



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:58 AM UTC

PDB ID : 9IMO / pdb_00009imo
Title : Crystal structure of Tubulin-RB3-TTL-Y12
Authors : Yan, W.; Yang, J.H.
Deposited on : 2024-07-04
Resolution : 2.75 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

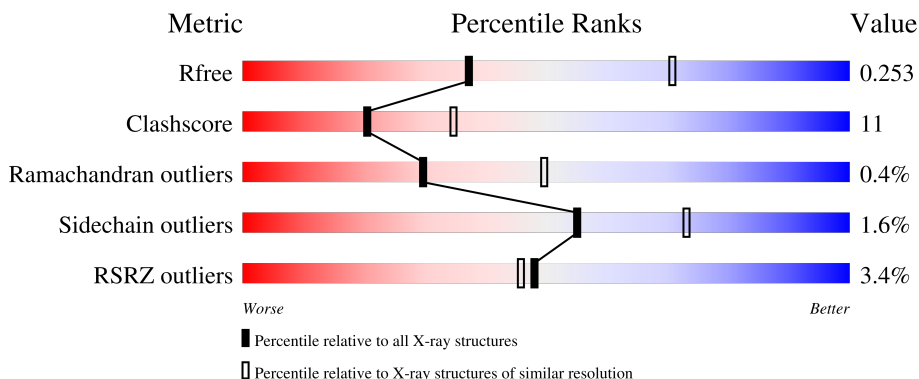
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



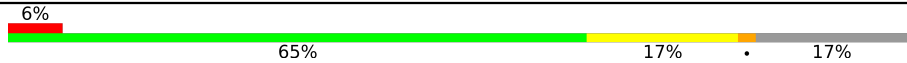
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	 2% 77% 20%
1	C	451	 2% 78% 19%
2	B	431	 2% 74% 23%
2	D	431	 3% 75% 21%
3	E	189	 5% 51% 12% 36%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>6% 65% 17% 17%</p>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 17121 atoms, of which 68 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	439	Total	C	N	O	S	0	6	0
			3409	2165	573	649	22			
1	C	440	Total	C	N	O	S	0	7	0
			3443	2185	577	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	422	Total	C	N	O	S	0	3	0
			3275	2066	551	634	24			
2	D	421	Total	C	N	O	S	0	2	0
			3224	2032	543	624	25			

- 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
			943	586	171	181	5			

- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	320	Total	C	N	O	S	0	3	0
			2478	1609	409	449	11			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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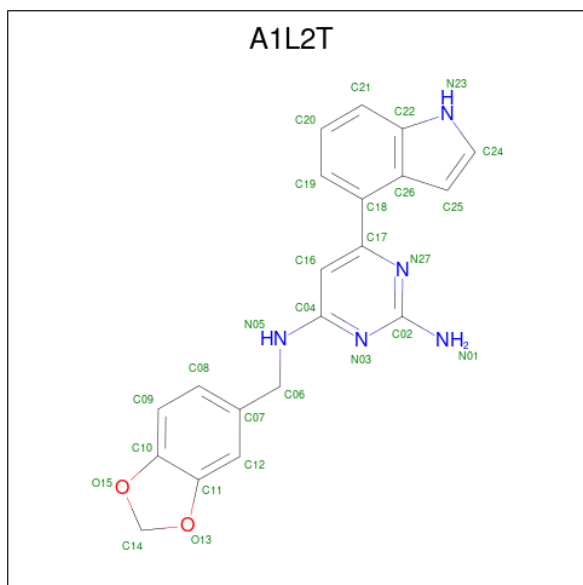
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

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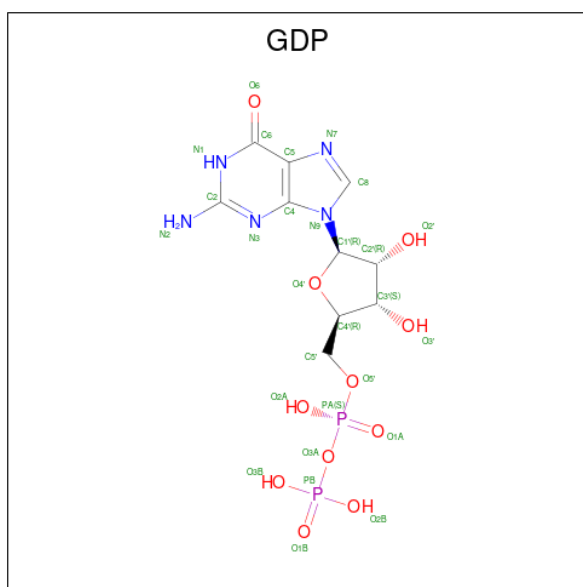
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is {N}4-(1,3-benzodioxol-5-ylmethyl)-6-(1 {H}-indol-4-yl)pyrimidine-2,4-diamine (CCD ID: A1L2T) (formula: C₂₀H₁₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



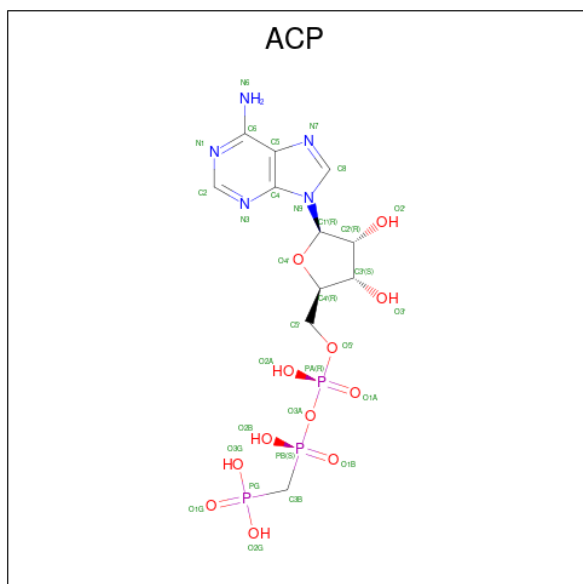
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H N O 44 20 17 5 2	0	0
8	B	1	Total C H N O 44 20 17 5 2	0	0
8	B	1	Total C H N O 44 20 17 5 2	0	0
8	D	1	Total C H N O 44 20 17 5 2	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

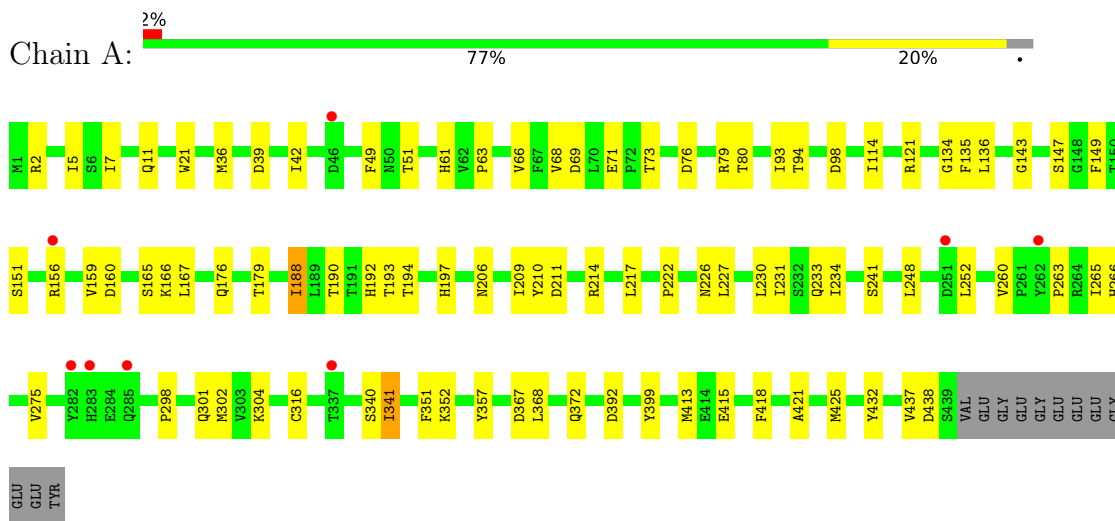
- Molecule 11 is water.

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

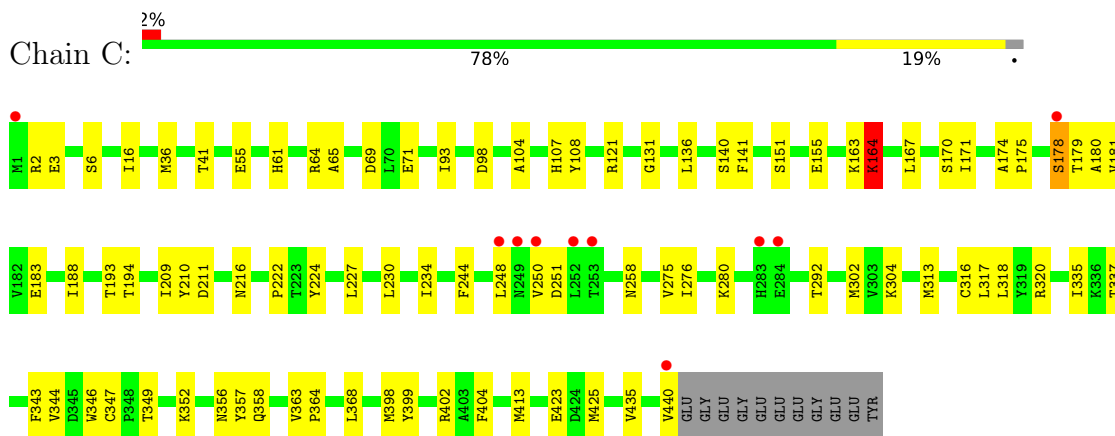
3 Residue-property plots

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.

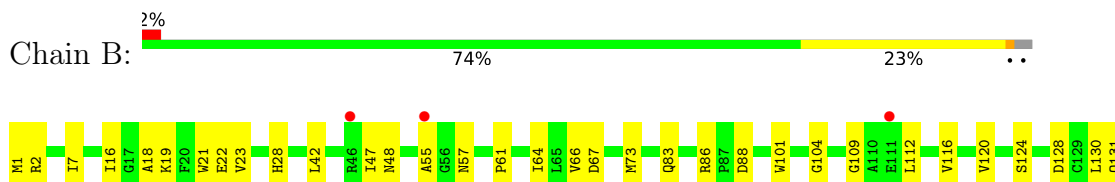
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



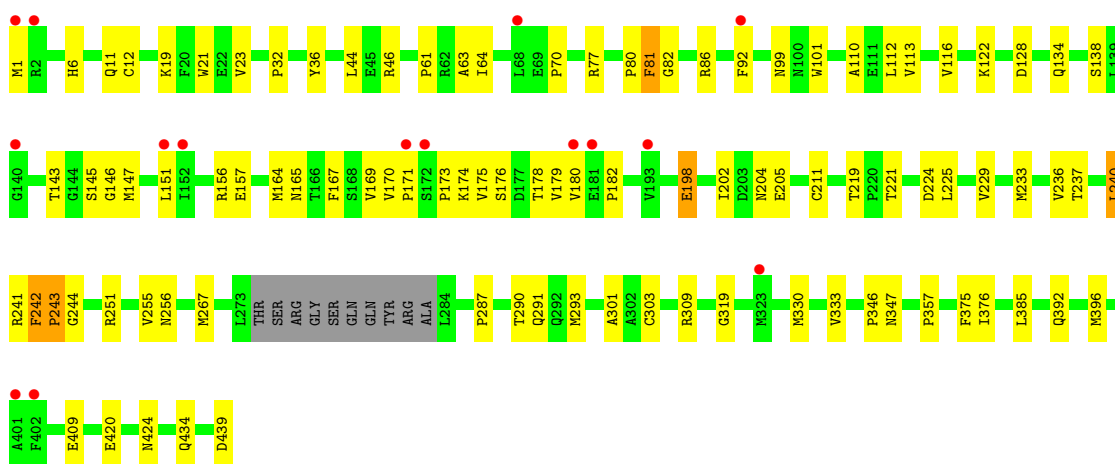
- Molecule 2: Tubulin beta chain





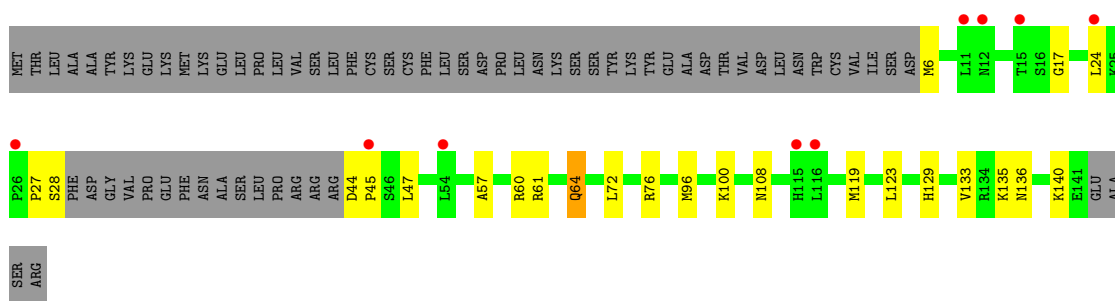
- Molecule 2: Tubulin beta chain

Chain D: 3% 75% 21%



- Molecule 3: Stathmin-4

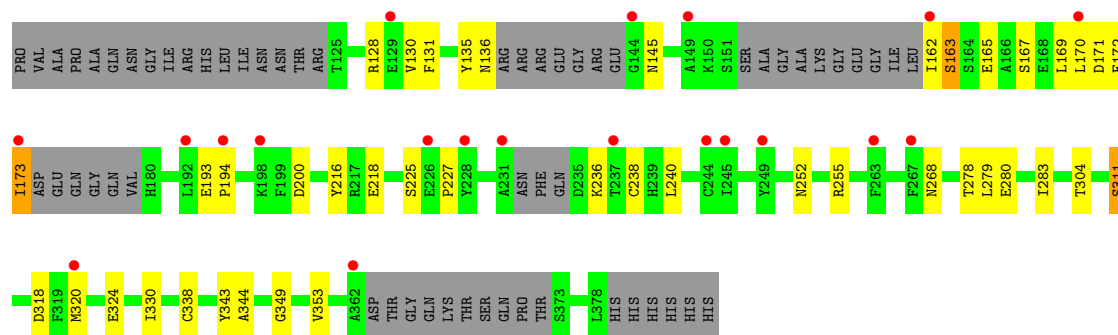
Chain E: 5% 51% 12% 36%



- Molecule 4: Tubulin-tyrosine ligase

Chain F: 6% 65% 17% 17%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.27Å 158.14Å 179.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.35 – 2.75 41.35 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.35-2.75) 99.8 (41.35-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.211 , 0.255 0.211 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.0	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	0.94	EDS
Total number of atoms	17121	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, A1L2T, MG, CA, ACP, GTP

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	0.24	0/3504	0.58	0/4767
1	C	0.27	0/3542	0.62	0/4814
2	B	0.29	0/3358	0.65	0/4561
2	D	0.25	0/3303	0.60	0/4496
3	E	0.32	0/951	0.66	0/1269
4	F	0.21	0/2543	0.59	0/3463
All	All	0.26	0/17201	0.61	0/23370

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	3409	0	3300	77	0
1	C	3443	0	3352	74	0
2	B	3275	0	3110	84	0
2	D	3224	0	3030	83	0
3	E	943	0	928	20	0
4	F	2478	0	2352	49	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	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	27	17	0	0	0
8	B	54	34	0	2	0
8	D	27	17	0	2	0
9	B	28	0	12	0	0
9	D	28	0	12	4	0
10	F	31	0	14	2	0
11	A	1	0	0	0	0
11	B	2	0	0	1	0
11	C	9	0	0	3	0
11	D	2	0	0	1	0
All	All	17053	68	16134	371	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 11.

All (371) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:HE3	1:A:39:ASP:HB2	1.17	1.11
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.30	1.06
4:F:81:ILE:HD13	4:F:87:LEU:HD13	1.38	1.03
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.43	0.99
2:D:101:TRP:HD1	2:D:145:SER:HG	1.14	0.96
2:B:16[B]:ILE:HD13	2:B:229:VAL:HG11	1.47	0.96
2:D:198:GLU:OE2	11:D:601:HOH:O	1.85	0.94
2:B:198:GLU:OE2	11:B:601:HOH:O	1.87	0.91
1:C:313:MET:HE1	1:C:435:VAL:CG2	2.03	0.89
1:A:11:GLN:OE1	2:B:247:ASN:ND2	2.10	0.84
2:D:101:TRP:CD1	2:D:145:SER:HG	1.98	0.82
1:C:178:SER:OG	1:C:224:TYR:OH	1.98	0.81
2:D:157:GLU:HG3	3:E:123:LEU:HD13	1.62	0.81
2:D:156:ARG:HE	3:E:119:MET:HE1	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ASP:HB3	2:B:307:HIS:ND1	1.95	0.80
2:D:46:ARG:HG3	2:D:243:PRO:HG2	1.63	0.80
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.17	0.80
2:B:179:VAL:HG13	1:C:258:ASN:OD1	1.82	0.80
2:D:80:PRO:O	2:D:81:PHE:HB2	1.80	0.79
2:B:165:ASN:OD1	2:B:198:GLU:HB2	1.82	0.79
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.64	0.78
2:B:86:ARG:NH1	2:B:88:ASP:HB2	1.98	0.78
2:B:157:GLU:HB2	3:E:72:LEU:HD13	1.66	0.77
1:C:398:MET:HE2	2:D:346:PRO:HD2	1.67	0.76
1:A:36:MET:HE1	1:A:49:PHE:CZ	2.21	0.75
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.67	0.75
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	1.86	0.74
1:A:36:MET:HE2	1:A:61:HIS:NE2	2.02	0.74
2:D:157:GLU:CG	3:E:123:LEU:HD13	2.18	0.74
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.89	0.73
1:A:234:ILE:HD13	1:A:302:MET:SD	2.28	0.72
2:B:296:ALA:H	2:B:306:ARG:HH12	1.35	0.72
1:A:156:ARG:O	1:A:159:VAL:HG22	1.91	0.71
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.73	0.71
1:A:36:MET:HE2	1:A:61:HIS:CD2	2.26	0.70
4:F:64:TYR:O	4:F:311:SER:OG	2.09	0.70
1:A:340:SER:C	1:A:341:ILE:HD12	2.17	0.69
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.19	0.69
2:D:165:ASN:OD1	2:D:198:GLU:HG3	1.92	0.69
4:F:320:MET:HG2	4:F:330:ILE:HG13	1.73	0.69
2:D:242:PHE:O	2:D:244:GLY:N	2.25	0.69
1:C:69:ASP:OD2	11:C:602:HOH:O	2.11	0.69
1:C:313:MET:HE1	1:C:435:VAL:HG21	1.75	0.68
2:D:267[A]:MET:HE2	2:D:303:CYS:HB2	1.76	0.68
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.76	0.68
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.77	0.67
2:D:242:PHE:N	2:D:243:PRO:HD2	2.09	0.67
2:B:66:VAL:C	2:B:73:MET:HE1	2.20	0.67
1:A:209[A]:ILE:HD11	1:A:302:MET:SD	2.34	0.67
4:F:3:THR:HG23	4:F:37:PHE:HA	1.76	0.67
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.59	0.67
1:C:2:ARG:HA	1:C:131:GLY:O	1.94	0.66
4:F:304:THR:HG21	4:F:311:SER:HB2	1.76	0.66
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.26	0.66
1:C:320:ARG:HA	1:C:356:ASN:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:CE	1:A:39:ASP:HB2	2.11	0.65
3:E:136:ASN:O	3:E:140:LYS:HG3	1.97	0.65
1:C:209:ILE:HD11	1:C:302:MET:SD	2.36	0.65
1:A:316:CYS:HB2	1:A:352:LYS:O	1.96	0.65
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.79	0.65
1:C:209:ILE:CG2	1:C:227:LEU:HD22	2.25	0.64
2:D:242:PHE:N	2:D:243:PRO:CD	2.60	0.64
4:F:268:ASN:OD1	4:F:278:THR:HG23	1.96	0.64
1:C:276:ILE:HD11	1:C:280:LYS:HG2	1.80	0.64
2:D:175:VAL:HG21	2:D:204:ASN:HB3	1.79	0.64
1:A:71:GLU:CD	1:A:73:THR:HG22	2.22	0.64
4:F:102:PRO:HB3	4:F:173:ILE:HB	1.80	0.63
2:B:66:VAL:CA	2:B:73:MET:HE1	2.27	0.63
1:A:71:GLU:OE1	1:A:73:THR:HG22	1.98	0.63
2:B:42:LEU:HD23	2:B:243:PRO:HG2	1.79	0.63
1:A:71:GLU:OE2	1:A:73:THR:HG22	1.99	0.63
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.31	0.63
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.34	0.62
2:B:1:MET:O	2:B:48:ASN:ND2	2.32	0.62
2:B:155:ILE:HG21	2:B:164:MET:CE	2.29	0.62
2:D:287:PRO:O	2:D:290:THR:HG22	1.99	0.62
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.30	0.62
1:A:341:ILE:HD12	1:A:341:ILE:N	2.15	0.62
2:B:301:ALA:O	2:B:303:CYS:N	2.33	0.62
2:D:420:GLU:O	2:D:424:ASN:ND2	2.31	0.62
2:D:11:GLN:N	9:D:503:GDP:O1B	2.24	0.61
4:F:91:CYS:O	4:F:92:THR:HG22	2.01	0.61
1:A:36:MET:HE3	1:A:39:ASP:CB	2.11	0.61
2:B:219:THR:HG22	2:B:219:THR:O	1.98	0.61
2:B:18:ALA:O	2:B:22[A]:GLU:HG3	2.01	0.61
1:C:398:MET:CE	2:D:346:PRO:HD2	2.30	0.61
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.31	0.60
2:B:236:VAL:HG13	2:B:376:ILE:HD11	1.84	0.60
1:C:313:MET:HE2	1:C:346:TRP:HZ2	1.67	0.60
4:F:324:GLU:O	4:F:324:GLU:HG3	2.02	0.59
4:F:2:TYR:O	4:F:27:TRP:HA	2.02	0.59
1:C:216:ASN:HB3	1:C:275:VAL:O	2.02	0.59
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.02	0.59
2:D:236:VAL:HG22	2:D:376:ILE:HD11	1.85	0.59
1:A:2:ARG:O	1:A:51[A]:THR:HG22	2.02	0.59
2:D:309:ARG:NH2	2:D:434:GLN:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:72:LEU:O	3:E:76:ARG:HG2	2.03	0.58
1:C:55:GLU:OE2	11:C:601:HOH:O	2.16	0.58
4:F:3:THR:HG23	4:F:38:ASN:H	1.68	0.58
2:D:143:THR:HB	9:D:503:GDP:O3B	2.04	0.58
4:F:278:THR:HG22	4:F:280:GLU:H	1.69	0.58
2:B:163:ILE:HA	2:B:197:ASP:OD1	2.04	0.58
4:F:193:GLU:CB	4:F:194:PRO:HD3	2.34	0.58
4:F:252:ASN:OD1	4:F:255:ARG:HD2	2.03	0.58
2:B:55:ALA:C	2:B:57:ASN:H	2.12	0.57
2:B:86:ARG:HH11	2:B:88:ASP:HB2	1.69	0.57
1:C:276:ILE:HG13	1:C:280:LYS:HD3	1.87	0.57
4:F:2:TYR:N	4:F:26:GLN:O	2.37	0.57
2:B:1:MET:CB	2:B:128:ASP:HB3	2.35	0.57
2:B:42:LEU:CD2	2:B:243:PRO:HG2	2.35	0.57
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.40	0.56
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.87	0.56
4:F:172:PHE:C	4:F:173:ILE:HD13	2.30	0.56
1:A:7:ILE:HG23	1:A:66:VAL:HG13	1.87	0.56
1:A:263:PRO:O	1:A:266:HIS:HD2	1.87	0.56
1:C:181:VAL:O	1:C:398:MET:HE1	2.06	0.56
1:A:134:GLY:HA3	1:A:165:SER:O	2.06	0.55
2:D:116:VAL:CG1	2:D:151:LEU:HD21	2.36	0.55
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.88	0.55
1:A:159:VAL:HG23	1:A:160:ASP:OD1	2.06	0.55
4:F:278:THR:HG22	4:F:279:LEU:N	2.22	0.55
1:C:180:ALA:HB1	2:D:256:ASN:HD21	1.72	0.55
2:D:1:MET:O	2:D:1:MET:HG2	2.07	0.55
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.55
3:E:47:LEU:HD23	3:E:47:LEU:O	2.06	0.55
2:D:167:PHE:CD1	2:D:233:MET:HE3	2.42	0.54
2:D:241:ARG:C	2:D:243:PRO:HD2	2.32	0.54
2:D:267[A]:MET:CE	2:D:303:CYS:HB2	2.36	0.54
2:D:287:PRO:HA	2:D:290:THR:HG22	1.89	0.54
2:B:2:ARG:HB3	2:B:131:GLN:NE2	2.22	0.54
2:B:272:PRO:HB3	2:B:284:LEU:HD22	1.90	0.54
2:D:180:VAL:HA	2:D:396:MET:HE1	1.89	0.54
2:D:169:VAL:HA	2:D:202:ILE:O	2.09	0.53
1:A:179:THR:HA	2:B:350:LYS:HD2	1.91	0.53
2:B:134:GLN:HA	2:B:165:ASN:O	2.08	0.53
1:A:241:SER:HB2	1:A:248:LEU:O	2.08	0.53
2:B:189:VAL:HB	2:B:423:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.39	0.53
2:D:134:GLN:HA	2:D:165:ASN:O	2.09	0.53
2:B:124:SER:HB2	2:B:130:LEU:HD22	1.90	0.53
2:B:155:ILE:HG21	2:B:164:MET:HE1	1.91	0.53
1:C:313:MET:HE1	1:C:435:VAL:CB	2.39	0.52
2:B:67:ASP:HB2	2:B:73:MET:HE3	1.92	0.52
1:C:230:LEU:O	1:C:234:ILE:HD12	2.10	0.52
2:D:164:MET:HE3	2:D:165:ASN:H	1.75	0.52
4:F:8:ASP:HB2	4:F:43:GLU:HA	1.92	0.52
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.35	0.52
4:F:169:LEU:O	4:F:172:PHE:HB3	2.09	0.52
2:B:7:ILE:O	2:B:135:LEU:HA	2.10	0.52
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.92	0.52
2:B:321:MET:HE2	2:B:371:MET:HE3	1.92	0.51
1:C:313:MET:CE	1:C:435:VAL:HB	2.40	0.51
2:D:77:ARG:O	2:D:82:GLY:HA3	2.09	0.51
4:F:21:LEU:O	4:F:24:THR:HG23	2.11	0.51
2:B:308:GLY:HA2	2:B:434:GLN:CD	2.35	0.51
2:D:174:LYS:NZ	2:D:205:GLU:OE2	2.43	0.51
2:B:66:VAL:C	2:B:73:MET:CE	2.83	0.51
2:D:165:ASN:CG	2:D:198:GLU:HG3	2.35	0.51
2:D:110:ALA:O	2:D:113:VAL:HG12	2.11	0.51
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.41	0.51
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.40	0.51
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.92	0.51
2:D:64:ILE:HD12	2:D:64:ILE:N	2.24	0.51
2:D:99:ASN:OD1	2:D:178:THR:HG21	2.11	0.51
10:F:402:ACP:O2G	10:F:402:ACP:O2B	2.30	0.50
1:A:42:ILE:HD12	1:A:42:ILE:O	2.11	0.50
1:A:413:MET:CE	1:A:418:PHE:CE1	2.94	0.50
2:D:385:LEU:HD23	2:D:385:LEU:C	2.36	0.50
2:D:116:VAL:HG11	2:D:151:LEU:HD21	1.93	0.50
3:E:60:ARG:O	3:E:64:GLN:HG2	2.11	0.50
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.11	0.50
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.92	0.50
1:C:151[B]:SER:HB3	1:C:193:THR:CG2	2.42	0.50
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	1.93	0.50
2:B:145:SER:HG	2:B:188:SER:HG	1.59	0.50
2:D:170:VAL:HG13	2:D:171:PRO:HD2	1.94	0.50
3:E:129:HIS:O	3:E:133:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.47	0.50
1:A:206:ASN:HA	1:A:209[B]:ILE:HG12	1.94	0.49
2:D:86:ARG:HH21	2:D:122:LYS:HE2	1.77	0.49
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.12	0.49
2:B:135:LEU:HD23	2:B:152:ILE:HD11	1.94	0.49
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.43	0.49
2:B:272:PRO:HB3	2:B:284:LEU:CD2	2.41	0.49
3:E:96:MET:O	3:E:100:LYS:HG2	2.13	0.49
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.13	0.49
2:B:86:ARG:HH12	2:B:88:ASP:HB2	1.77	0.49
2:B:321:MET:CE	2:B:371:MET:HE3	2.43	0.49
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.47	0.49
2:D:293:MET:CG	2:D:375:PHE:HB2	2.42	0.49
2:B:386:PHE:CD1	2:B:423:MET:HE2	2.48	0.49
2:D:164:MET:HE3	2:D:165:ASN:N	2.27	0.49
4:F:73:ARG:HE	4:F:75:ALA:HB3	1.78	0.49
2:B:256:ASN:HD22	8:B:503:A1L2T:C14	2.26	0.48
2:B:83:GLN:CD	2:B:83:GLN:H	2.21	0.48
1:C:399:TYR:O	1:C:402:ARG:NH2	2.45	0.48
1:C:423:GLU:OE1	1:C:423:GLU:HA	2.12	0.48
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.94	0.48
1:C:174:ALA:O	1:C:179:THR:CG2	2.61	0.48
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.43	0.48
2:B:200:TYR:CE1	2:B:266:PHE:HD2	2.31	0.48
2:D:179:VAL:HG22	2:D:396:MET:HE3	1.96	0.48
1:C:104:ALA:HB2	1:C:413:MET:SD	2.54	0.48
2:B:289:LEU:HD12	2:B:371:MET:HE2	1.94	0.48
2:B:170:VAL:HG11	2:B:385:LEU:HD21	1.95	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.49	0.48
4:F:320:MET:HG2	4:F:330:ILE:CG1	2.41	0.47
2:B:170:VAL:HG13	2:B:171:PRO:HD2	1.96	0.47
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.50	0.47
2:B:201:CYS:O	2:B:301:ALA:HB2	2.14	0.47
2:B:293:MET:CE	2:B:373:ALA:HB1	2.45	0.47
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.97	0.47
1:A:7:ILE:HG12	1:A:66:VAL:CG1	2.44	0.47
1:A:413:MET:HE2	1:A:418:PHE:CE1	2.50	0.47
2:D:240:LEU:HD12	2:D:240:LEU:HA	1.70	0.47
4:F:135:TYR:O	4:F:145:ASN:ND2	2.48	0.47
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.47
2:B:64:ILE:CD1	2:B:120:VAL:HG22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:HB3	3:E:108:ASN:ND2	2.31	0.46
2:D:46:ARG:HG3	2:D:243:PRO:CG	2.41	0.46
4:F:73:ARG:HB3	4:F:76[B]:SER:OG	2.14	0.46
4:F:227:PRO:O	4:F:238:CYS:HB2	2.15	0.46
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.46	0.46
2:D:409:GLU:OE2	2:D:409:GLU:HA	2.15	0.46
1:A:188:ILE:HD11	1:A:392:ASP:OD1	2.15	0.46
1:C:16:ILE:HD13	1:C:171:ILE:HD11	1.97	0.46
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.98	0.46
1:A:437:VAL:HG12	1:A:438:ASP:N	2.30	0.46
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.46
2:B:112:LEU:HD23	2:B:147:MET:HE1	1.96	0.46
2:B:19:LYS:O	2:B:23:VAL:HG23	2.15	0.46
2:B:293:MET:HE3	2:B:373:ALA:HB1	1.96	0.46
2:D:63:ALA:C	2:D:64:ILE:HD12	2.40	0.46
4:F:2:TYR:HB2	4:F:27:TRP:CE2	2.51	0.46
4:F:98:TYR:CG	4:F:131:PHE:HB2	2.51	0.46
1:A:5:ILE:O	1:A:135:PHE:HA	2.16	0.46
1:C:313:MET:HE1	1:C:435:VAL:HB	1.96	0.46
4:F:83:THR:O	4:F:83:THR:HG22	2.16	0.46
1:A:351:PHE:CE1	3:E:24:LEU:HD11	2.46	0.46
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.46
1:C:175:PRO:HB3	2:D:347:ASN:CG	2.41	0.46
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.97	0.46
2:D:237:THR:HA	8:D:502:A1L2T:C24	2.46	0.46
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.98	0.45
1:C:140:SER:HA	1:C:171:ILE:HB	1.98	0.45
2:B:393:PHE:CE1	2:B:420:GLU:HB2	2.51	0.45
1:A:341:ILE:N	1:A:341:ILE:CD1	2.78	0.45
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.51	0.45
1:C:313:MET:HE1	1:C:435:VAL:HG23	1.92	0.45
2:D:211:CYS:SG	2:D:225:LEU:HD23	2.56	0.45
2:D:251:ARG:O	2:D:255:VAL:HG23	2.16	0.45
4:F:32:LYS:HB2	4:F:32:LYS:NZ	2.31	0.45
1:A:7:ILE:HG12	1:A:66:VAL:HG12	1.99	0.45
2:B:189:VAL:HG11	2:B:423:MET:CE	2.46	0.45
1:A:210:TYR:CE2	1:A:222:PRO:HD2	2.52	0.45
1:C:230:LEU:O	1:C:234:ILE:CD1	2.64	0.45
4:F:14:TYR:HA	4:F:17:VAL:HB	1.98	0.44
2:B:189:VAL:CB	2:B:423:MET:HE3	2.47	0.44
2:B:385:LEU:C	2:B:385:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:LEU:HD12	1:C:318:LEU:N	2.33	0.44
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.18	0.44
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.98	0.44
3:E:44:ASP:N	3:E:45:PRO:HD2	2.33	0.44
2:B:66:VAL:N	2:B:73:MET:HE1	2.33	0.44
2:D:167:PHE:CE1	2:D:233:MET:HE3	2.53	0.44
4:F:3:THR:OG1	4:F:30:LEU:HD11	2.18	0.44
2:B:189:VAL:CG1	2:B:423:MET:HE3	2.48	0.44
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	2.00	0.44
1:A:69:ASP:O	1:A:94:THR:HA	2.17	0.44
1:A:298:PRO:HA	1:A:301:GLN:CD	2.43	0.44
8:B:504:A1L2T:C08	3:E:64:GLN:HB2	2.47	0.44
1:C:2:ARG:HA	1:C:2:ARG:HD2	1.72	0.44
2:D:112:LEU:HD23	2:D:147:MET:HE1	1.99	0.44
2:D:165:ASN:HD22	8:D:502:A1L2T:C20	2.31	0.44
2:D:175:VAL:HG21	2:D:204:ASN:CB	2.48	0.44
2:D:330:MET:O	2:D:333:VAL:HG12	2.18	0.44
2:D:36:TYR:CD1	2:D:44:LEU:HD21	2.53	0.43
2:B:101:TRP:HB2	2:B:184:ASN:OD1	2.18	0.43
2:B:289:LEU:CD1	2:B:371:MET:HE2	2.48	0.43
1:A:151:SER:HB2	1:A:193:THR:HG22	1.98	0.43
2:B:347:ASN:O	2:B:350:LYS:HE2	2.18	0.43
1:C:244:PHE:CZ	1:C:358[A]:GLN:HG2	2.54	0.43
4:F:173:ILE:HD13	4:F:173:ILE:N	2.34	0.43
1:C:313:MET:CE	1:C:435:VAL:CG2	2.87	0.43
1:C:337:THR:O	1:C:337:THR:HG22	2.18	0.43
1:A:263:PRO:O	1:A:266:HIS:CD2	2.69	0.43
1:A:265:ILE:O	1:A:265:ILE:HG22	2.18	0.43
1:C:175:PRO:HB3	2:D:347:ASN:OD1	2.18	0.43
2:D:221:THR:HG22	2:D:224:ASP:OD2	2.18	0.43
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.01	0.43
2:D:267[A]:MET:HG3	2:D:301:ALA:HB3	2.00	0.43
1:C:244:PHE:CE1	1:C:358[B]:GLN:HG2	2.53	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.54	0.43
2:D:70:PRO:HB3	2:D:92:PHE:CD2	2.54	0.43
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.01	0.43
1:C:41:THR:OG1	11:C:601:HOH:O	2.08	0.43
2:D:173:PRO:HA	2:D:176:SER:O	2.19	0.43
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.45	0.43
2:B:387:LYS:O	2:B:388:ARG:C	2.62	0.43
2:B:104:GLY:O	2:B:109:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:44:ASP:N	3:E:45:PRO:CD	2.82	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.53	0.42
2:B:116:VAL:CG1	2:B:151:LEU:HD21	2.49	0.42
1:C:181:VAL:HG21	1:C:404:PHE:CZ	2.54	0.42
4:F:5:VAL:HG12	4:F:30:LEU:HB2	2.00	0.42
4:F:278:THR:CG2	4:F:279:LEU:N	2.80	0.42
2:B:172:SER:CB	2:B:205:GLU:HB2	2.50	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.42
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.99	0.42
4:F:343:TYR:O	4:F:344:ALA:C	2.61	0.42
2:B:116:VAL:HG11	2:B:151:LEU:HD21	2.02	0.42
1:C:6:SER:O	1:C:65:ALA:HA	2.19	0.42
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	2.02	0.42
1:A:93:ILE:HG22	1:A:114:ILE:HD11	2.02	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
2:D:182:PRO:HG2	2:D:392:GLN:HB3	2.01	0.42
4:F:167:SER:O	4:F:171:ASP:HB2	2.19	0.42
1:C:163:LYS:O	1:C:164:LYS:C	2.62	0.42
1:A:156:ARG:HA	1:A:159:VAL:HG22	2.02	0.42
2:D:86:ARG:NH2	2:D:122:LYS:HE2	2.34	0.42
2:B:189:VAL:HG11	2:B:423:MET:HE3	2.00	0.42
1:C:174:ALA:O	1:C:179:THR:HG21	2.19	0.42
4:F:200:ASP:OD1	4:F:200:ASP:C	2.63	0.42
1:A:7:ILE:HG23	1:A:66:VAL:CG1	2.50	0.42
2:B:202:ILE:HD13	2:B:229:VAL:HG13	2.01	0.42
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.42
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.55	0.42
2:D:143:THR:N	9:D:503:GDP:O3B	2.49	0.42
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.68	0.41
2:B:55:ALA:O	2:B:57:ASN:N	2.53	0.41
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.01	0.41
3:E:135:LYS:O	3:E:136:ASN:C	2.62	0.41
1:A:176:GLN:HG3	4:F:56:PRO:CG	2.49	0.41
2:B:237:THR:O	2:B:241:ARG:HG3	2.20	0.41
2:D:12:CYS:HB2	9:D:503:GDP:C8	2.54	0.41
1:A:135:PHE:C	1:A:136[B]:LEU:HD12	2.44	0.41
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.55	0.41
2:B:272:PRO:HD2	2:B:369:LEU:HD13	2.01	0.41
3:E:57:ALA:HA	3:E:60:ARG:HH21	1.84	0.41
1:C:317:LEU:C	1:C:318:LEU:HD12	2.45	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:ARG:O	2:B:255:VAL:HG23	2.21	0.41
2:D:12:CYS:SG	2:D:138:SER:HB3	2.60	0.41
2:D:256:ASN:HD22	2:D:256:ASN:HA	1.65	0.41
2:B:28:HIS:HB3	2:B:47:ILE:HD13	2.03	0.41
2:B:398:ARG:HG3	2:B:399:ARG:HG2	2.02	0.41
1:C:316:CYS:HA	1:C:352:LYS:O	2.21	0.41
1:C:363:VAL:CG1	1:C:364:PRO:HD2	2.49	0.41
1:C:343:PHE:HB2	1:C:349:THR:HG22	2.03	0.41
1:A:93:ILE:HD11	1:A:121:ARG:HG3	2.03	0.41
1:C:107:HIS:HE1	1:C:155:GLU:OE1	2.04	0.41
1:A:399:TYR:OH	1:A:415:GLU:HG2	2.20	0.40
4:F:81:ILE:HD13	4:F:87:LEU:CD1	2.27	0.40
4:F:338:CYS:O	4:F:343:TYR:HE1	2.05	0.40
1:A:194:THR:O	1:A:194:THR:HG22	2.21	0.40
2:B:19:LYS:HA	2:B:22[B]:GLU:HG2	2.04	0.40
2:B:155:ILE:CG2	2:B:164:MET:CE	2.98	0.40
2:B:301:ALA:O	2:B:302:ALA:C	2.64	0.40
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.03	0.40
1:C:174:ALA:O	1:C:179:THR:HG23	2.22	0.40
2:D:290:THR:HG23	2:D:291:GLN:N	2.37	0.40
4:F:73:ARG:HB3	4:F:76[A]:SER:OG	2.21	0.40
2:B:156:ARG:HD3	2:B:156:ARG:HA	1.72	0.40
2:B:206:ALA:HB2	2:B:302:ALA:H	1.86	0.40
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.40
2:D:1:MET:HA	2:D:128:ASP:HB3	2.04	0.40
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.36	0.40
2:D:287:PRO:C	2:D:290:THR:HG22	2.46	0.40
4:F:318:ASP:OD2	10:F:402:ACP:O1G	2.40	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	443/451 (98%)	433 (98%)	10 (2%)	0	100	100
1	C	445/451 (99%)	434 (98%)	9 (2%)	2 (0%)	30	50
2	B	421/431 (98%)	410 (97%)	10 (2%)	1 (0%)	43	64
2	D	419/431 (97%)	406 (97%)	10 (2%)	3 (1%)	18	34
3	E	117/189 (62%)	113 (97%)	3 (3%)	1 (1%)	14	28
4	F	309/384 (80%)	287 (93%)	20 (6%)	2 (1%)	21	38
All	All	2154/2337 (92%)	2083 (97%)	62 (3%)	9 (0%)	30	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	ALA
2	D	243	PRO
3	E	27	PRO
4	F	92	THR
1	C	178	SER
4	F	91	CYS
1	C	164	LYS
2	D	81	PHE
2	D	242	PHE

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	363/379 (96%)	360 (99%)	3 (1%)	73	84
1	C	372/379 (98%)	367 (99%)	5 (1%)	61	76
2	B	352/370 (95%)	348 (99%)	4 (1%)	65	79
2	D	342/370 (92%)	339 (99%)	3 (1%)	70	82
3	E	95/171 (56%)	92 (97%)	3 (3%)	34	58
4	F	256/342 (75%)	245 (96%)	11 (4%)	26	47
All	All	1780/2011 (88%)	1751 (98%)	29 (2%)	55	73

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

Mol	Chain	Res	Type
1	A	188	ILE
1	A	214	ARG
1	A	341	ILE
2	B	156	ARG
2	B	219	THR
2	B	225	LEU
2	B	240	LEU
1	C	164	LYS
1	C	251	ASP
1	C	347	CYS
1	C	368	LEU
1	C	440	VAL
2	D	198	GLU
2	D	240	LEU
2	D	439	ASP
3	E	28	SER
3	E	61	ARG
3	E	64	GLN
4	F	12	SER
4	F	32	LYS
4	F	130	VAL
4	F	136	ASN
4	F	162	ILE
4	F	163	SER
4	F	165	GLU
4	F	170	LEU
4	F	173	ILE
4	F	225	SER
4	F	311	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	285	GLN
1	A	300	ASN
1	A	301	GLN
1	A	309	HIS
1	A	393	HIS
2	B	329	GLN
2	B	335	ASN

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Mol	Chain	Res	Type
1	C	393	HIS
2	D	329	GLN
4	F	333	ASN
4	F	348	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 8 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$
9	GDP	B	505	6	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)
8	A1L2T	A	504	-	31,31,31	1.35	5 (16%)	42,44,44	1.32	4 (9%)
9	GDP	D	503	6	29,30,30	1.22	3 (10%)	45,47,47	1.81	5 (11%)
8	A1L2T	B	504	-	31,31,31	1.57	7 (22%)	42,44,44	1.79	9 (21%)
8	A1L2T	D	502	-	31,31,31	1.75	6 (19%)	42,44,44	1.77	9 (21%)
10	ACP	F	402	-	31,33,33	1.82	9 (29%)	47,52,52	1.77	9 (19%)
5	GTP	A	501	6	33,34,34	1.14	4 (12%)	50,54,54	1.56	10 (20%)
5	GTP	C	501	6	33,34,34	1.03	3 (9%)	50,54,54	1.59	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	A1L2T	B	503	-	31,31,31	1.66	5 (16%)	42,44,44	1.88	10 (23%)

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
9	GDP	B	505	6	-	3/16/32/32	0/3/3/3
8	A1L2T	A	504	-	-	2/9/15/15	0/5/5/5
9	GDP	D	503	6	-	4/16/32/32	0/3/3/3
8	A1L2T	B	504	-	-	1/9/15/15	0/5/5/5
8	A1L2T	D	502	-	-	2/9/15/15	0/5/5/5
10	ACP	F	402	-	-	5/19/38/38	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
8	A1L2T	B	503	-	-	2/9/15/15	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	A1L2T	C04-N05	5.66	1.44	1.36
8	B	503	A1L2T	C04-N05	5.23	1.44	1.36
10	F	402	ACP	C5-C4	4.90	1.47	1.39
8	B	504	A1L2T	C26-C22	4.19	1.45	1.41
10	F	402	ACP	PB-O3A	3.81	1.62	1.58
8	B	504	A1L2T	C04-N05	3.68	1.41	1.36
9	D	503	GDP	C5-C4	3.40	1.48	1.38
10	F	402	ACP	PG-O3G	3.11	1.61	1.55
5	A	501	GTP	PA-O3A	3.02	1.62	1.59
10	F	402	ACP	PA-O3A	2.92	1.62	1.59
9	B	505	GDP	C5-C4	2.89	1.46	1.38
10	F	402	ACP	PG-O2G	2.87	1.61	1.55
8	B	503	A1L2T	C02-N01	2.82	1.39	1.33
10	F	402	ACP	C5-C6	2.79	1.48	1.41
8	B	504	A1L2T	C16-C04	2.76	1.46	1.39
8	D	502	A1L2T	C02-N03	2.68	1.40	1.35
8	A	504	A1L2T	C02-N03	2.66	1.40	1.35
5	C	501	GTP	PB-O3B	2.64	1.62	1.59
8	D	502	A1L2T	C02-N01	2.62	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	A1L2T	C16-C04	2.59	1.46	1.39
8	B	503	A1L2T	C26-C22	2.50	1.44	1.41
9	D	503	GDP	C6-N1	-2.48	1.34	1.38
8	D	502	A1L2T	C04-N03	2.47	1.39	1.34
5	A	501	GTP	PB-O3B	2.45	1.62	1.59
10	F	402	ACP	C8-N7	2.43	1.36	1.31
8	A	504	A1L2T	C04-N05	2.40	1.39	1.36
8	A	504	A1L2T	C02-N01	2.33	1.38	1.33
5	A	501	GTP	PB-O3A	2.32	1.62	1.59
8	B	503	A1L2T	C02-N03	2.27	1.39	1.35
8	D	502	A1L2T	C26-C22	2.27	1.43	1.41
10	F	402	ACP	PB-O2B	2.24	1.61	1.56
8	B	504	A1L2T	C02-N27	2.24	1.39	1.35
9	B	505	GDP	C6-N1	-2.22	1.34	1.38
8	A	504	A1L2T	C12-C07	2.21	1.43	1.39
8	A	504	A1L2T	C02-N27	2.20	1.39	1.35
9	D	503	GDP	C5-N7	-2.19	1.34	1.39
5	C	501	GTP	PA-O3A	2.16	1.61	1.59
8	B	504	A1L2T	C16-C17	2.14	1.43	1.39
10	F	402	ACP	C5-N7	-2.10	1.35	1.39
5	A	501	GTP	C2-N3	2.07	1.38	1.33
8	B	503	A1L2T	C06-N05	2.04	1.51	1.45
8	B	504	A1L2T	C24-C25	2.02	1.39	1.36
8	B	504	A1L2T	C09-C08	2.02	1.42	1.38
9	B	505	GDP	C5-N7	-2.01	1.35	1.39
5	C	501	GTP	C2-N3	2.01	1.38	1.33

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	GDP	C5-C4-N3	-6.53	118.00	128.39
10	F	402	ACP	C5-C4-N3	-6.12	118.30	126.72
8	B	503	A1L2T	C26-C18-C17	5.97	128.04	123.02
8	B	504	A1L2T	C26-C18-C17	5.76	127.86	123.02
9	B	505	GDP	C5-C4-N3	-5.66	119.38	128.39
9	B	505	GDP	C2-N3-C4	5.06	121.02	112.30
8	D	502	A1L2T	C26-C18-C17	5.01	127.23	123.02
9	D	503	GDP	C2-N3-C4	5.00	120.91	112.30
9	D	503	GDP	N9-C4-N3	4.75	135.45	125.95
10	F	402	ACP	N3-C4-N9	4.74	135.24	127.17
5	A	501	GTP	C5-C4-N3	-4.74	120.85	128.39
5	C	501	GTP	C5-C4-N3	-4.60	121.06	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	4.46	119.98	112.30
5	A	501	GTP	C2-N3-C4	4.39	119.86	112.30
9	B	505	GDP	N9-C4-N3	4.17	134.28	125.95
8	B	503	A1L2T	C06-N05-C04	4.06	131.13	123.04
8	D	502	A1L2T	C06-N05-C04	4.06	131.13	123.04
8	B	504	A1L2T	C06-N05-C04	4.02	131.04	123.04
10	F	402	ACP	C2-N3-C4	3.75	120.98	111.83
9	B	505	GDP	C6-C5-N7	3.63	136.90	130.29
10	F	402	ACP	C4-C5-N7	-3.58	106.49	110.58
8	B	503	A1L2T	C26-C22-N23	3.47	109.07	107.09
8	B	503	A1L2T	C17-N27-C02	-3.46	114.30	116.35
8	B	504	A1L2T	C26-C22-N23	3.28	108.96	107.09
8	A	504	A1L2T	C17-N27-C02	-3.24	114.44	116.35
8	D	502	A1L2T	C16-C17-C18	3.15	127.93	121.98
8	D	502	A1L2T	C26-C22-N23	3.13	108.88	107.09
10	F	402	ACP	N3-C2-N1	-3.11	123.88	128.58
5	C	501	GTP	N9-C8-N7	-3.09	107.66	113.40
9	D	503	GDP	C6-C5-N7	3.04	135.83	130.29
8	D	502	A1L2T	C18-C17-N27	-2.97	109.65	116.69
5	A	501	GTP	N9-C4-N3	2.89	131.73	125.95
5	C	501	GTP	N9-C4-N3	2.87	131.69	125.95
5	A	501	GTP	N9-C8-N7	-2.83	108.15	113.40
5	C	501	GTP	C8-N7-C5	2.80	109.25	104.26
5	A	501	GTP	C8-N7-C5	2.76	109.18	104.26
9	D	503	GDP	C4-C5-N7	-2.68	106.42	110.67
5	C	501	GTP	C2-N1-C6	-2.66	120.29	125.11
9	B	505	GDP	C4-C5-N7	-2.64	106.49	110.67
8	B	503	A1L2T	C07-C06-N05	2.61	120.86	113.60
5	A	501	GTP	C2-N1-C6	-2.57	120.46	125.11
8	B	503	A1L2T	C09-C08-C07	2.56	124.36	121.00
10	F	402	ACP	C5-N7-C8	2.53	107.42	103.45
8	D	502	A1L2T	C09-C08-C07	2.50	124.28	121.00
8	B	503	A1L2T	C22-C26-C25	-2.49	105.21	107.02
8	B	504	A1L2T	C22-C26-C25	-2.45	105.24	107.02
5	C	501	GTP	C5-C6-N1	2.43	119.45	113.25
8	B	504	A1L2T	N27-C02-N03	2.42	129.19	125.48
8	A	504	A1L2T	C09-C08-C07	2.39	124.13	121.00
5	A	501	GTP	C5-C6-N1	2.37	119.29	113.25
5	C	501	GTP	O2B-PB-O3A	2.37	113.67	107.27
8	D	502	A1L2T	C22-C26-C25	-2.34	105.32	107.02
8	B	504	A1L2T	C16-C04-N05	2.30	124.52	120.79
8	A	504	A1L2T	C26-C22-N23	2.30	108.40	107.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	402	ACP	PB-O3A-PA	-2.25	125.02	132.37
10	F	402	ACP	C4-N9-C8	2.24	108.09	105.74
5	C	501	GTP	O6-C6-C5	-2.23	120.65	126.53
9	B	505	GDP	O6-C6-C5	-2.21	120.69	126.53
8	B	503	A1L2T	C18-C17-N27	-2.21	111.47	116.69
8	B	504	A1L2T	C16-C17-C18	2.18	126.10	121.98
10	F	402	ACP	O3G-PG-C3B	2.17	111.67	106.40
8	D	502	A1L2T	C07-C06-N05	2.17	119.62	113.60
5	C	501	GTP	O2A-PA-O3A	2.17	113.13	107.27
8	B	504	A1L2T	C17-N27-C02	-2.16	115.07	116.35
8	B	503	A1L2T	C16-C17-C18	2.11	125.97	121.98
5	A	501	GTP	C4-C5-N7	-2.10	107.34	110.67
9	B	505	GDP	O2A-PA-O3A	2.10	112.94	107.27
5	A	501	GTP	O6-C6-C5	-2.09	121.02	126.53
5	A	501	GTP	O2B-PB-O3A	2.08	112.88	107.27
8	B	504	A1L2T	C19-C18-C26	-2.05	116.08	118.61
8	A	504	A1L2T	N27-C02-N03	2.04	128.61	125.48
8	D	502	A1L2T	N27-C02-N03	2.02	128.57	125.48
8	B	503	A1L2T	N27-C02-N03	2.01	128.56	125.48

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	503	A1L2T	C16-C04-N05-C06
8	B	503	A1L2T	N03-C04-N05-C06
8	D	502	A1L2T	C16-C04-N05-C06
8	D	502	A1L2T	N03-C04-N05-C06
9	B	505	GDP	C5'-O5'-PA-O3A
9	B	505	GDP	C5'-O5'-PA-O1A
9	B	505	GDP	C5'-O5'-PA-O2A
9	D	503	GDP	PA-O3A-PB-O2B
9	D	503	GDP	C5'-O5'-PA-O3A
9	D	503	GDP	C5'-O5'-PA-O1A
9	D	503	GDP	C5'-O5'-PA-O2A
10	F	402	ACP	PB-C3B-PG-O1G

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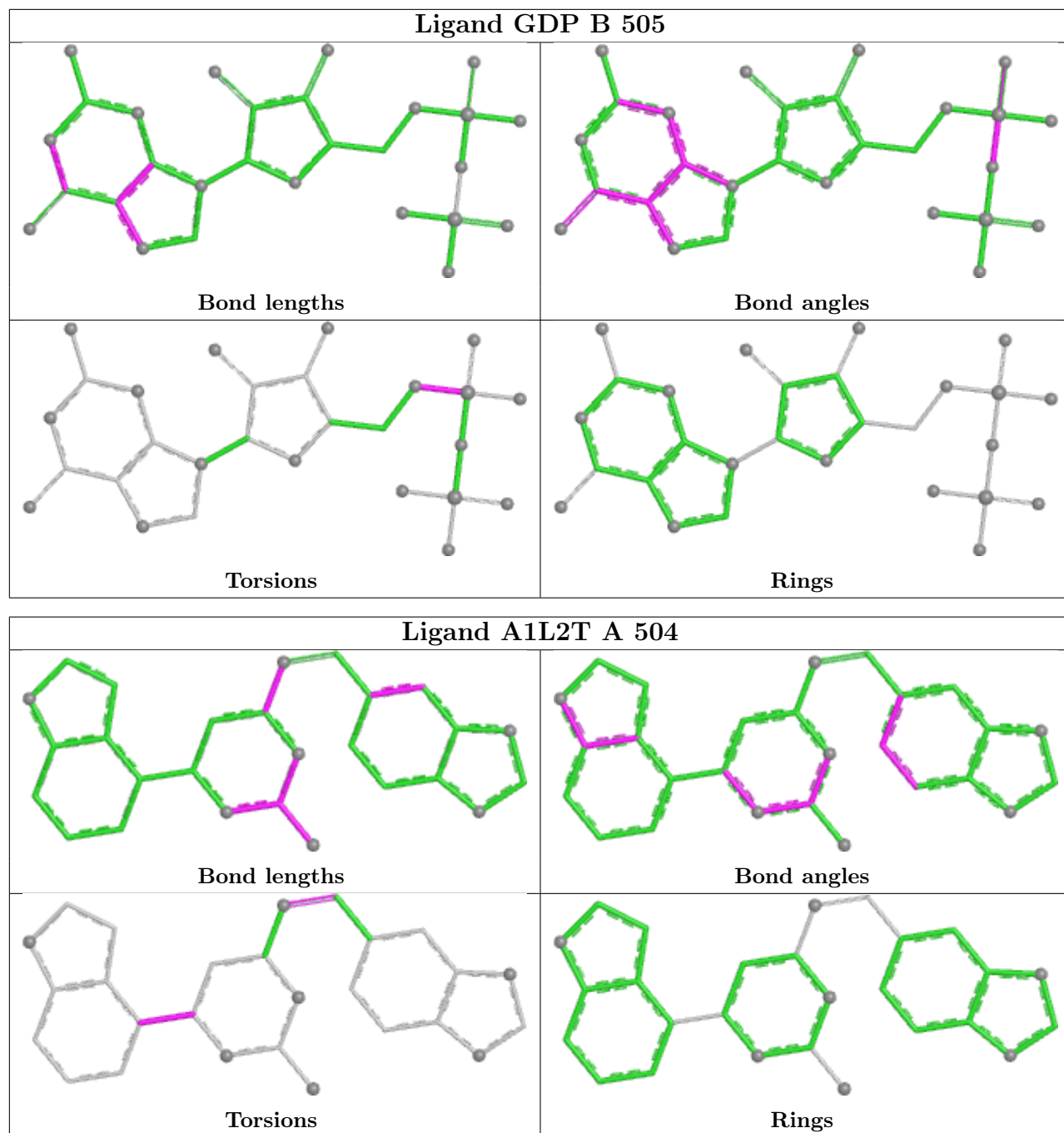
Mol	Chain	Res	Type	Atoms
10	F	402	ACP	PG-C3B-PB-O1B
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
10	F	402	ACP	PB-C3B-PG-O2G
10	F	402	ACP	PB-C3B-PG-O3G
10	F	402	ACP	PG-C3B-PB-O2B
8	A	504	A1L2T	C16-C17-C18-C26
8	A	504	A1L2T	C07-C06-N05-C04
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	B	504	A1L2T	C07-C06-N05-C04
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A

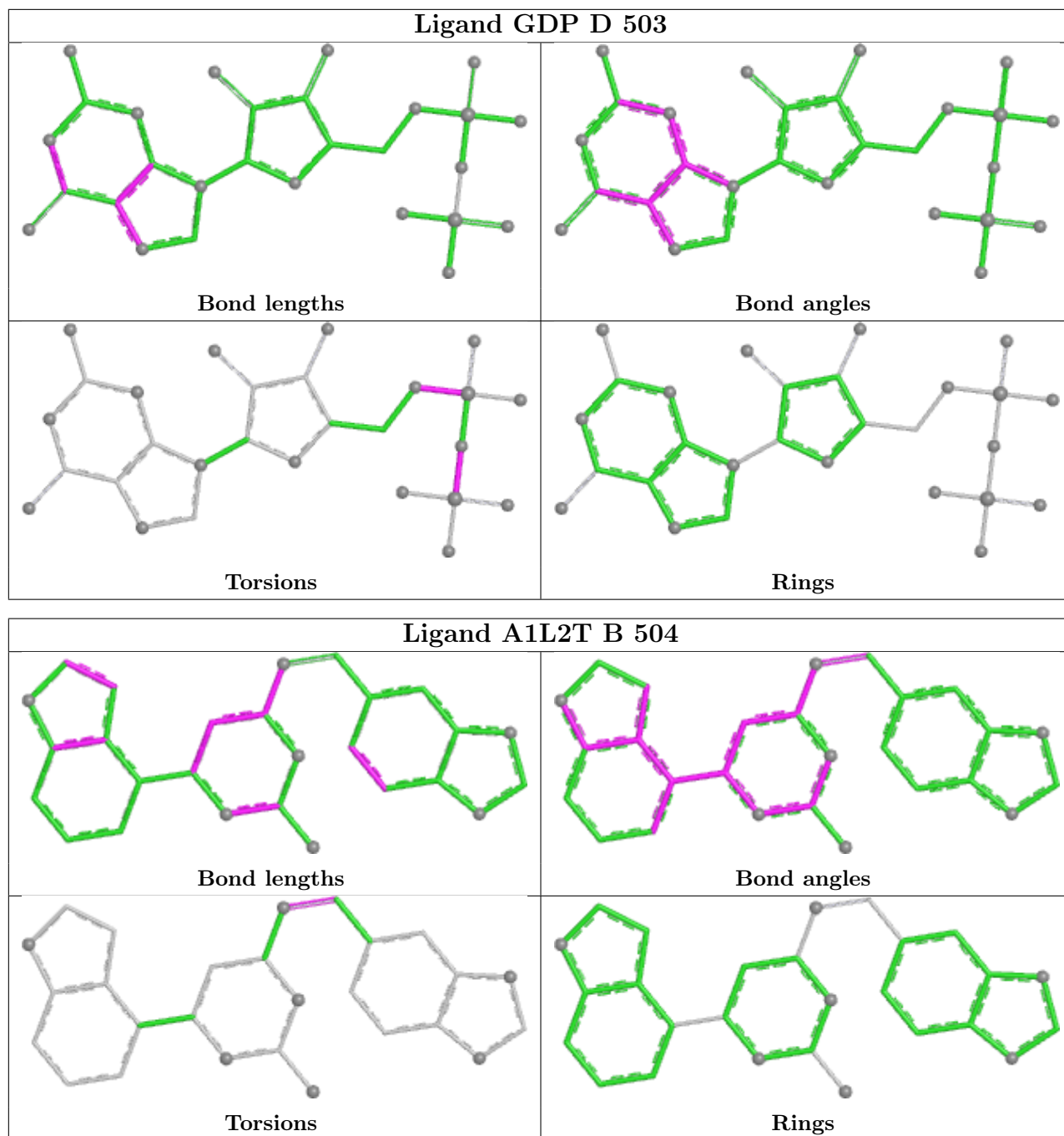
There are no ring outliers.

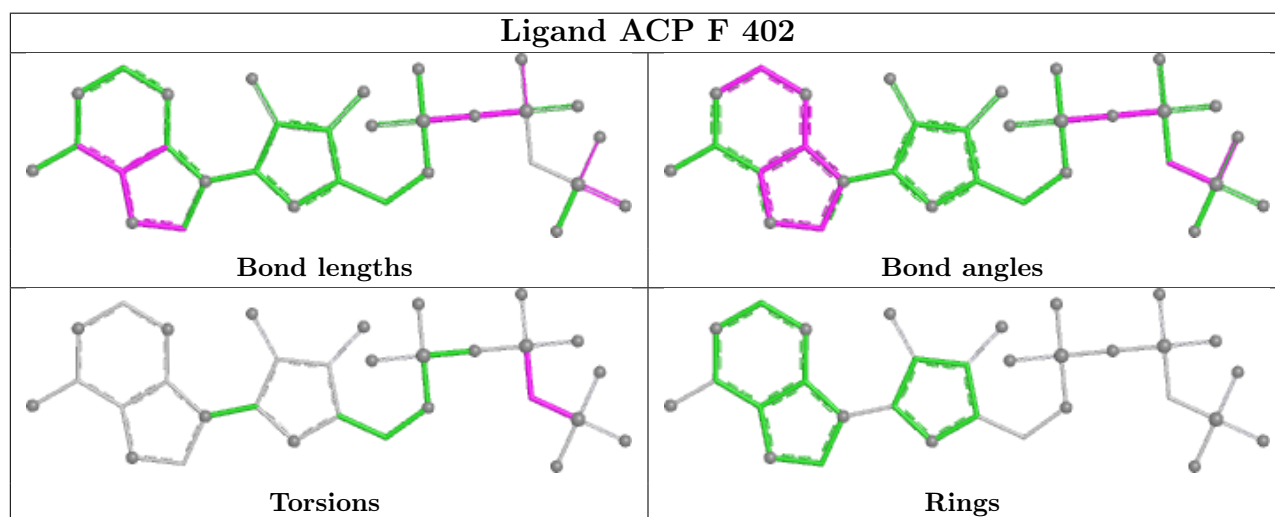
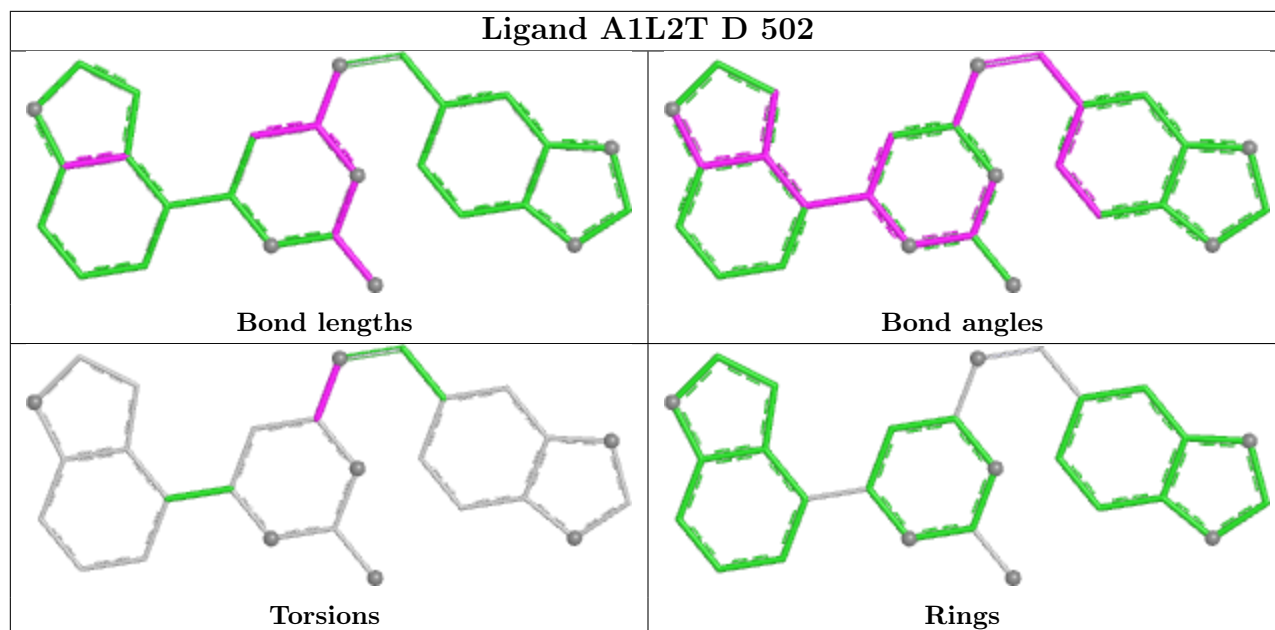
6 monomers are involved in 11 short contacts:

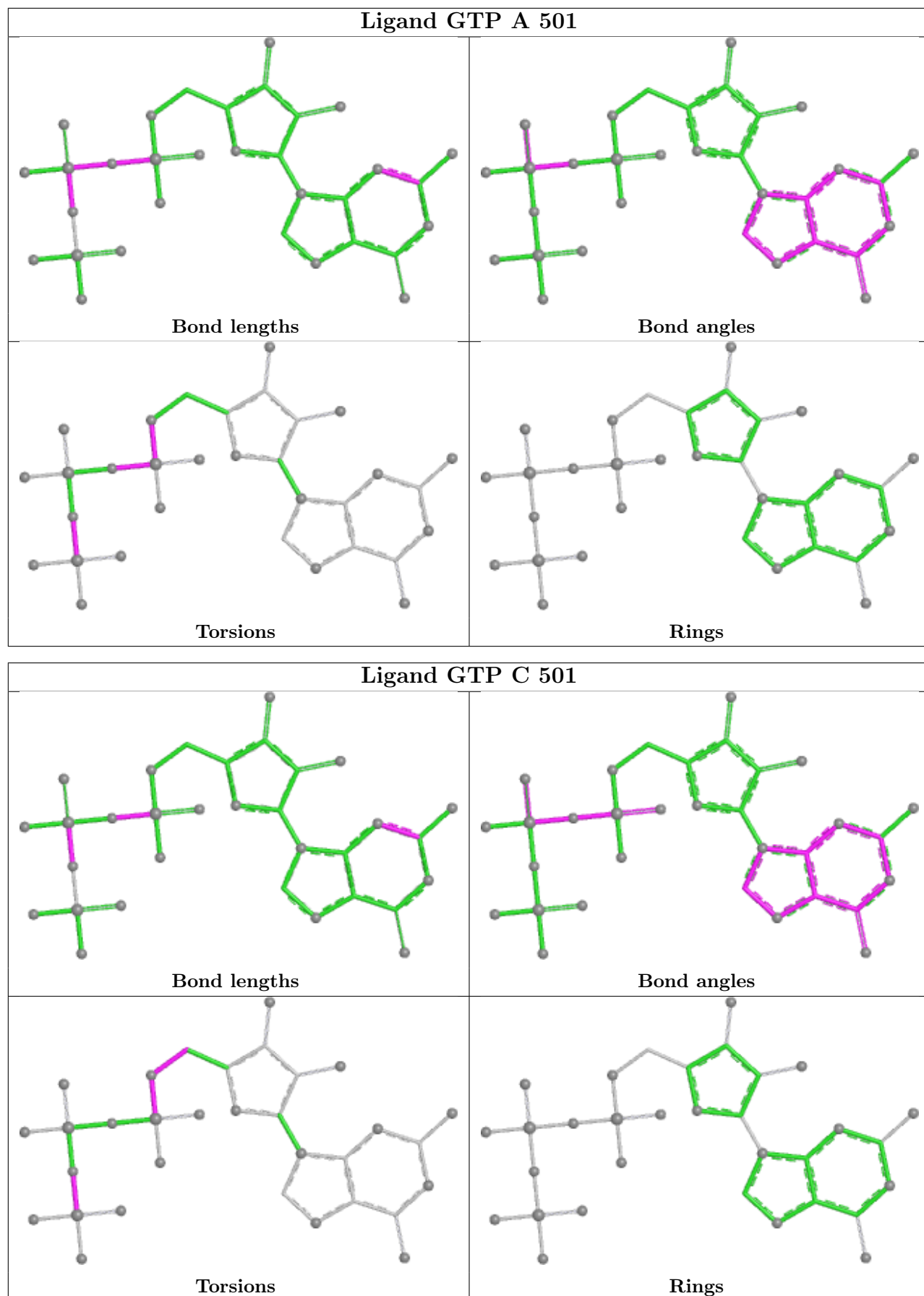
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	503	GDP	4	0
8	B	504	A1L2T	1	0
8	D	502	A1L2T	2	0
10	F	402	ACP	2	0
5	A	501	GTP	1	0
8	B	503	A1L2T	1	0

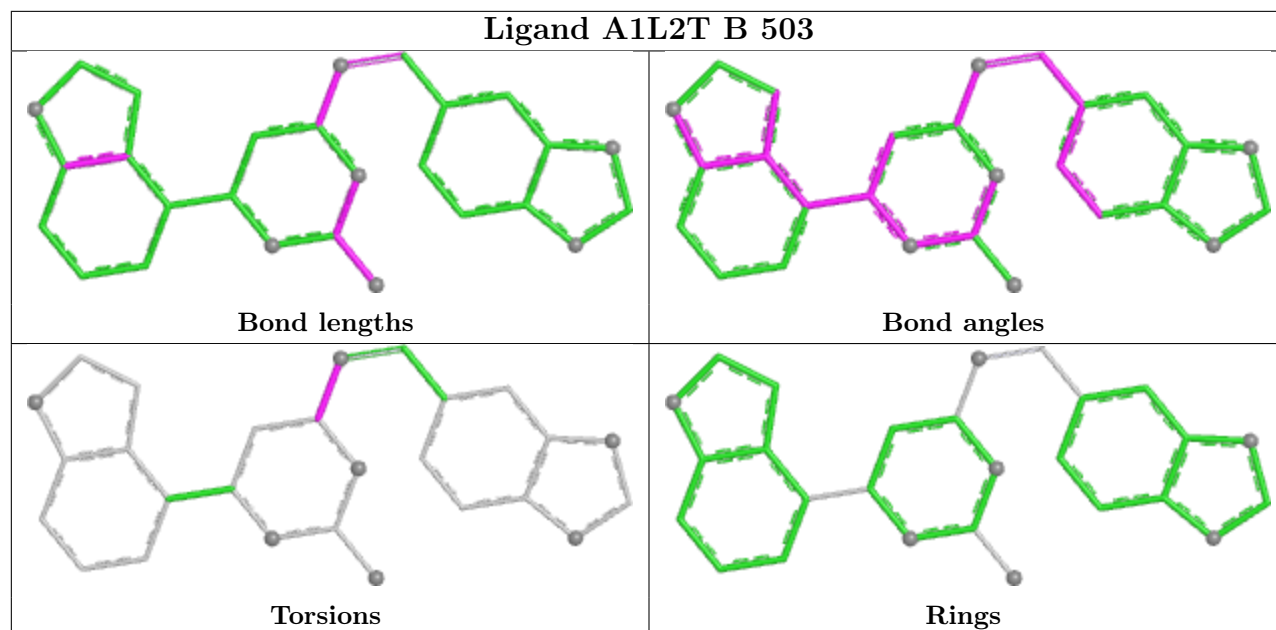
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	439/451 (97%)	0.32	8 (1%) 67 65	39, 75, 106, 136	6 (1%)
1	C	440/451 (97%)	0.11	10 (2%) 61 59	33, 64, 92, 115	7 (1%)
2	B	422/431 (97%)	0.28	9 (2%) 63 61	39, 73, 106, 128	4 (0%)
2	D	421/431 (97%)	0.58	15 (3%) 46 44	47, 91, 115, 132	3 (0%)
3	E	121/189 (64%)	0.57	9 (7%) 20 20	60, 88, 126, 137	0
4	F	320/384 (83%)	0.74	23 (7%) 21 21	59, 105, 139, 154	3 (0%)
All	All	2163/2337 (92%)	0.40	74 (3%) 48 46	33, 81, 120, 154	23 (1%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	178	SER	5.0
4	F	149	ALA	4.3
1	C	249	ASN	4.1
4	F	170	LEU	3.8
1	C	1	MET	3.7
4	F	198	LYS	3.5
1	A	46	ASP	3.5
4	F	362	ALA	3.4
2	D	402	PHE	3.3
1	A	156	ARG	3.3
1	C	283	HIS	3.2
4	F	245	ILE	3.2
4	F	226	GLU	3.1
2	B	281	TYR	2.9
4	F	129	GLU	2.9
3	E	12	ASN	2.8
3	E	26	PRO	2.8
1	C	253	THR	2.8
4	F	237	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	283	ALA	2.7
2	D	92	PHE	2.7
2	D	323	MET	2.7
3	E	15	THR	2.7
2	B	243	PRO	2.7
4	F	194	PRO	2.7
1	C	248	LEU	2.6
4	F	102	PRO	2.6
4	F	244	CYS	2.6
2	B	282	ARG	2.6
4	F	99	VAL	2.6
4	F	320	MET	2.6
2	D	2	ARG	2.5
4	F	249	TYR	2.5
1	C	440	VAL	2.5
4	F	173	ILE	2.5
4	F	34	ASN	2.4
1	A	285	GLN	2.4
1	C	252	LEU	2.4
2	D	172	SER	2.4
2	D	1	MET	2.4
1	C	250	VAL	2.4
2	D	193	VAL	2.3
2	B	246	LEU	2.3
2	D	140	GLY	2.3
4	F	263	PHE	2.3
1	A	283	HIS	2.3
3	E	115	HIS	2.3
4	F	162	ILE	2.2
1	A	337	THR	2.2
2	D	171	PRO	2.2
2	D	151	LEU	2.2
3	E	24	LEU	2.2
2	B	111	GLU	2.2
3	E	45	PRO	2.2
1	C	284	GLU	2.2
3	E	116	LEU	2.2
1	A	251	ASP	2.2
2	D	180	VAL	2.2
3	E	11	LEU	2.1
2	B	55	ALA	2.1
2	D	181	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.1
4	F	192	LEU	2.1
2	B	46	ARG	2.1
4	F	144	GLY	2.1
4	F	228	TYR	2.1
2	D	401	ALA	2.1
3	E	54	LEU	2.1
2	D	152	ILE	2.1
4	F	231	ALA	2.0
4	F	267	PHE	2.0
2	D	68	LEU	2.0
2	B	170	VAL	2.0
1	A	282	TYR	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 oligosaccharides 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.

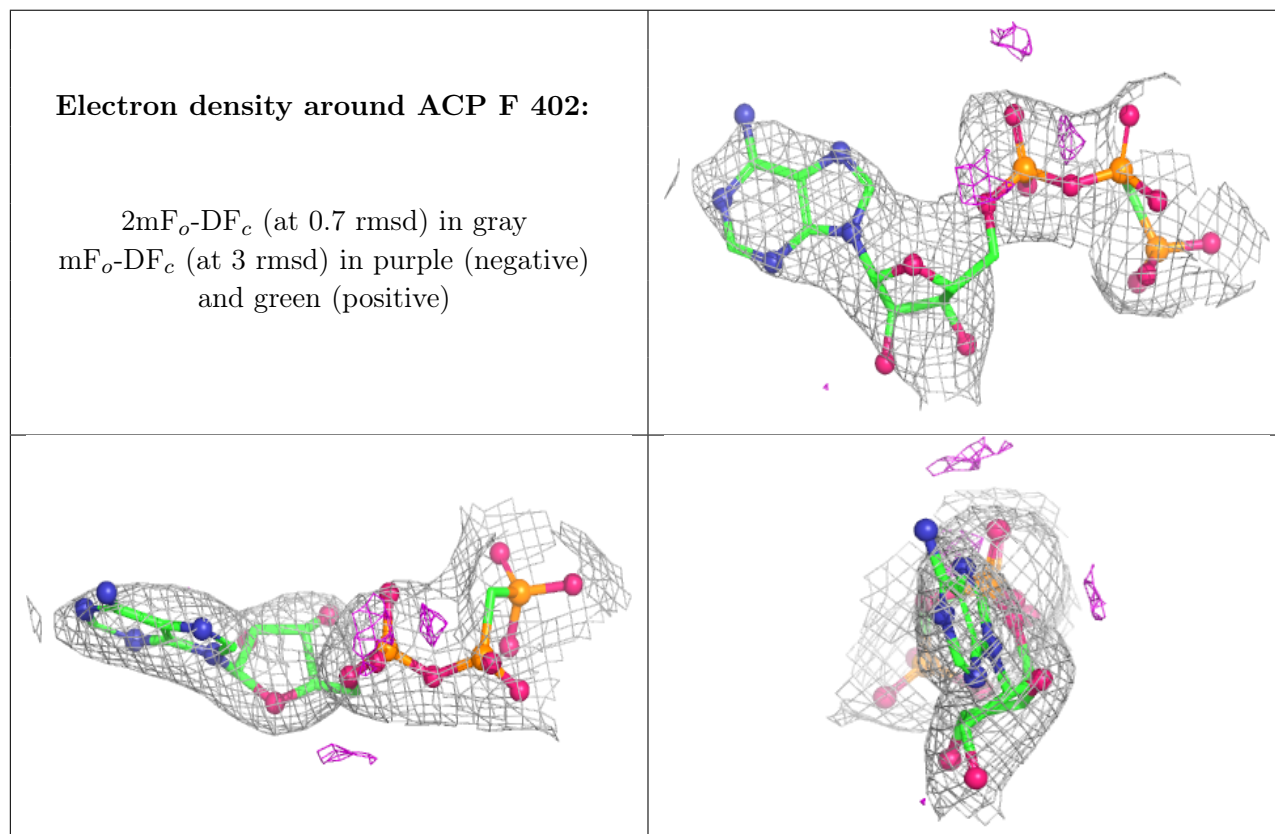
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	401	1/1	0.73	0.14	123,123,123,123	0
6	MG	A	502	1/1	0.75	0.39	71,71,71,71	0
6	MG	C	502	1/1	0.77	0.33	71,71,71,71	0
7	CA	C	503	1/1	0.83	0.12	129,129,129,129	0
10	ACP	F	402	31/31	0.84	0.10	116,127,152,158	0
9	GDP	D	503	28/28	0.85	0.12	71,80,96,107	0
6	MG	B	501	1/1	0.86	0.25	88,88,88,88	0
8	A1L2T	B	504	27/27	0.88	0.13	66,83,103,110	0
8	A1L2T	A	504	27/27	0.91	0.10	64,78,93,103	0
6	MG	D	501	1/1	0.91	0.28	68,68,68,68	0

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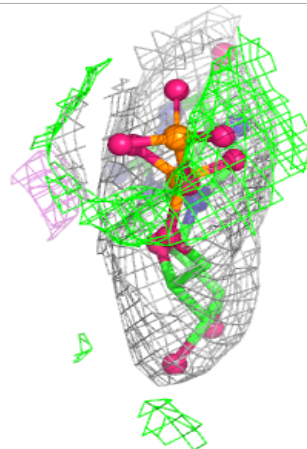
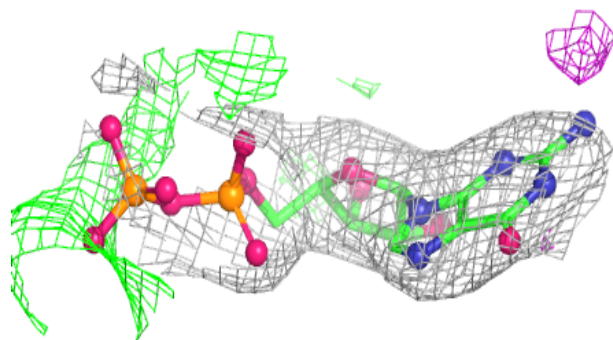
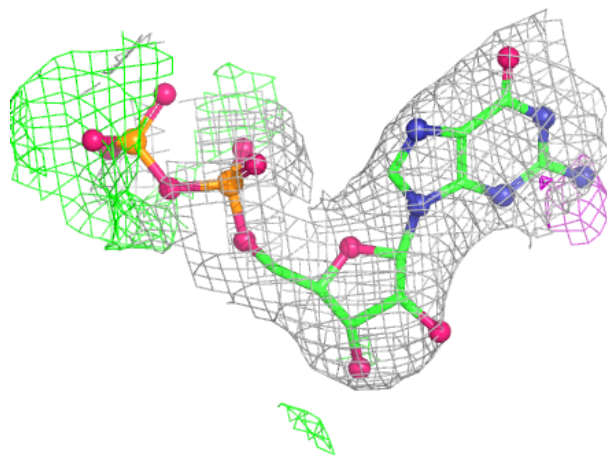
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	A1L2T	D	502	27/27	0.93	0.10	58,77,97,101	0
7	CA	B	502	1/1	0.94	0.11	121,121,121,121	0
9	GDP	B	505	28/28	0.94	0.08	50,59,74,76	0
8	A1L2T	B	503	27/27	0.94	0.11	51,68,98,109	0
5	GTP	A	501	32/32	0.94	0.08	49,62,71,82	0
7	CA	A	503	1/1	0.95	0.05	117,117,117,117	0
5	GTP	C	501	32/32	0.96	0.08	49,57,65,69	0

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



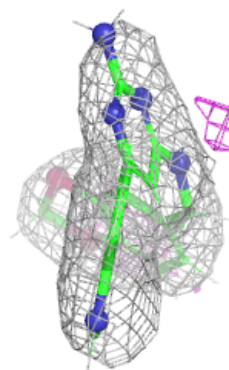
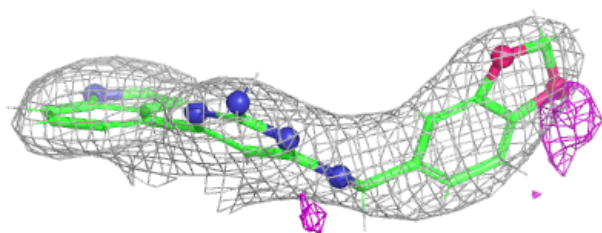
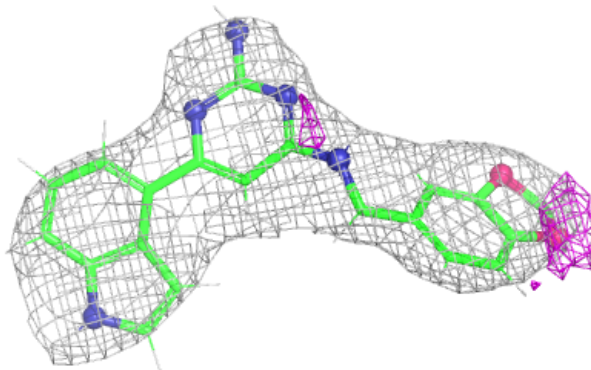
Electron density around GDP D 503:

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

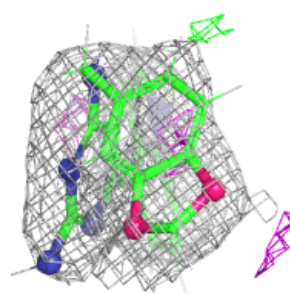
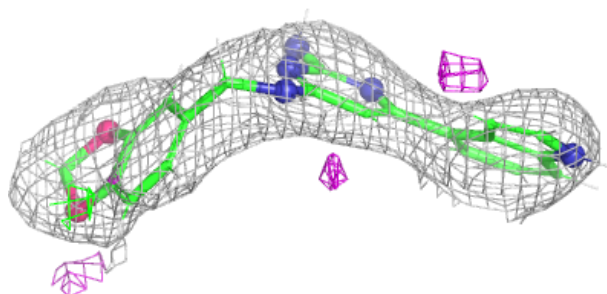
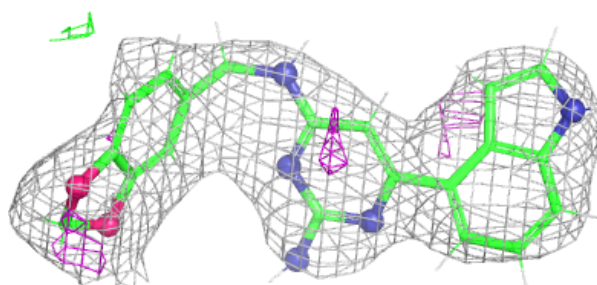


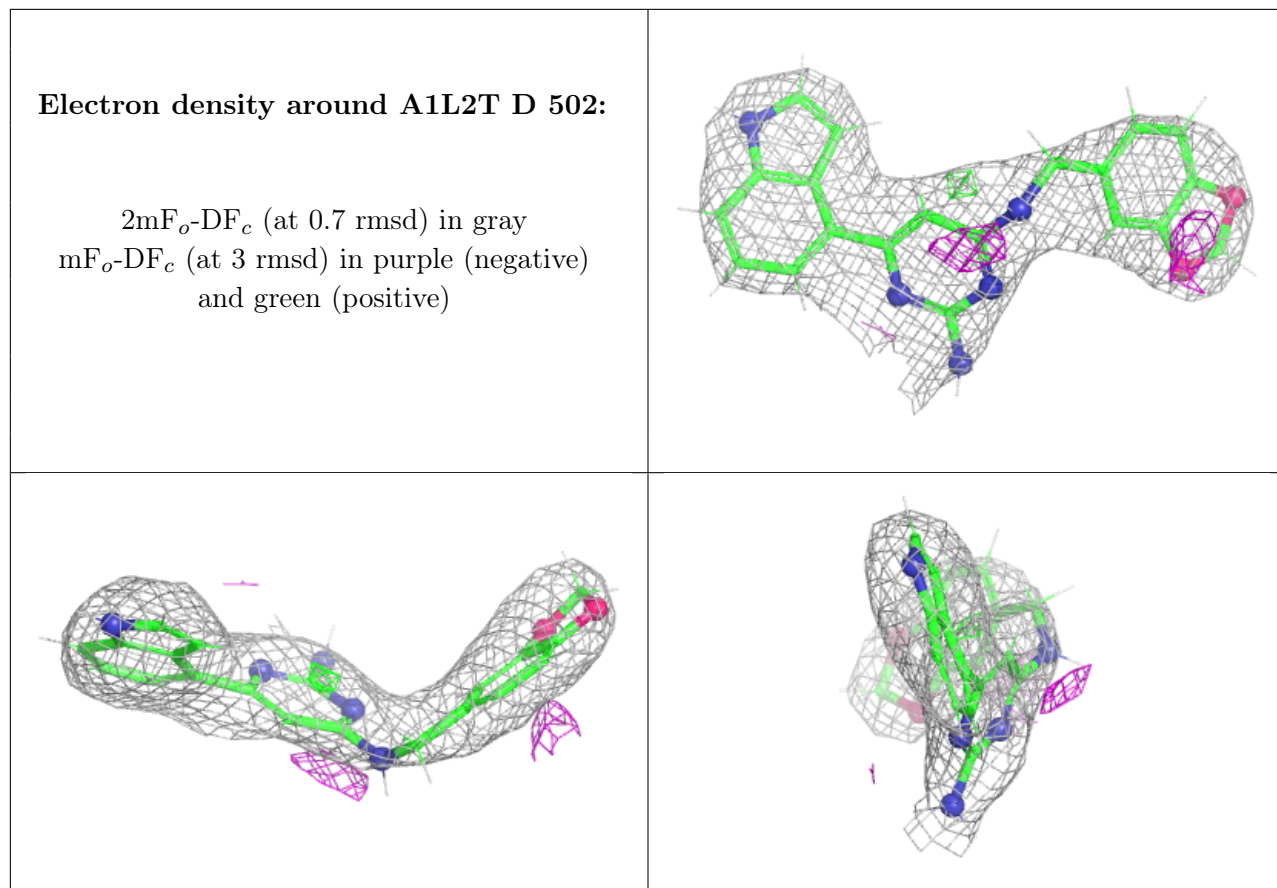
Electron density around A1L2T B 504:

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

**Electron density around A1L2T A 504:**

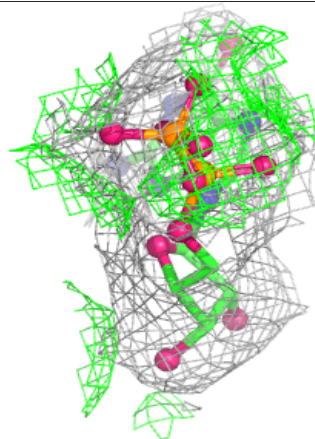
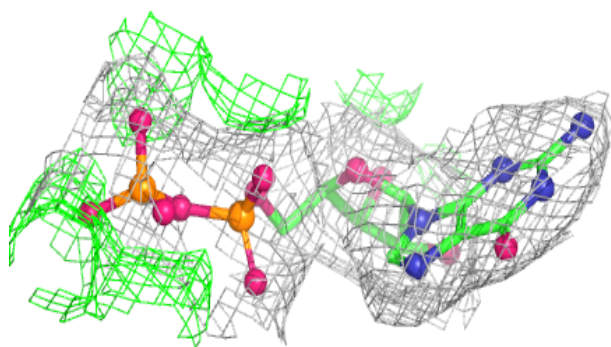
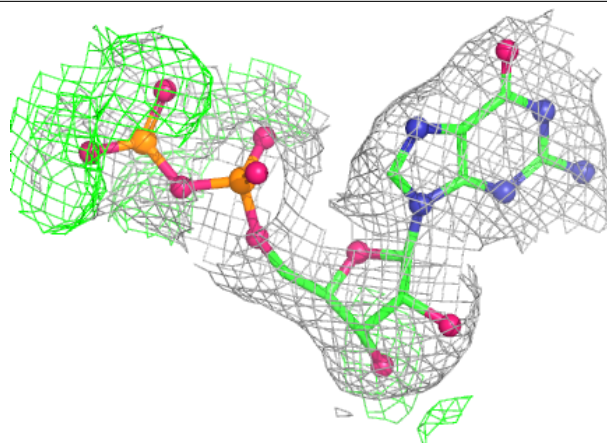
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





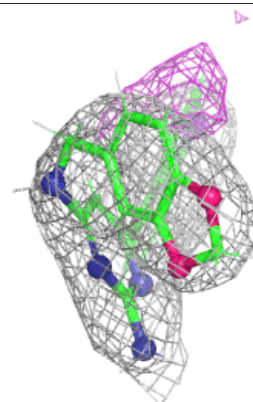
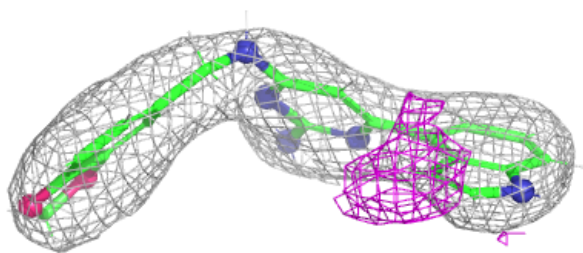
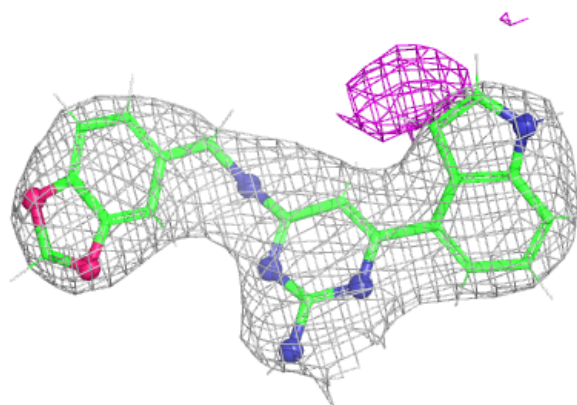
Electron density around GDP B 505:

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

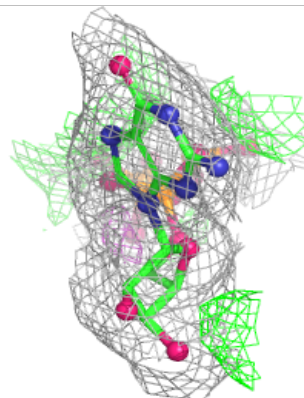
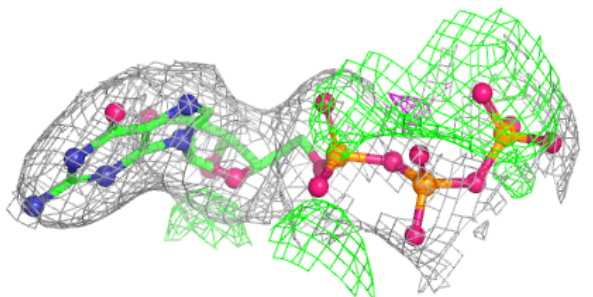
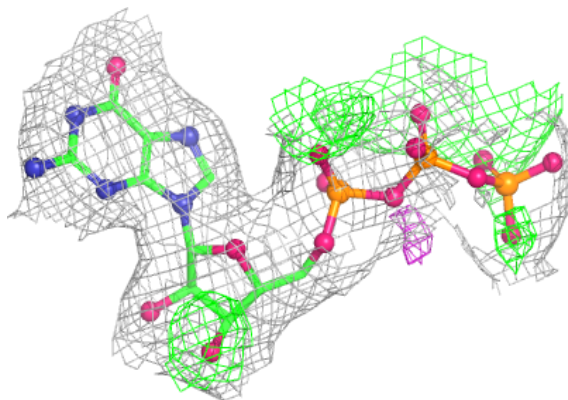


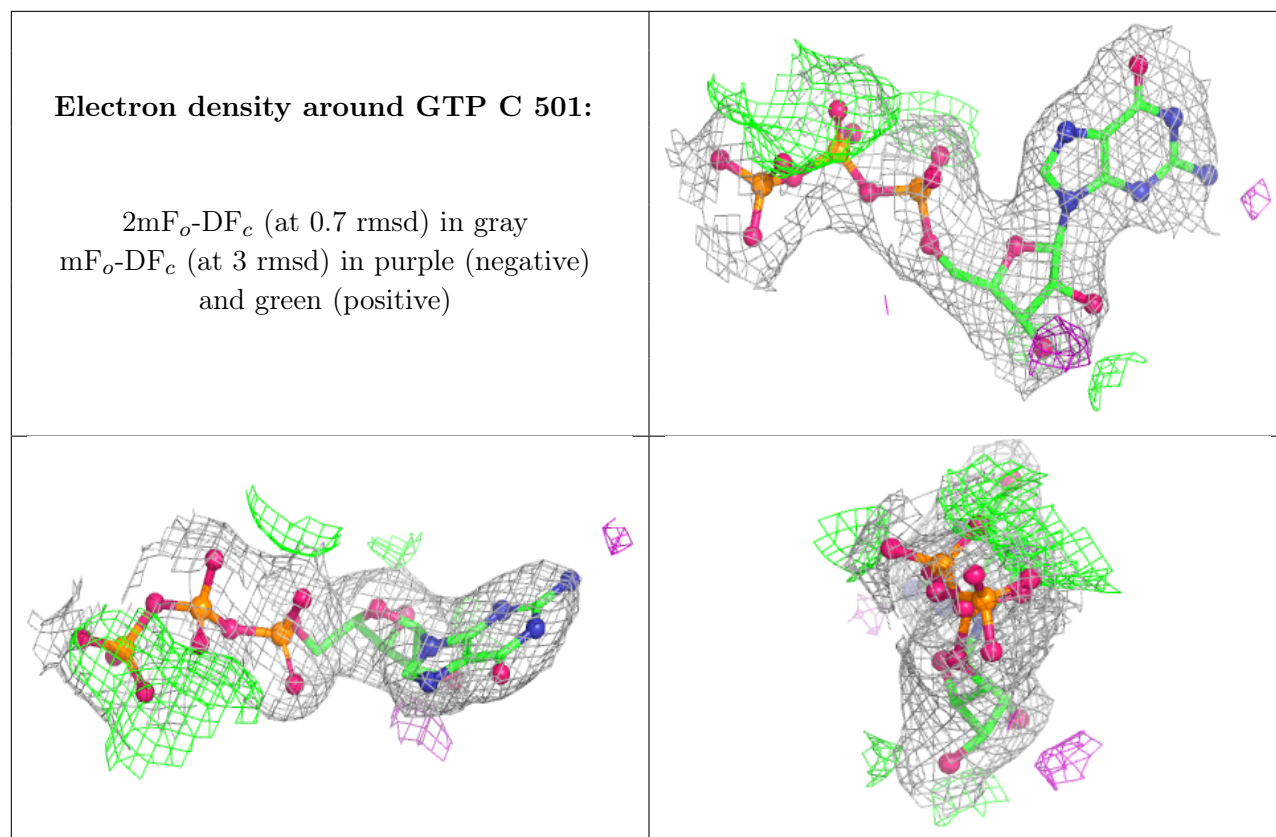
Electron density around A1L2T B 503:

$2mF_o-DF_c$ (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.