU:OE1	12:B:601:HOH:O	2.18	0.53
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.91	0.53
4:F:88:SER:O	4:F:90:SER:N	2.33	0.53
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.92	0.51
4:F:200:ASP:OD2	4:F:222:ARG:NH2	2.42	0.51
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.43	0.51
4:F:36:ARG:NH1	12:F:507:HOH:O	2.42	0.51
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.93	0.51
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.42	0.51
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.94	0.50
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.91	0.50
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.38	0.50
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.93	0.50
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.76	0.50
1:C:320:ARG:HA	1:C:356:ASN:O	2.12	0.50
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.92	0.49
2:B:422:GLU:HG3	12:B:613:HOH:O	2.12	0.49
1:A:381:THR:HG22	1:A:383:ALA:H	1.77	0.49
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.46	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.49
2:B:136:GLN:HA	2:B:167:ASN:O	2.12	0.49
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.94	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.48
2:D:172:MET:HB2	2:D:205:ASP:HA	1.96	0.48
2:D:414:ASP:N	2:D:414:ASP:OD1	2.47	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.97	0.46
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.33	0.46
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.34	0.46
1:C:167:LEU:HD13	10:C:504:4FK:C17	2.47	0.45
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.45
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.99	0.44
4:F:138:ARG:NH1	4:F:144:GLY:O	2.50	0.44
2:B:424:ASN:HB3	12:B:609:HOH:O	2.16	0.44
1:A:83:TYR:HB3	1:A:86:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.99	0.44
4:F:175:GLU:O	12:F:501:HOH:O	2.20	0.44
2:D:2:ARG:NH1	12:D:606:HOH:O	2.43	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.36	0.44
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.53	0.43
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.00	0.43
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.00	0.43
4:F:14:TYR:HA	4:F:17:VAL:HB	2.00	0.43
1:A:319:TYR:HB2	1:A:355:ILE:HG12	2.00	0.43
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.01	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.43
1:C:209:ILE:HD11	1:C:302:MET:SD	2.59	0.43
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.43
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.42
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.00	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
1:C:209:ILE:HD11	1:C:302:MET:HE1	2.02	0.42
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.55	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.20	0.42
2:B:159:GLU:OE2	12:B:602:HOH:O	2.22	0.42
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.54	0.42
2:B:119:LEU:HD11	2:B:156:LYS:HB3	2.00	0.42
4:F:184:LYS:NZ	4:F:185:TYR:O	2.52	0.42
2:B:295:MET:CG	2:B:377:PHE:HB2	2.49	0.42
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.20	0.42
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.20	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.41
4:F:226:GLU:HB2	4:F:238:CYS:HB3	2.02	0.41
1:C:133:GLN:HG2	10:C:504:4FK:S1	2.60	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.41
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.53	0.41
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.21	0.41
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.36	0.41
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.02	0.41
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.20	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.56	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.41
1:C:76:ASP:O	1:C:80:THR:HG22	2.21	0.41
3:E:140:LYS:HE2	3:E:140:LYS:HB3	1.93	0.41
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:VAL:HA	2:D:204:ILE:O	2.21	0.40
3:E:72:LEU:O	3:E:76:ARG:HG2	2.20	0.40
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.02	0.40
2:B:105:LYS:HA	2:B:109:THR:OG1	2.21	0.40
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.02	0.40
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.03	0.40
2:D:11:GLN:HA	2:D:74:THR:HG21	2.03	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	435/451 (96%)	424 (98%)	11 (2%)	0	100	100
1	C	438/451 (97%)	428 (98%)	10 (2%)	0	100	100
2	B	420/445 (94%)	411 (98%)	9 (2%)	0	100	100
2	D	422/445 (95%)	415 (98%)	7 (2%)	0	100	100
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	318/384 (83%)	306 (96%)	12 (4%)	0	100	100
All	All	2150/2319 (93%)	2099 (98%)	51 (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	368/379 (97%)	366 (100%)	2 (0%)	88	95
1	C	371/379 (98%)	369 (100%)	2 (0%)	88	95
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	97
2	D	367/383 (96%)	366 (100%)	1 (0%)	92	97
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	296/342 (86%)	294 (99%)	2 (1%)	84	92
All	All	1879/1993 (94%)	1871 (100%)	8 (0%)	91	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	A	221	ARG
2	B	139	HIS
1	C	71	GLU
1	C	381	THR
2	D	139	HIS
4	F	89	GLU
4	F	217	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
2	B	434	GLN
1	C	285	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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
8	GDP	B	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.92	8 (25%)
10	4FK	C	504	-	22,25,25	1.45	3 (13%)	28,34,34	0.82	1 (3%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	2.00	4 (28%)
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.68	6 (18%)
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.94	7 (22%)
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.73	7 (21%)
11	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.45	4 (12%)

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.52	1.66	1.77
8	D	501	GDP	C5-C6	4.13	1.48	1.41
8	B	501	GDP	C5-C6	4.07	1.48	1.41
10	C	504	4FK	C10-S1	3.27	1.75	1.70
10	C	504	4FK	C7-N1	3.27	1.42	1.36
5	C	501	GTP	C6-N1	2.93	1.38	1.33
5	A	501	GTP	C6-N1	2.92	1.38	1.33
11	F	401	ACP	PG-O3G	2.90	1.61	1.54
11	F	401	ACP	PG-O2G	2.88	1.61	1.54
11	F	401	ACP	PB-O3A	2.74	1.61	1.58
10	C	504	4FK	C11-N3	2.55	1.41	1.36
11	F	401	ACP	C5-C4	2.52	1.47	1.40
8	D	501	GDP	C5-C4	2.42	1.47	1.40
8	B	501	GDP	C5-C4	2.41	1.47	1.40
11	F	401	ACP	PB-O2B	2.25	1.61	1.56

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.41	120.00	127.22
5	C	501	GTP	N3-C2-N1	-5.11	120.40	127.22
8	D	501	GDP	C2-N3-C4	4.80	120.84	115.36
8	B	501	GDP	C2-N3-C4	4.63	120.64	115.36
9	B	504	MES	O1S-S-C8	4.31	112.10	106.92
8	B	501	GDP	C4-C5-C6	-4.27	116.72	120.80
8	D	501	GDP	C4-C5-C6	-4.14	116.85	120.80
5	A	501	GTP	C2-N3-C4	4.12	120.06	115.36
8	D	501	GDP	C2-N1-C6	4.11	122.46	115.93
8	B	501	GDP	C2-N1-C6	4.06	122.38	115.93
8	B	501	GDP	C5-C6-N1	-3.90	118.10	123.43
8	D	501	GDP	C5-C6-N1	-3.89	118.11	123.43
11	F	401	ACP	PB-O3A-PA	-3.74	120.70	132.56
5	C	501	GTP	C2-N3-C4	3.74	119.62	115.36
9	B	504	MES	C5-N4-C3	3.61	116.95	108.83
11	F	401	ACP	C3'-C2'-C1'	3.48	106.22	100.98
8	D	501	GDP	N3-C2-N1	-3.41	122.67	127.22
8	B	501	GDP	N3-C2-N1	-3.35	122.75	127.22
5	C	501	GTP	PA-O3A-PB	-3.19	121.89	132.83
11	F	401	ACP	N3-C2-N1	-3.17	123.72	128.68
5	C	501	GTP	C5-C6-N1	-3.14	119.14	123.43
5	A	501	GTP	C5-C6-N1	-3.02	119.30	123.43
5	A	501	GTP	PA-O3A-PB	-2.96	122.68	132.83
8	D	501	GDP	PA-O3A-PB	-2.88	122.94	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C4-C5-N7	-2.87	106.40	109.40
8	B	501	GDP	PA-O3A-PB	-2.83	123.12	132.83
9	B	504	MES	C7-N4-C5	2.80	118.41	111.23
5	A	501	GTP	C2-N1-C6	2.77	120.33	115.93
5	C	501	GTP	C2-N1-C6	2.73	120.26	115.93
9	B	504	MES	C6-C5-N4	-2.72	105.98	110.10
8	D	501	GDP	C4-C5-N7	-2.71	106.57	109.40
11	F	401	ACP	C4-C5-N7	-2.60	106.69	109.40
5	C	501	GTP	PB-O3B-PG	-2.55	124.06	132.83
5	A	501	GTP	PB-O3B-PG	-2.37	124.71	132.83
10	C	504	4FK	C12-N3-C11	-2.12	124.02	129.39
8	B	501	GDP	C1'-N9-C4	-2.11	122.94	126.64
5	A	501	GTP	N2-C2-N1	2.00	120.36	117.25

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
10	C	504	4FK	C17-C12-N3-C11
10	C	504	4FK	C13-C12-N3-C11
8	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S

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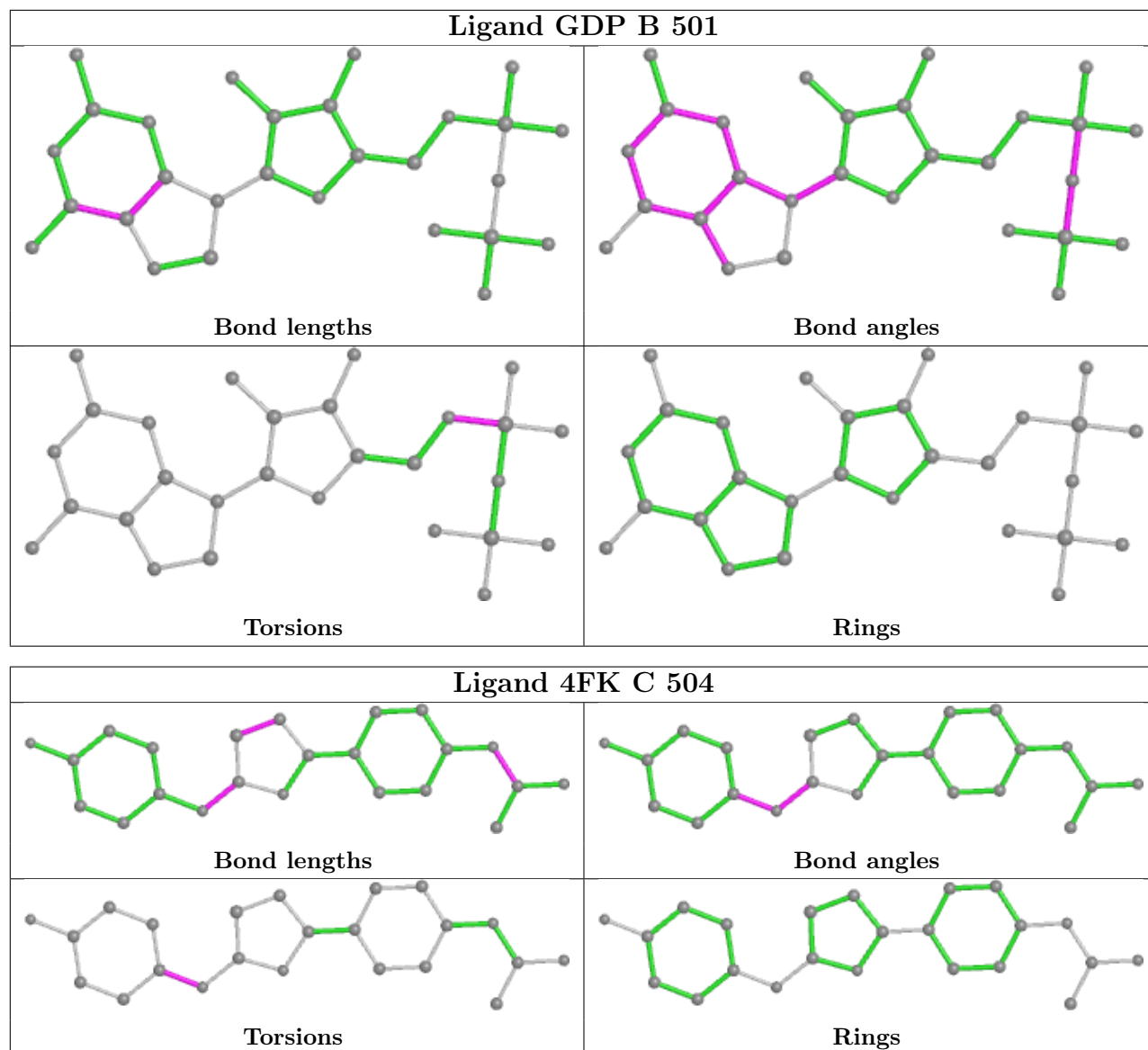
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	PG-C3B-PB-O1B
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
9	B	504	MES	C8-C7-N4-C3

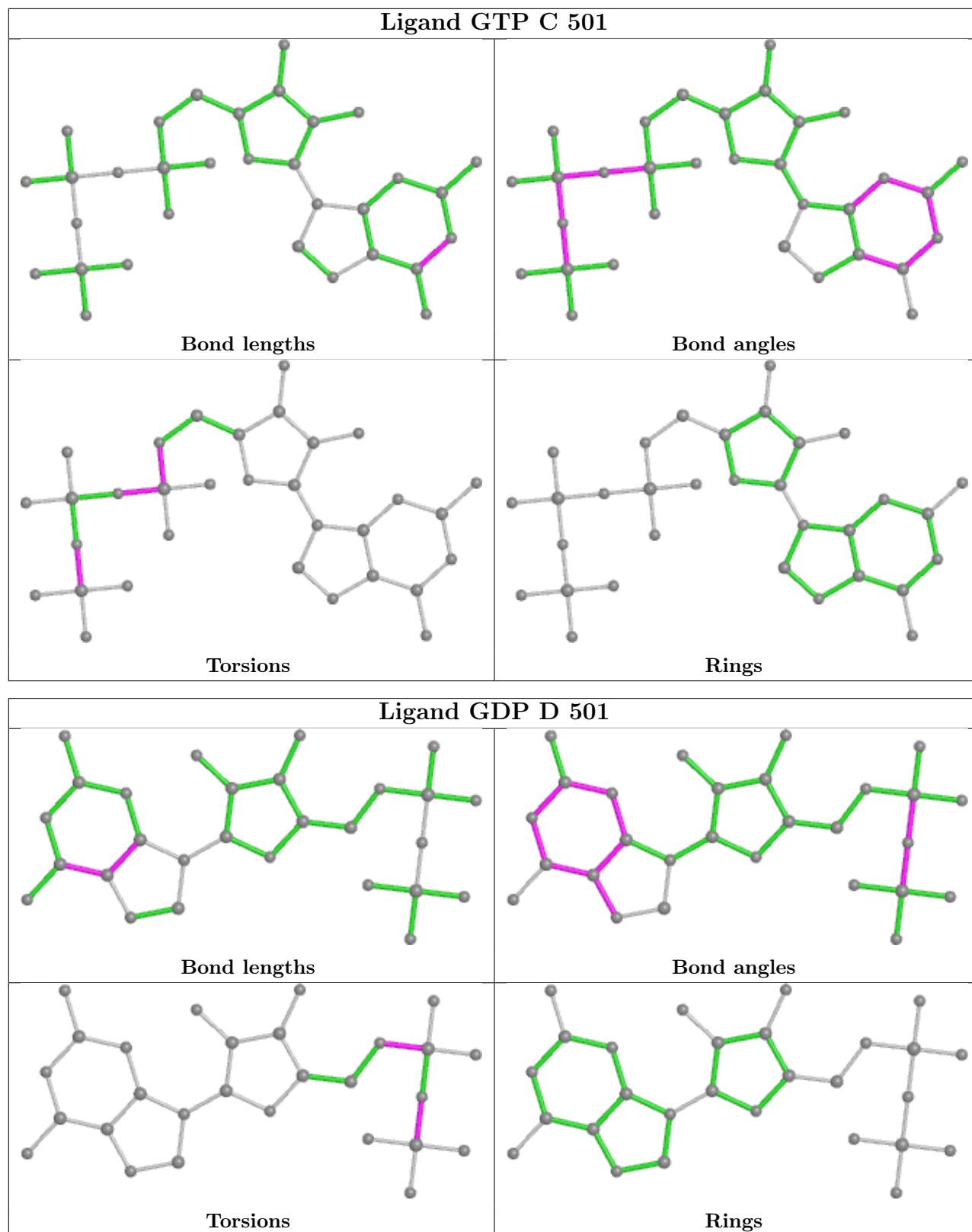
There are no ring outliers.

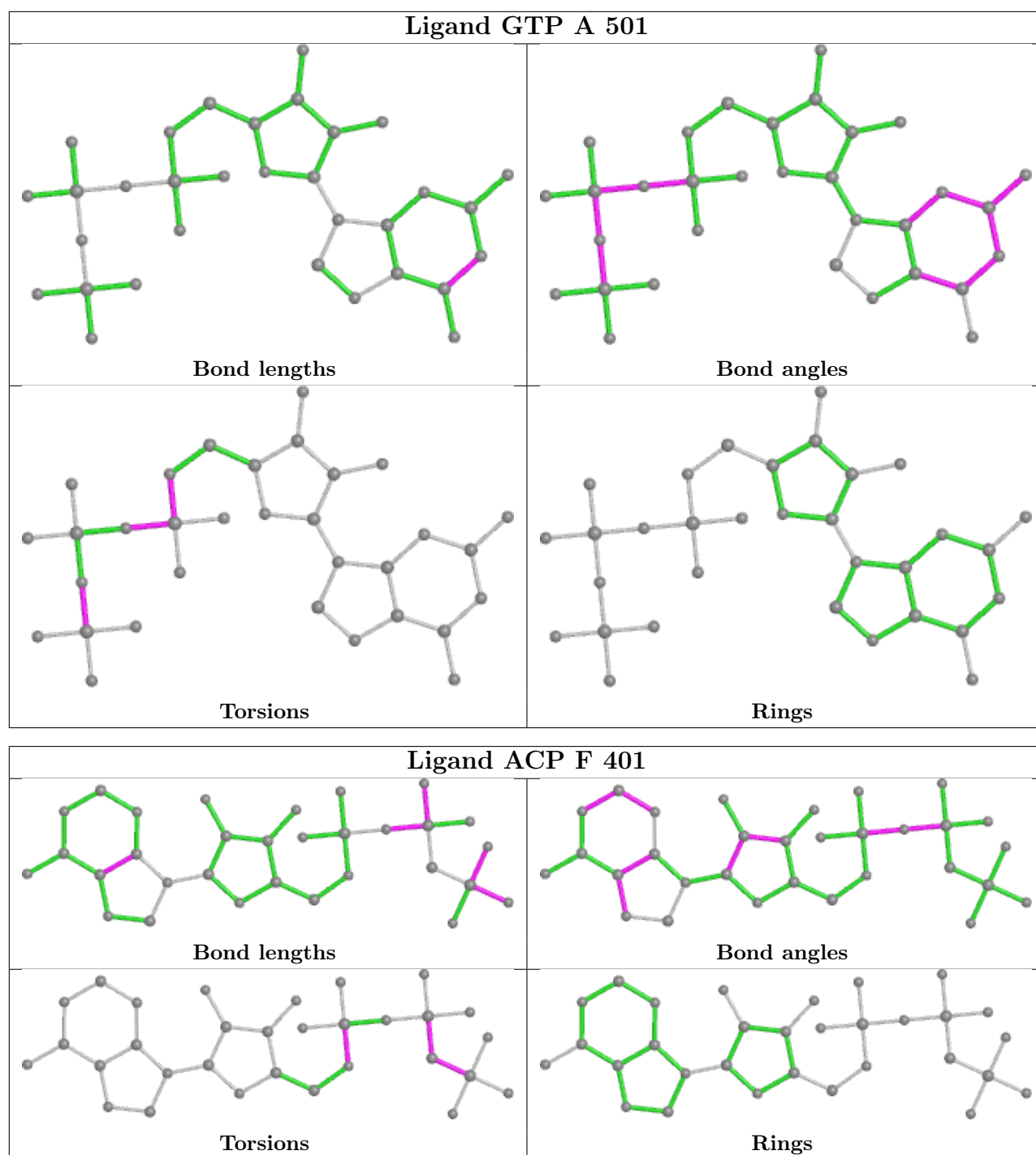
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	504	4FK	2	0
8	D	501	GDP	2	0
5	A	501	GTP	1	0
11	F	401	ACP	3	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	437/451 (96%)	0.48	22 (5%) 28 35	41, 59, 89, 134	0
1	C	440/451 (97%)	0.10	5 (1%) 80 85	34, 47, 70, 104	0
2	B	423/445 (95%)	0.35	17 (4%) 38 45	34, 54, 88, 129	0
2	D	426/445 (95%)	0.67	49 (11%) 4 7	42, 65, 97, 126	2 (0%)
3	E	121/143 (84%)	0.52	9 (7%) 14 19	47, 69, 106, 120	0
4	F	332/384 (86%)	1.59	114 (34%) 0 0	55, 84, 146, 164	0
All	All	2179/2319 (93%)	0.59	216 (9%) 7 10	34, 60, 110, 164	2 (0%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	11.9
4	F	244	CYS	9.8
4	F	133	ALA	9.4
4	F	253	TYR	9.3
4	F	130	VAL	9.3
4	F	100	ILE	8.2
4	F	161	LEU	8.1
2	B	276	THR	7.7
4	F	169	LEU	7.4
4	F	131	PHE	7.4
2	B	1	MET	7.3
4	F	132	LEU	7.1
4	F	240	LEU	6.9
4	F	134	ALA	6.9
4	F	129	GLU	6.8
4	F	135	TYR	6.7
1	A	282	TYR	6.4
2	D	57	THR	6.4
2	B	57	THR	6.3

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Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	6.0
4	F	167	SER	6.0
4	F	239	HIS	5.8
4	F	99	VAL	5.6
4	F	153	ALA	5.5
4	F	254	GLY	5.4
2	B	59	ASN	5.4
4	F	259	GLY	5.4
4	F	101	TYR	5.3
4	F	182	ILE	5.3
4	F	142	ARG	5.3
4	F	245	ILE	5.1
4	F	170	LEU	5.1
1	A	42	ILE	5.0
3	E	26	PRO	4.9
2	D	94	PHE	4.9
4	F	163	SER	4.8
4	F	172	PHE	4.8
4	F	225	SER	4.8
4	F	181	VAL	4.8
4	F	136	ASN	4.8
3	E	27	PRO	4.8
4	F	147	TRP	4.7
4	F	252	ASN	4.7
4	F	143	GLU	4.6
4	F	231	ALA	4.5
4	F	256	TYR	4.4
2	B	284	ARG	4.4
4	F	238	CYS	4.4
2	D	400	ARG	4.4
4	F	137	ARG	4.4
4	F	243	HIS	4.4
4	F	248	GLU	4.4
1	C	440	VAL	4.3
4	F	168	GLU	4.3
4	F	139	ARG	4.3
2	D	415	GLU	4.3
3	E	139	LEU	4.3
2	D	401	ARG	4.2
4	F	145	ASN	4.0
4	F	247	LYS	4.0
4	F	162	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	241	THR	4.0
1	C	340	SER	4.0
4	F	361	LEU	3.9
4	F	165	GLU	3.9
2	B	33	THR	3.8
4	F	224	SER	3.8
4	F	242	ASN	3.8
2	B	58	GLY	3.8
1	A	262	TYR	3.8
4	F	223	THR	3.7
2	D	58	GLY	3.7
4	F	199	PHE	3.7
2	D	59	ASN	3.6
4	F	20	LEU	3.6
4	F	255	ARG	3.6
4	F	230	SER	3.6
4	F	228	TYR	3.6
4	F	17	VAL	3.5
2	D	407	TRP	3.5
4	F	144	GLY	3.4
2	D	182	VAL	3.4
4	F	138	ARG	3.4
4	F	151	SER	3.4
4	F	227	PRO	3.4
1	A	283	HIS	3.3
4	F	362	ALA	3.3
2	D	202	TYR	3.3
2	D	96	GLN	3.3
4	F	174	ASP	3.3
2	D	56	ALA	3.3
4	F	343	TYR	3.2
1	C	357	TYR	3.2
4	F	229	ASN	3.2
4	F	126	ASP	3.2
4	F	98	TYR	3.2
4	F	89	GLU	3.1
2	D	82	PRO	3.1
1	A	41	THR	3.1
3	E	45	PRO	3.1
2	D	97	SER	3.1
4	F	27	TRP	3.0
4	F	21	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	37	HIS	3.0
3	E	135	LYS	3.0
2	D	201	THR	3.0
4	F	258	GLU	3.0
2	D	406	HIS	3.0
2	D	404	PHE	3.0
4	F	44	ARG	3.0
4	F	22	LEU	3.0
1	A	346	TRP	3.0
4	F	260	ASN	3.0
4	F	9	GLU	3.0
4	F	263	PHE	3.0
4	F	194	PRO	3.0
4	F	150	LYS	2.9
1	A	179	THR	2.9
2	D	268	PHE	2.9
4	F	10	ASN	2.9
4	F	160	ILE	2.8
4	F	26	GLN	2.8
4	F	164	SER	2.8
1	A	171	ILE	2.8
4	F	25	GLY	2.8
4	F	152	SER	2.8
2	B	82	PRO	2.8
1	A	43	GLY	2.8
4	F	128	ARG	2.8
4	F	246	GLN	2.8
2	D	252	LEU	2.8
2	D	405	LEU	2.8
2	D	279	GLY	2.7
4	F	6	VAL	2.7
1	A	345	ASP	2.7
4	F	146	VAL	2.7
2	D	60	LYS	2.7
4	F	257	GLU	2.7
4	F	28	LYS	2.7
1	A	364	PRO	2.7
4	F	320	MET	2.6
1	C	80	THR	2.6
2	D	285	ALA	2.6
3	E	28	SER	2.6
4	F	183	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	127	GLU	2.6
4	F	23	ALA	2.6
3	E	25	LYS	2.6
1	A	177	VAL	2.5
2	D	33	THR	2.5
4	F	148	ILE	2.5
4	F	149	ALA	2.5
1	A	280	LYS	2.5
2	D	276	THR	2.5
4	F	196	HIS	2.5
1	A	146	GLY	2.5
4	F	226	GLU	2.5
2	D	259	MET	2.5
4	F	31	ARG	2.5
4	F	141	GLY	2.5
3	E	140	LYS	2.4
2	B	60	LYS	2.4
1	A	180	ALA	2.4
4	F	337	ALA	2.4
2	D	260	VAL	2.4
2	D	198	THR	2.4
2	B	144	GLY	2.4
2	B	437	ASP	2.4
2	D	76	ASP	2.4
2	B	36	TYR	2.4
2	D	267	PHE	2.4
2	D	416	MET	2.3
4	F	198	LYS	2.3
4	F	24	THR	2.3
4	F	18	SER	2.3
4	F	140	GLU	2.3
2	D	85	GLN	2.3
2	D	179	ASP	2.3
1	A	178	SER	2.3
2	B	85	GLN	2.3
1	A	58	ALA	2.3
2	D	402	LYS	2.2
4	F	171	ASP	2.2
2	B	143	GLY	2.2
2	D	37	HIS	2.2
2	D	399	PHE	2.2
4	F	11	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	56	ALA	2.2
2	D	220	THR	2.2
2	D	79	ARG	2.2
2	D	221	THR	2.2
2	D	256	ALA	2.2
3	E	141	GLU	2.2
4	F	175	GLU	2.2
4	F	237	THR	2.2
2	D	1	MET	2.2
4	F	32	LYS	2.1
2	D	169	PHE	2.1
1	A	201	ALA	2.1
4	F	191	LEU	2.1
2	D	270	PRO	2.1
1	A	12	ALA	2.1
1	A	224	TYR	2.1
1	A	143	GLY	2.1
2	B	275	LEU	2.1
4	F	379	HIS	2.1
2	D	83	PHE	2.1
4	F	95	PRO	2.1
1	C	1	MET	2.1
2	D	203	CYS	2.1
2	D	396	THR	2.0
4	F	90	SER	2.0
2	D	255	LEU	2.0
1	A	9	VAL	2.0
2	D	269	MET	2.0
2	D	376	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

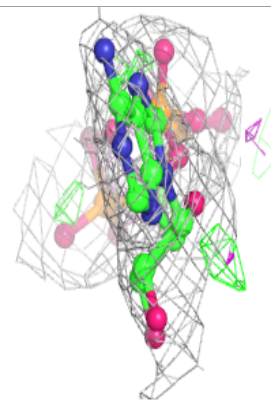
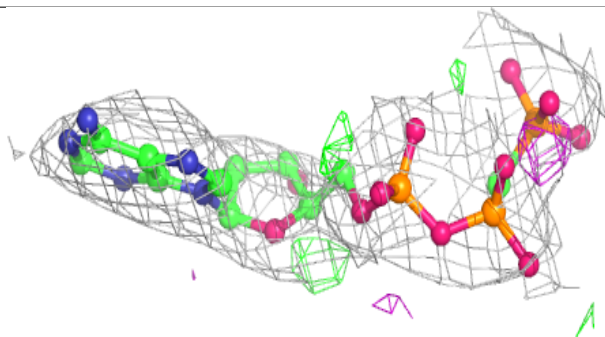
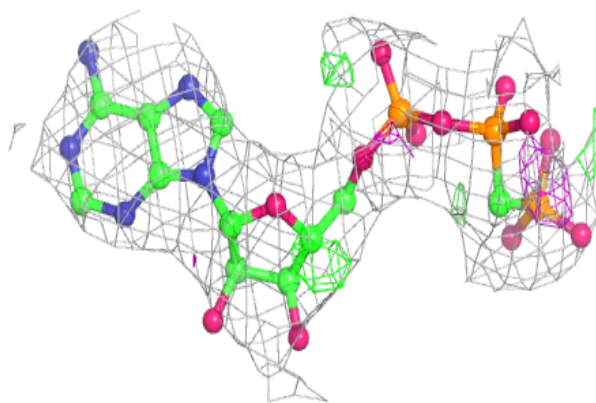
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.58	0.19	79,79,79,79	0
11	ACP	F	401	31/31	0.84	0.21	93,104,114,117	0
7	CA	B	503	1/1	0.89	0.25	91,91,91,91	0
6	MG	A	502	1/1	0.89	0.18	44,44,44,44	0
7	CA	A	504	1/1	0.90	0.07	90,90,90,90	0
10	4FK	C	504	23/23	0.94	0.22	37,47,51,54	23
7	CA	A	503	1/1	0.94	0.04	78,78,78,78	0
6	MG	F	402	1/1	0.95	0.04	93,93,93,93	0
8	GDP	D	501	28/28	0.95	0.13	57,63,72,74	0
5	GTP	A	501	32/32	0.97	0.22	37,44,49,51	0
9	MES	B	504	12/12	0.97	0.14	45,51,58,59	0
6	MG	B	502	1/1	0.98	0.25	34,34,34,34	0
5	GTP	C	501	32/32	0.98	0.16	32,38,43,47	0
7	CA	C	503	1/1	0.99	0.05	65,65,65,65	0
8	GDP	B	501	28/28	0.99	0.18	34,40,46,47	0
6	MG	C	502	1/1	0.99	0.09	37,37,37,37	0

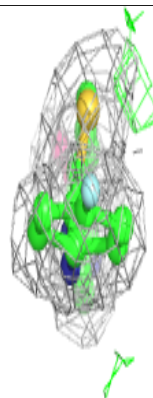
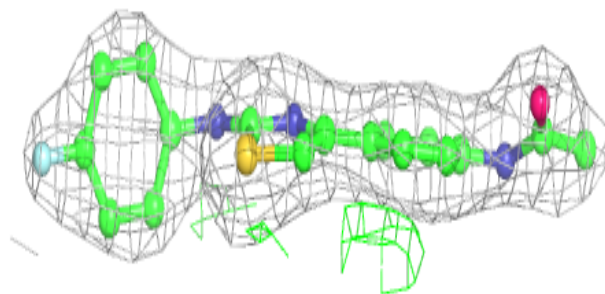
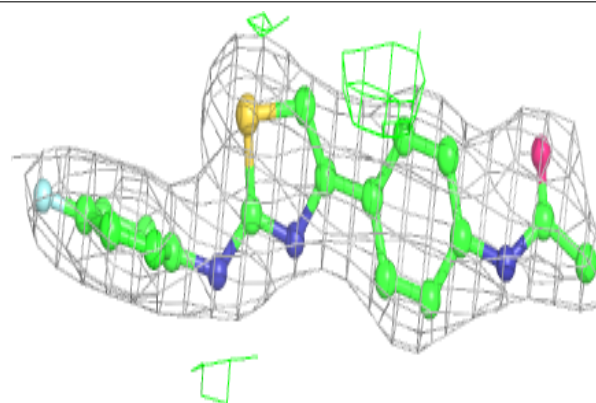
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

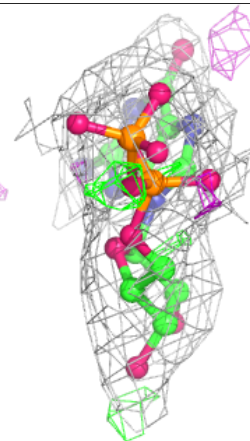
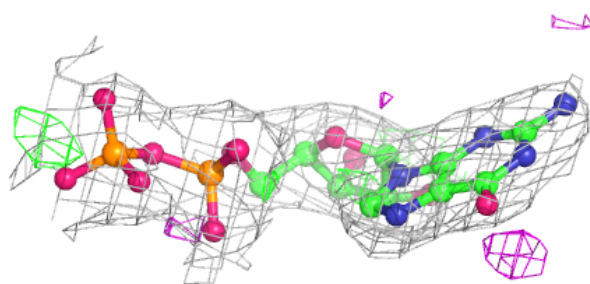
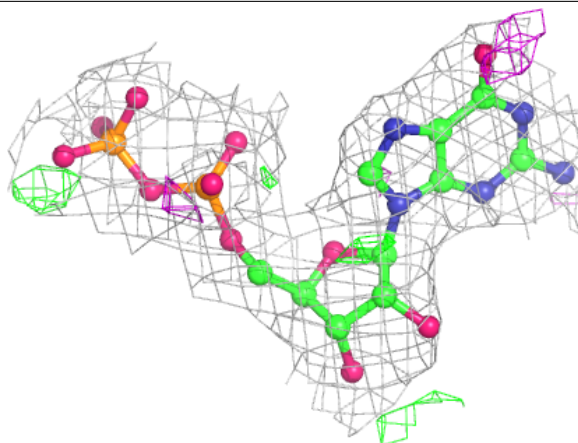
**Electron density around 4FK C 504:**

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

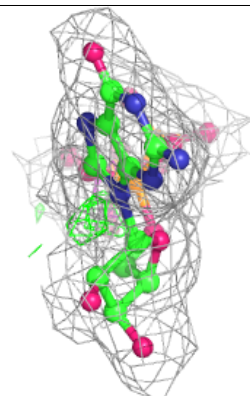
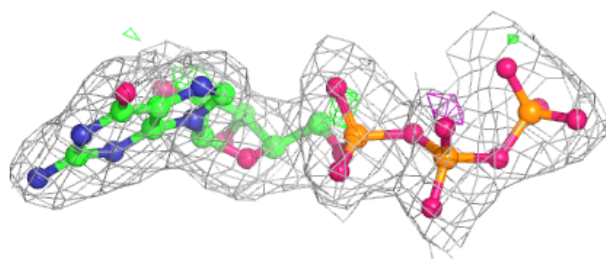
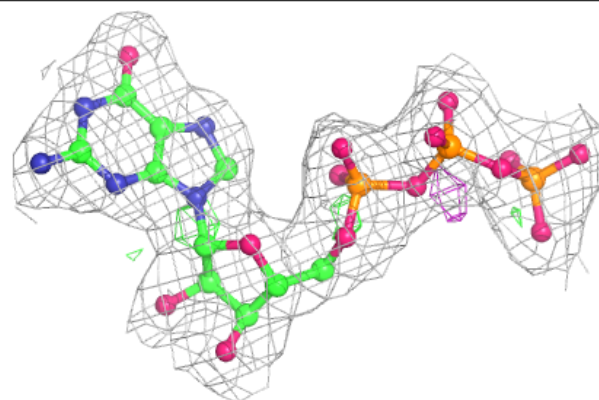


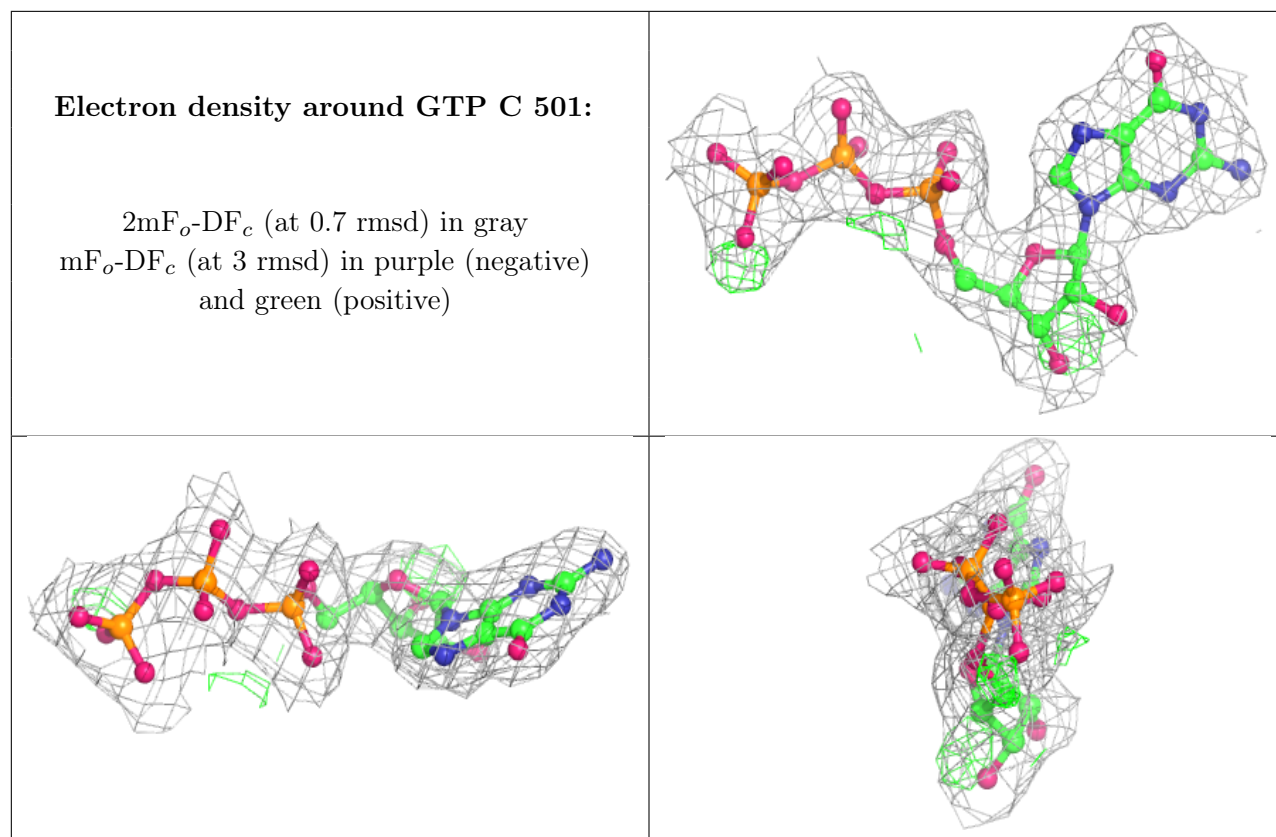
Electron density around GDP D 501:

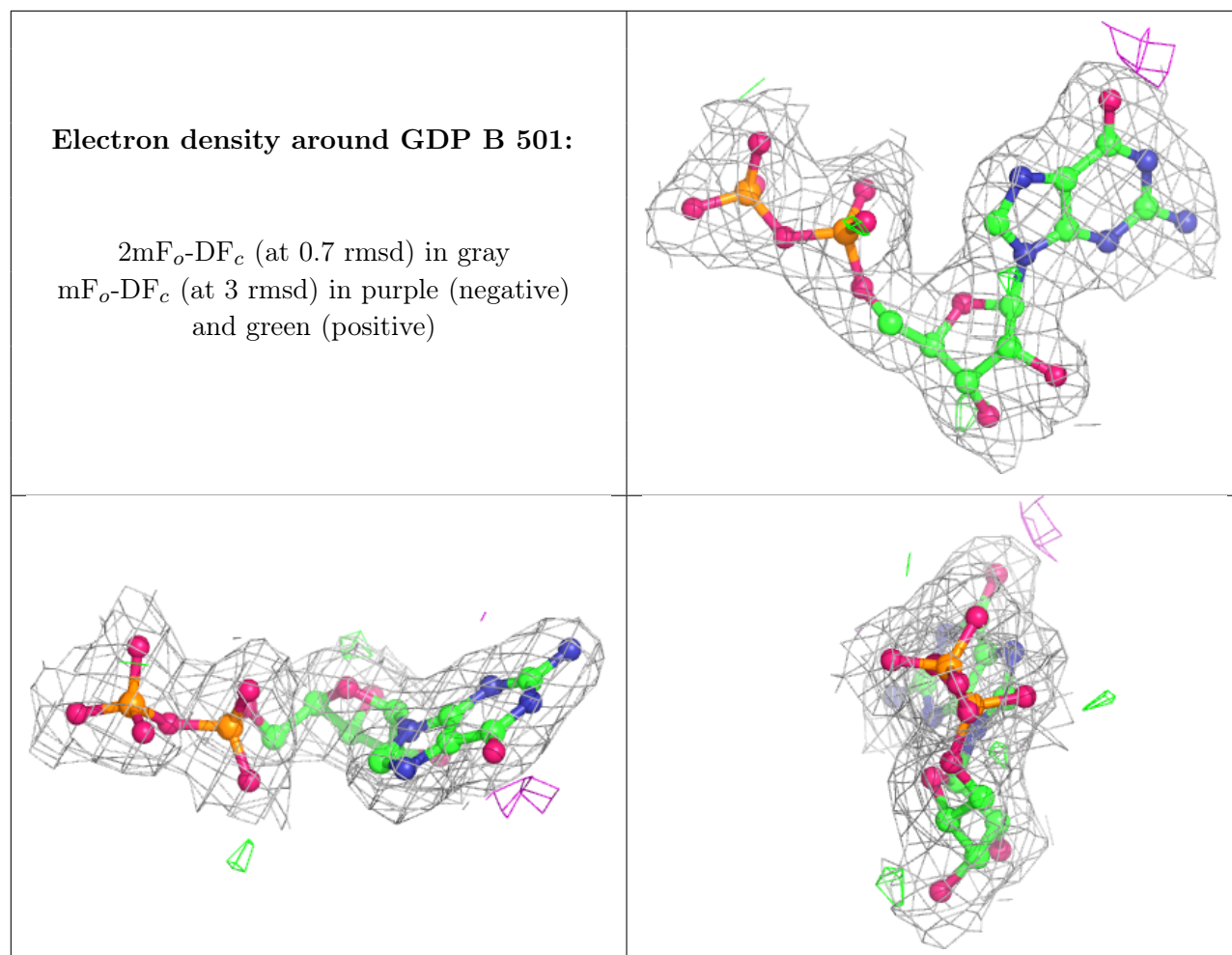
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**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)







6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.