



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:33 AM UTC

PDB ID : 9KBL / pdb_00009kbl
Title : Crystal structure of T2R-TTL-IKP104
Authors : Yan, W.; Yang, J.
Deposited on : 2024-10-31
Resolution : 3.14 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

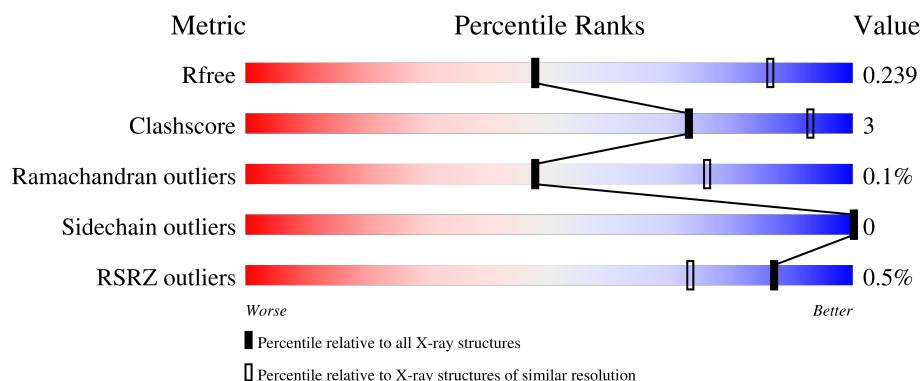
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	
1	C	451	
2	B	431	
2	D	431	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	% 80% 11% 9%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 34541 atoms, of which 16931 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	S	0	3	0
			6778	2176	3338	584	656	24			
1	C	439	Total	C	H	N	O	S	0	5	0
			6744	2173	3317	577	656	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	418	Total	C	H	N	O	S	0	3	0
			6484	2076	3179	566	635	28			
2	D	426	Total	C	H	N	O	S	0	1	0
			6533	2089	3202	568	647	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	1	0
			2033	624	1018	185	201	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

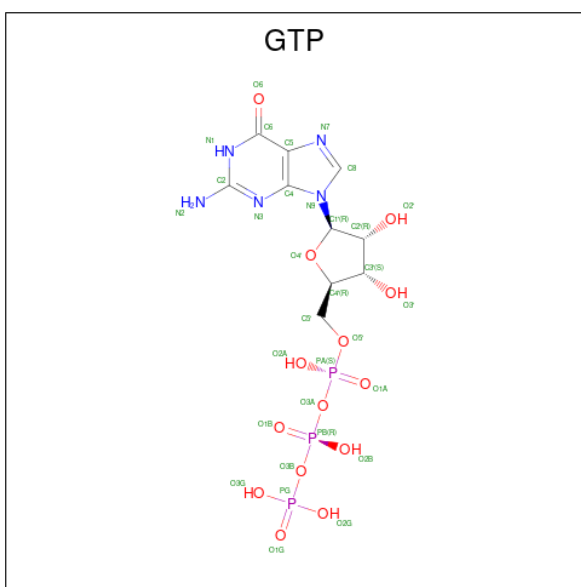
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	351	Total	C	H	N	O	S	0	0	0
			5638	1824	2790	488	522	14			

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
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: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0
5	C	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0
5	D	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	C	2	Total Mg 2 2	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

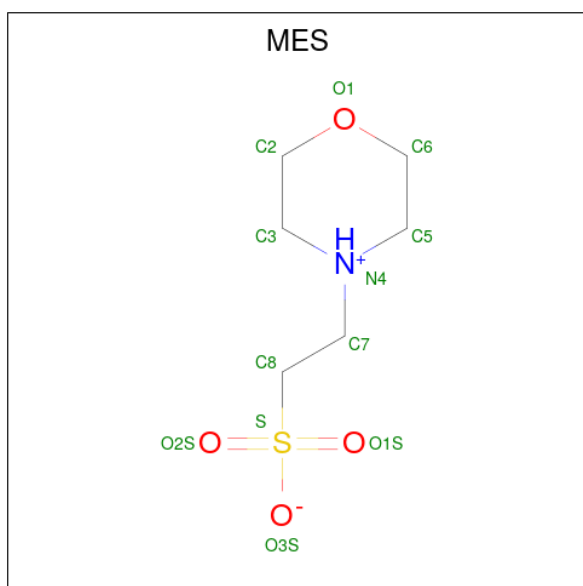
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	2	Total Ca 2 2	0	0

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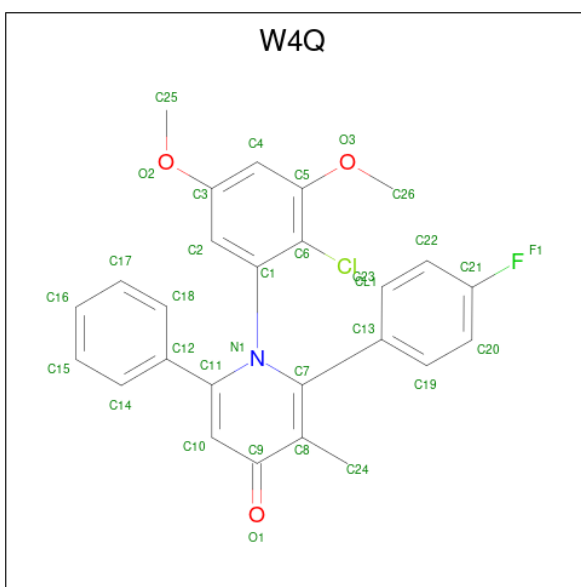
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total	Ca	0	0
			2	2		
7	D	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



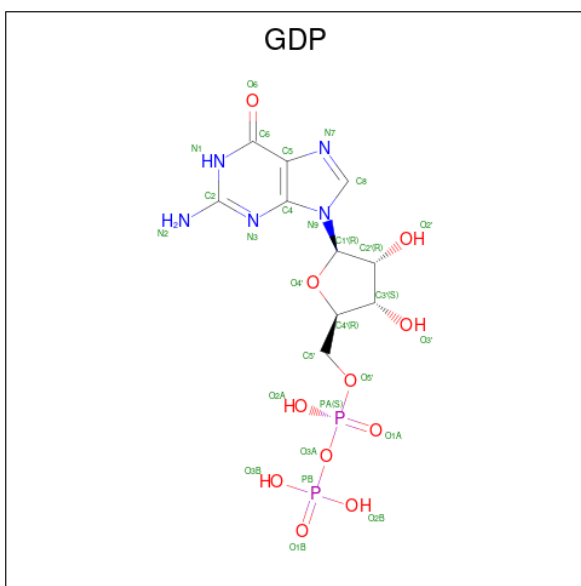
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 9 is 1-(2-chloranyl-3,5-dimethoxy-phenyl)-2-(4-fluorophenyl)-3-methyl-6-phenyl-pyridin-4-one (CCD ID: W4Q) (formula: $C_{26}H_{21}ClFNO_3$) (labeled as "Ligand of Interest" by depositor).



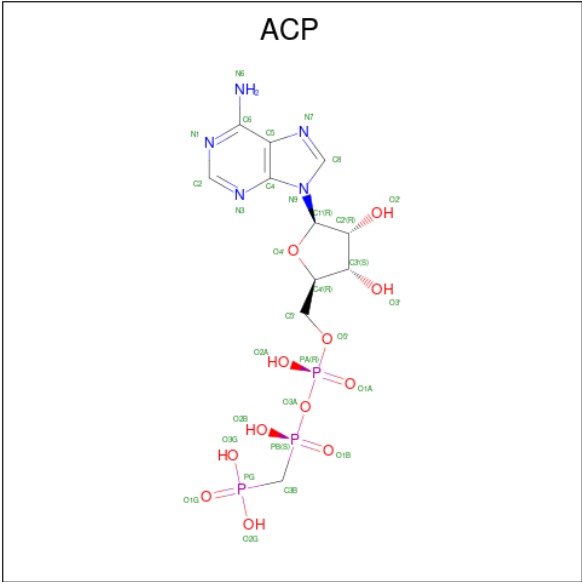
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	Cl	F	H	N	O	
			53	26	1	1	21	1	3	0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	P		
			38	10	10	5	11	2	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

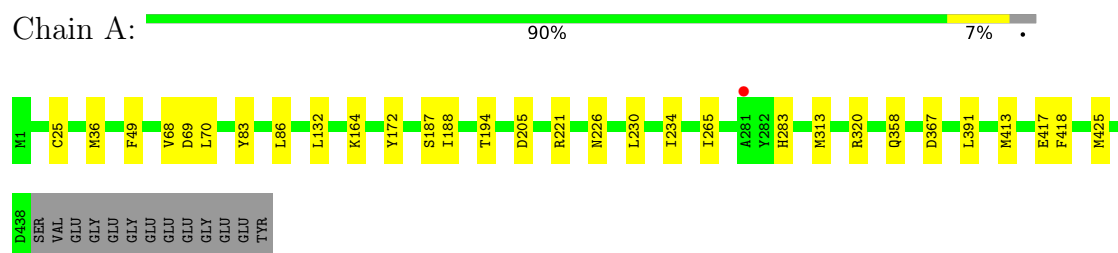
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	8	Total	O	0
			8	8	
12	B	4	Total	O	0
			4	4	
12	C	9	Total	O	0
			9	9	
12	D	8	Total	O	0
			8	8	
12	E	4	Total	O	0
			4	4	

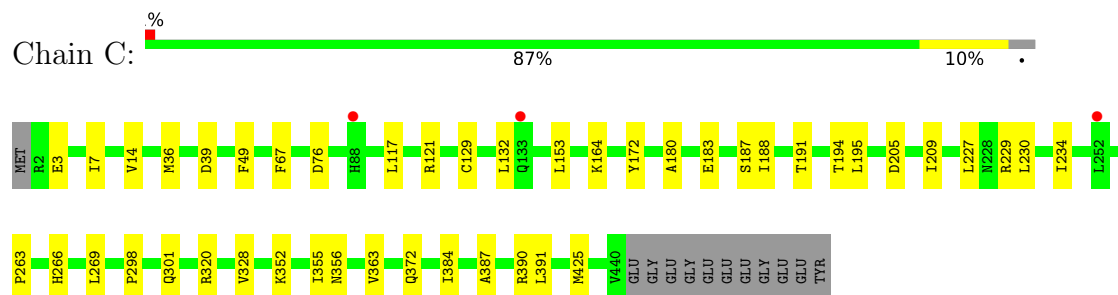
3 Residue-property plots [i](#)

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

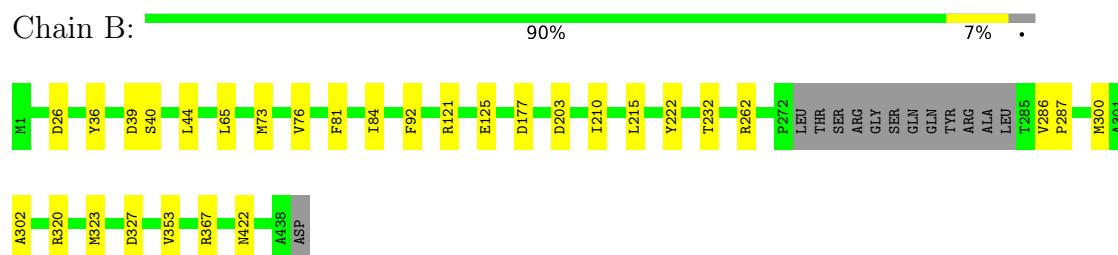
• Molecule 1: Tubulin alpha-1B chain



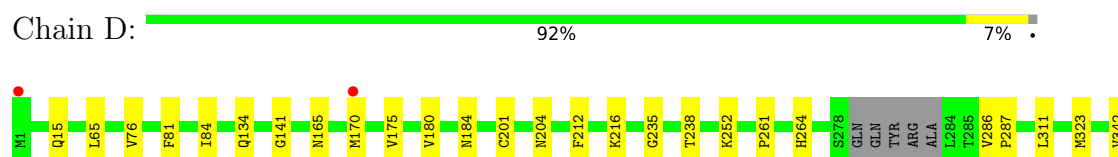
• Molecule 1: Tubulin alpha-1B chain



• Molecule 2: Tubulin beta chain

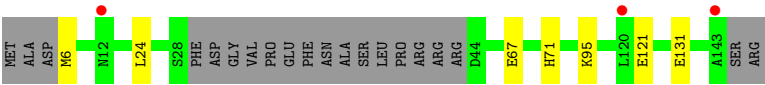
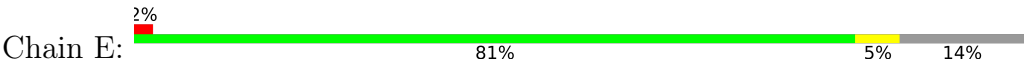


• Molecule 2: Tubulin beta chain

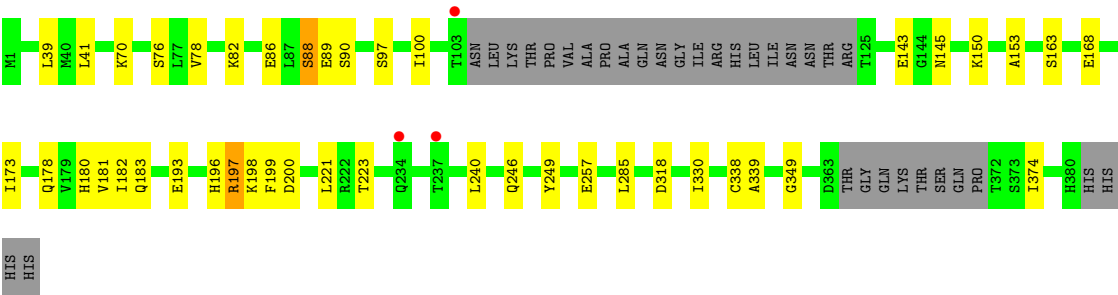
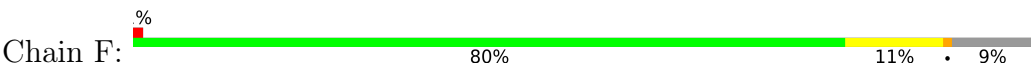




● Molecule 3: Stathmin-4



● 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	104.33Å 159.24Å 176.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.84 – 3.14 38.84 – 3.14	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.84-3.14) 99.9 (38.84-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.184 , 0.238 0.185 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34541	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, W4Q, GTP, ACP, MES, CA

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	0.20	0/3521	0.34	0/4780
1	C	0.23	0/3525	0.37	0/4791
2	B	0.21	0/3384	0.32	0/4581
2	D	0.19	0/3405	0.33	0/4612
3	E	0.21	0/1023	0.33	0/1358
4	F	0.24	0/2913	0.43	3/3938 (0.1%)
All	All	0.21	0/17771	0.36	3/24060 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	285	LEU	N-CA-C	-6.63	104.14	111.36
4	F	197	ARG	NE-CZ-NH1	-5.69	115.81	121.50
4	F	285	LEU	CB-CG-CD2	5.01	125.72	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	3338	3350	23	0
1	C	3427	3317	3319	29	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3305	3179	3188	18	1
2	D	3331	3202	3211	17	0
3	E	1015	1018	1021	3	2
4	F	2848	2790	2802	24	0
5	A	32	10	12	1	0
5	C	32	10	12	0	0
5	D	32	10	12	1	0
6	A	1	0	0	0	0
6	C	2	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	2	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	B	12	12	12	0	0
9	B	32	21	0	1	0
10	B	28	10	12	0	0
11	F	31	14	14	0	0
12	A	8	0	0	4	0
12	B	4	0	0	0	0
12	C	9	0	0	4	0
12	D	8	0	0	0	0
12	E	4	0	0	1	0
All	All	17610	16931	16965	112	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ASP:OD1	12:C:602:HOH:O	2.05	0.74
1:C:76:ASP:OD2	12:C:603:HOH:O	2.07	0.71
1:A:320:ARG:NE	12:A:602:HOH:O	2.26	0.68
1:A:283:HIS:NE2	12:A:603:HOH:O	2.27	0.68
1:A:187:SER:CB	1:A:391:LEU:HD21	2.24	0.67
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.76	0.67
1:C:390:ARG:NH2	12:C:602:HOH:O	2.30	0.64
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLN:O	12:A:602:HOH:O	2.16	0.61
5:A:501:GTP:O1G	12:A:601:HOH:O	2.16	0.60
2:B:73:MET:HE3	2:B:92:PHE:HB3	1.83	0.59
2:B:262:ARG:NH2	2:B:422:ASN:OD1	2.36	0.59
1:C:36:MET:HE2	1:C:39:ASP:HB2	1.82	0.59
1:A:83:TYR:CD2	1:A:86:LEU:HD22	2.38	0.59
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.38	0.58
4:F:86:GLU:N	4:F:86:GLU:OE1	2.35	0.58
2:D:175:VAL:HG21	2:D:204:ASN:HB3	1.85	0.58
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.86	0.57
2:B:323:MET:SD	2:B:353:VAL:HG21	2.45	0.57
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.85	0.56
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.70	0.56
2:D:235:GLY:O	2:D:238:THR:HG22	2.07	0.55
2:D:81:PHE:O	2:D:84:ILE:HG22	2.07	0.55
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.88	0.55
4:F:318:ASP:HB3	4:F:330:ILE:HD11	1.90	0.54
1:A:187:SER:HB2	1:A:391:LEU:HD21	1.90	0.53
2:D:15:GLN:NE2	5:D:503:GTP:O6	2.41	0.53
2:B:65:LEU:CD2	2:B:76:VAL:HG11	2.39	0.52
1:C:172:TYR:OH	1:C:387:ALA:O	2.23	0.52
2:B:81:PHE:O	2:B:84:ILE:HG22	2.10	0.52
2:D:134:GLN:HA	2:D:165:ASN:O	2.10	0.52
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.40	0.52
2:B:39:ASP:OD1	2:B:40:SER:N	2.37	0.51
2:B:210:ILE:HG22	2:B:215:LEU:HD13	1.92	0.51
1:A:413:MET:HE2	1:A:418:PHE:CE2	2.46	0.50
1:C:191:THR:O	1:C:195:LEU:HB2	2.11	0.50
1:A:36:MET:HE1	1:A:49:PHE:CE2	2.46	0.50
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.92	0.50
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.93	0.49
2:B:26:ASP:OD2	2:B:367:ARG:HG2	2.12	0.49
2:B:203:ASP:OD2	2:B:302:ALA:HB2	2.13	0.49
4:F:100:ILE:HD12	4:F:182:ILE:HD12	1.95	0.49
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.46	0.49
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.94	0.49
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.95	0.49
1:C:194:THR:O	1:C:194:THR:HG22	2.13	0.48
4:F:150:LYS:NZ	4:F:183:GLN:OE1	2.47	0.48
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.95	0.48
4:F:143:GLU:O	4:F:145:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:198:LYS:HG2	4:F:199:PHE:H	1.79	0.48
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.47
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.54	0.47
4:F:82:LYS:NZ	4:F:97:SER:O	2.42	0.47
1:C:328:VAL:HG21	1:C:355:ILE:HD11	1.96	0.47
4:F:240:LEU:O	4:F:246:GLN:NE2	2.47	0.47
4:F:249:TYR:CD2	4:F:249:TYR:O	2.68	0.47
2:D:323:MET:SD	2:D:353:VAL:HG21	2.54	0.47
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.97	0.47
1:A:221:ARG:NE	2:B:327:ASP:OD2	2.48	0.46
1:C:269:LEU:H	1:C:269:LEU:HD23	1.79	0.46
1:C:132:LEU:O	1:C:164:LYS:NZ	2.47	0.46
2:B:222:TYR:N	9:B:504:W4Q:O1	2.39	0.46
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.46
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.51	0.46
2:D:437:THR:HG22	2:D:438:ALA:N	2.31	0.46
1:C:263:PRO:O	1:C:266:HIS:ND1	2.36	0.46
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.31	0.45
2:D:141:GLY:O	2:D:184:ASN:ND2	2.48	0.45
4:F:197:ARG:HH21	4:F:223:THR:HG21	1.82	0.45
3:E:67:GLU:O	3:E:71:HIS:ND1	2.48	0.45
4:F:163:SER:OG	4:F:168:GLU:OE1	2.33	0.45
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.52	0.45
1:A:68:VAL:O	1:A:68:VAL:HG23	2.16	0.44
2:D:170:MET:HE1	2:D:201:CYS:SG	2.57	0.44
4:F:70:LYS:HA	4:F:76:SER:HB3	1.99	0.44
2:B:121:ARG:O	2:B:125:GLU:HG3	2.18	0.44
12:C:601:HOH:O	2:D:252:LYS:NZ	2.40	0.44
2:B:203:ASP:OD1	2:B:203:ASP:C	2.60	0.44
4:F:173:ILE:HD13	4:F:180:HIS:CG	2.52	0.44
3:E:121:GLU:N	12:E:301:HOH:O	2.51	0.44
1:C:229:ARG:HD3	1:C:363:VAL:HG21	2.00	0.44
2:D:261:PRO:O	2:D:264:HIS:ND1	2.42	0.44
1:C:298:PRO:HA	1:C:301:GLN:HG2	1.99	0.43
1:A:221:ARG:HG2	2:B:323:MET:HG2	2.00	0.43
4:F:198:LYS:O	4:F:199:PHE:HB3	2.17	0.43
1:A:132:LEU:O	1:A:164:LYS:NZ	2.41	0.43
1:A:230:LEU:O	1:A:234:ILE:HD12	2.18	0.43
1:A:69:ASP:OD1	1:A:70:LEU:N	2.51	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.91	0.43
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HB3	1:C:384:ILE:HD13	2.01	0.43
1:A:194:THR:O	1:A:194:THR:HG22	2.17	0.42
2:B:232:THR:OG1	2:B:300:MET:HE3	2.17	0.42
1:C:187:SER:CB	1:C:391:LEU:HD21	2.49	0.42
4:F:193:GLU:OE1	4:F:196:HIS:ND1	2.49	0.42
2:B:286:VAL:HB	2:B:287:PRO:HD3	2.01	0.42
1:C:3:GLU:OE1	1:C:129:CYS:SG	2.77	0.42
1:C:230:LEU:O	1:C:234:ILE:HD12	2.19	0.42
2:D:212:PHE:O	2:D:216:LYS:HE2	2.19	0.42
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.02	0.42
1:A:188:ILE:HG23	1:A:425:MET:HG3	2.02	0.42
4:F:153:ALA:HB2	4:F:178:GLN:HG2	2.01	0.42
2:D:180:VAL:HA	2:D:396:MET:HE1	2.01	0.42
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.01	0.41
2:D:65:LEU:HD12	2:D:65:LEU:N	2.36	0.41
2:D:311:LEU:HD23	2:D:342:VAL:HG11	2.02	0.41
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.54	0.41
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.54	0.41
4:F:88:SER:C	4:F:90:SER:N	2.78	0.40
4:F:200:ASP:OD1	4:F:200:ASP:C	2.64	0.40
3:E:6:MET:HE3	3:E:24:LEU:HD21	2.02	0.40
2:B:177:ASP:O	1:C:352:LYS:HD2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:GLN:OE1	3:E:95:LYS:NZ[4_455]	2.01	0.19
2:B:320:ARG:HH21	3:E:131:GLU:OE1[4_455]	1.58	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/451 (97%)	431 (98%)	8 (2%)	0	100	100
1	C	442/451 (98%)	426 (96%)	16 (4%)	0	100	100
2	B	417/431 (97%)	410 (98%)	7 (2%)	0	100	100
2	D	423/431 (98%)	417 (99%)	6 (1%)	0	100	100
3	E	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
4	F	345/384 (90%)	337 (98%)	6 (2%)	2 (1%)	21	50
All	All	2186/2291 (95%)	2138 (98%)	46 (2%)	2 (0%)	48	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU
4	F	88	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/379 (98%)	372 (100%)	0	100	100
1	C	371/379 (98%)	371 (100%)	0	100	100
2	B	363/372 (98%)	363 (100%)	0	100	100
2	D	366/372 (98%)	366 (100%)	0	100	100
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	309/342 (90%)	309 (100%)	0	100	100
All	All	1890/1971 (96%)	1890 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN

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Mol	Chain	Res	Type
1	A	329	ASN
1	A	393	HIS
2	B	334	GLN
2	B	383	GLN
2	B	434	GLN
1	C	393	HIS
2	D	8	GLN
2	D	134	GLN
2	D	165	ASN
2	D	334	GLN
2	D	383	GLN
2	D	434	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 19 ligands modelled in this entry, 12 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	$\# Z > 2$
5	GTP	A	501	6	33,34,34	0.99	2 (6%)	50,54,54	1.51	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	ACP	F	402	6	31,33,33	1.64	8 (25%)	47,52,52	1.91	12 (25%)
10	GDP	B	505	-	29,30,30	1.17	2 (6%)	45,47,47	1.73	6 (13%)
8	MES	B	501	-	12,12,12	2.29	1 (8%)	15,16,16	1.56	2 (13%)
5	GTP	D	503	6	33,34,34	1.00	2 (6%)	50,54,54	1.57	8 (16%)
9	W4Q	B	504	-	35,35,35	5.14	24 (68%)	44,50,50	1.12	2 (4%)
5	GTP	C	502	6	33,34,34	0.97	3 (9%)	50,54,54	1.57	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
11	ACP	F	402	6	-	3/19/38/38	0/3/3/3
10	GDP	B	505	-	-	0/16/32/32	0/3/3/3
8	MES	B	501	-	-	0/6/14/14	0/1/1/1
5	GTP	D	503	6	-	7/22/38/38	0/3/3/3
9	W4Q	B	504	-	-	3/16/16/16	0/4/4/4
5	GTP	C	502	6	-	5/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	W4Q	C1-C6	-10.16	1.31	1.40
9	B	504	W4Q	C4-C3	8.84	1.53	1.39
9	B	504	W4Q	C19-C13	8.66	1.52	1.39
9	B	504	W4Q	C23-C22	8.63	1.52	1.38
9	B	504	W4Q	C18-C12	8.60	1.52	1.39
9	B	504	W4Q	C5-C6	8.12	1.52	1.40
9	B	504	W4Q	C2-C1	8.06	1.52	1.39
9	B	504	W4Q	C15-C14	7.80	1.52	1.38
9	B	504	W4Q	C20-C21	7.67	1.52	1.37
8	B	501	MES	C8-S	-7.65	1.66	1.77
9	B	504	W4Q	C16-C17	6.55	1.52	1.38
9	B	504	W4Q	O1-C9	6.03	1.40	1.24
9	B	504	W4Q	C23-C13	-4.92	1.32	1.39
9	B	504	W4Q	C14-C12	-4.86	1.32	1.39
11	F	402	ACP	C5-C4	4.44	1.47	1.39
9	B	504	W4Q	C19-C20	-4.35	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	W4Q	C2-C3	-4.17	1.32	1.39
9	B	504	W4Q	C17-C18	-4.06	1.32	1.38
9	B	504	W4Q	C4-C5	-3.81	1.32	1.38
9	B	504	W4Q	C11-N1	3.72	1.47	1.40
9	B	504	W4Q	C12-C11	3.38	1.53	1.48
11	F	402	ACP	PG-O2G	3.22	1.62	1.55
10	B	505	GDP	C5-C4	3.20	1.47	1.38
9	B	504	W4Q	C13-C7	3.16	1.52	1.48
11	F	402	ACP	PG-O3G	3.03	1.61	1.55
9	B	504	W4Q	C16-C15	-2.77	1.32	1.38
5	D	503	GTP	PB-O3B	2.74	1.62	1.59
9	B	504	W4Q	C7-N1	2.68	1.47	1.41
10	B	505	GDP	C6-N1	-2.67	1.33	1.38
9	B	504	W4Q	C22-C21	-2.67	1.31	1.37
11	F	402	ACP	C5-C6	2.57	1.48	1.41
5	A	501	GTP	PB-O3B	2.44	1.62	1.59
9	B	504	W4Q	C6-CL1	2.33	1.77	1.72
11	F	402	ACP	C8-N7	2.31	1.36	1.31
11	F	402	ACP	PB-O3A	2.29	1.61	1.58
11	F	402	ACP	C5-N7	-2.29	1.34	1.39
11	F	402	ACP	PB-O2B	2.27	1.62	1.56
5	D	503	GTP	C2-N3	2.23	1.38	1.33
5	A	501	GTP	C2-N3	2.08	1.38	1.33
5	C	502	GTP	PB-O3B	2.04	1.61	1.59
5	C	502	GTP	C5-N7	-2.01	1.35	1.39
5	C	502	GTP	C2-N3	2.00	1.38	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C5-C4-N3	-5.84	118.67	126.72
10	B	505	GDP	C5-C4-N3	-5.80	119.16	128.39
5	C	502	GTP	C5-C4-N3	-5.05	120.35	128.39
5	D	503	GTP	C5-C4-N3	-4.88	120.62	128.39
11	F	402	ACP	N3-C4-N9	4.74	135.23	127.17
5	A	501	GTP	C5-C4-N3	-4.71	120.89	128.39
10	B	505	GDP	C2-N3-C4	4.56	120.15	112.30
5	C	502	GTP	C2-N3-C4	4.54	120.11	112.30
8	B	501	MES	C5-N4-C3	4.36	118.24	108.84
5	D	503	GTP	C2-N3-C4	4.33	119.76	112.30
10	B	505	GDP	N9-C4-N3	4.13	134.21	125.95
5	A	501	GTP	C2-N3-C4	4.13	119.41	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C2-N3-C4	3.87	121.28	111.83
11	F	402	ACP	N3-C2-N1	-3.74	122.92	128.58
11	F	402	ACP	PB-O3A-PA	-3.73	120.19	132.37
11	F	402	ACP	C4-C5-N7	-3.49	106.59	110.58
10	B	505	GDP	C6-C5-N7	3.35	136.38	130.29
5	C	502	GTP	N9-C4-N3	3.31	132.58	125.95
11	F	402	ACP	C4-N9-C8	3.19	109.09	105.74
5	D	503	GTP	N9-C4-N3	3.16	132.27	125.95
5	D	503	GTP	C2-N1-C6	-3.01	119.66	125.11
5	A	501	GTP	C2-N1-C6	-2.94	119.78	125.11
5	A	501	GTP	N9-C4-N3	2.92	131.79	125.95
9	B	504	W4Q	C24-C8-C9	2.90	121.22	115.28
9	B	504	W4Q	O3-C5-C6	2.81	118.52	115.44
5	D	503	GTP	N9-C8-N7	-2.79	108.23	113.40
5	C	502	GTP	C2-N1-C6	-2.77	120.09	125.11
11	F	402	ACP	C5-N7-C8	2.71	107.70	103.45
5	D	503	GTP	C8-N7-C5	2.70	109.06	104.26
10	B	505	GDP	C4-C5-N7	-2.63	106.51	110.67
5	C	502	GTP	N9-C8-N7	-2.56	108.66	113.40
5	A	501	GTP	N9-C8-N7	-2.52	108.72	113.40
10	B	505	GDP	C3'-C2'-C1'	2.48	106.16	101.46
5	C	502	GTP	C8-N7-C5	2.48	108.68	104.26
5	D	503	GTP	C5-C6-N1	2.47	119.54	113.25
5	A	501	GTP	C8-N7-C5	2.47	108.65	104.26
5	C	502	GTP	C5-C6-N1	2.44	119.45	113.25
11	F	402	ACP	N9-C8-N7	-2.41	110.52	113.94
11	F	402	ACP	C3'-C2'-C1'	2.37	105.94	101.46
5	A	501	GTP	C5-C6-N1	2.37	119.28	113.25
5	A	501	GTP	O6-C6-C5	-2.32	120.41	126.53
5	C	502	GTP	O6-C6-C5	-2.25	120.58	126.53
5	C	502	GTP	O3G-PG-O3B	2.14	111.81	104.64
11	F	402	ACP	C6-C5-N7	2.12	136.18	132.09
11	F	402	ACP	C2-N1-C6	2.11	122.19	118.73
5	D	503	GTP	O6-C6-C5	-2.06	121.10	126.53
8	B	501	MES	O2S-S-C8	2.02	109.78	106.73

There are no chirality outliers.

All (24) 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

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
5	D	503	GTP	PB-O3B-PG-O2G
5	D	503	GTP	C5'-O5'-PA-O3A
5	D	503	GTP	C5'-O5'-PA-O1A
5	D	503	GTP	C5'-O5'-PA-O2A
11	F	402	ACP	C5'-O5'-PA-O1A
9	B	504	W4Q	C4-C3-O2-C25
9	B	504	W4Q	C2-C3-O2-C25
5	C	502	GTP	PB-O3A-PA-O2A
11	F	402	ACP	C5'-O5'-PA-O2A
11	F	402	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	502	GTP	C4'-C5'-O5'-PA
9	B	504	W4Q	C6-C5-O3-C26
5	A	501	GTP	C4'-C5'-O5'-PA
5	D	503	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O1A
5	D	503	GTP	PB-O3A-PA-O1A
5	D	503	GTP	PB-O3A-PA-O2A

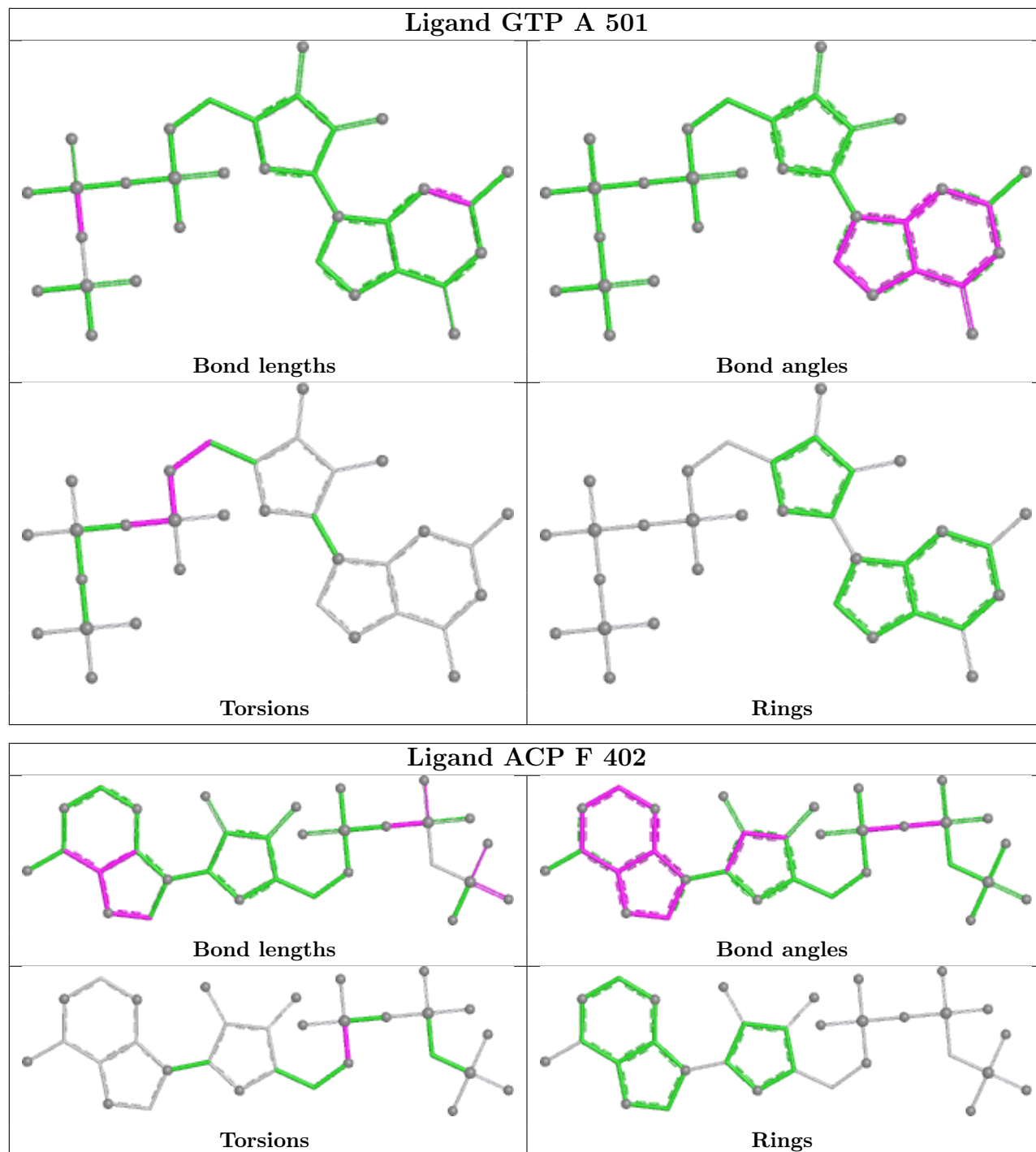
There are no ring outliers.

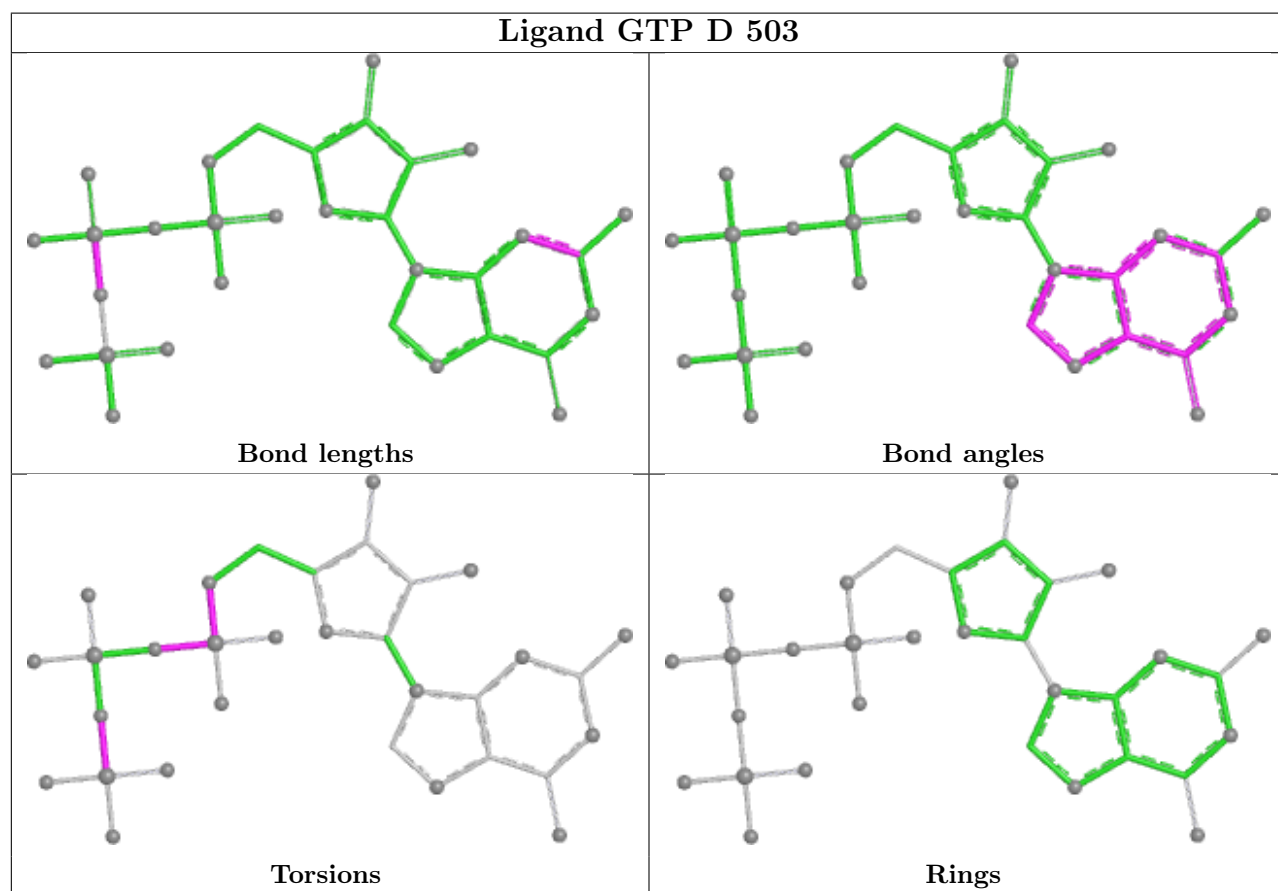
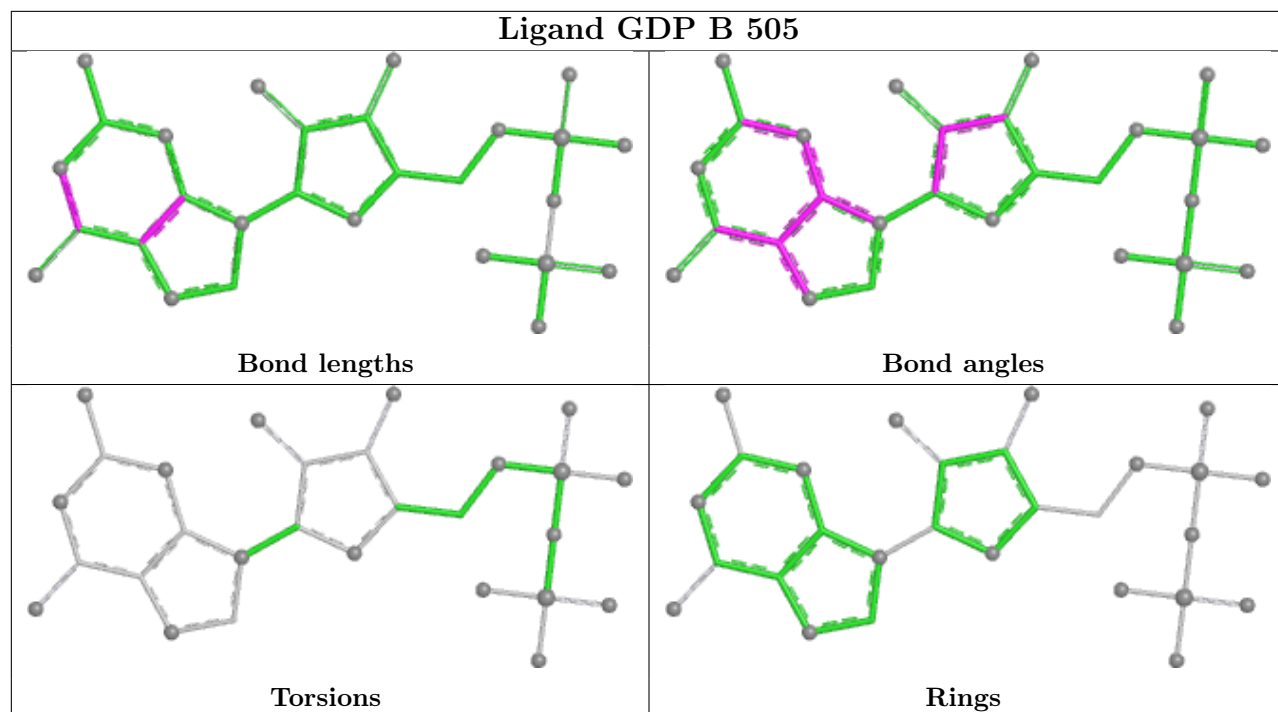
3 monomers are involved in 3 short contacts:

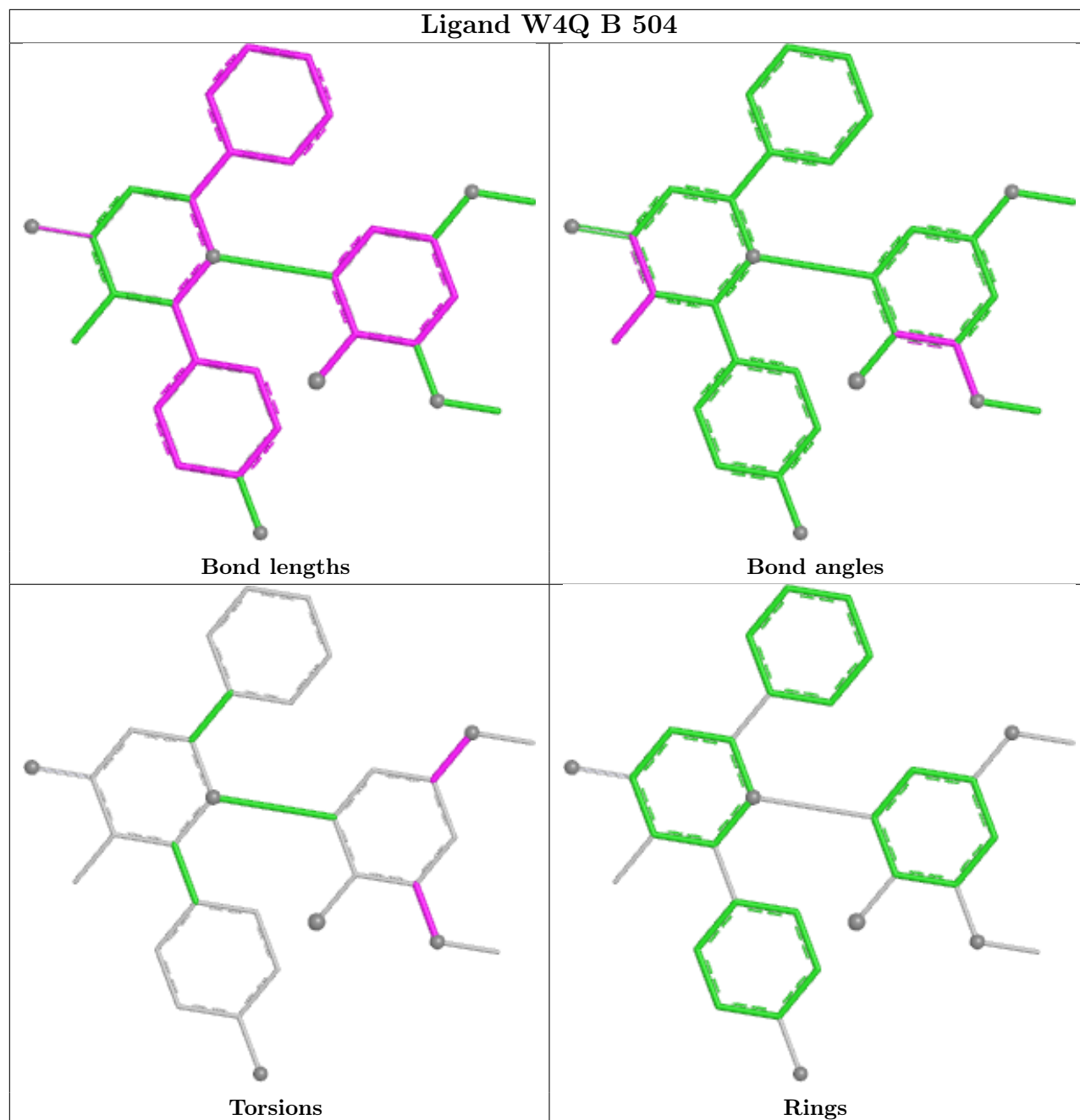
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
5	D	503	GTP	1	0
9	B	504	W4Q	1	0

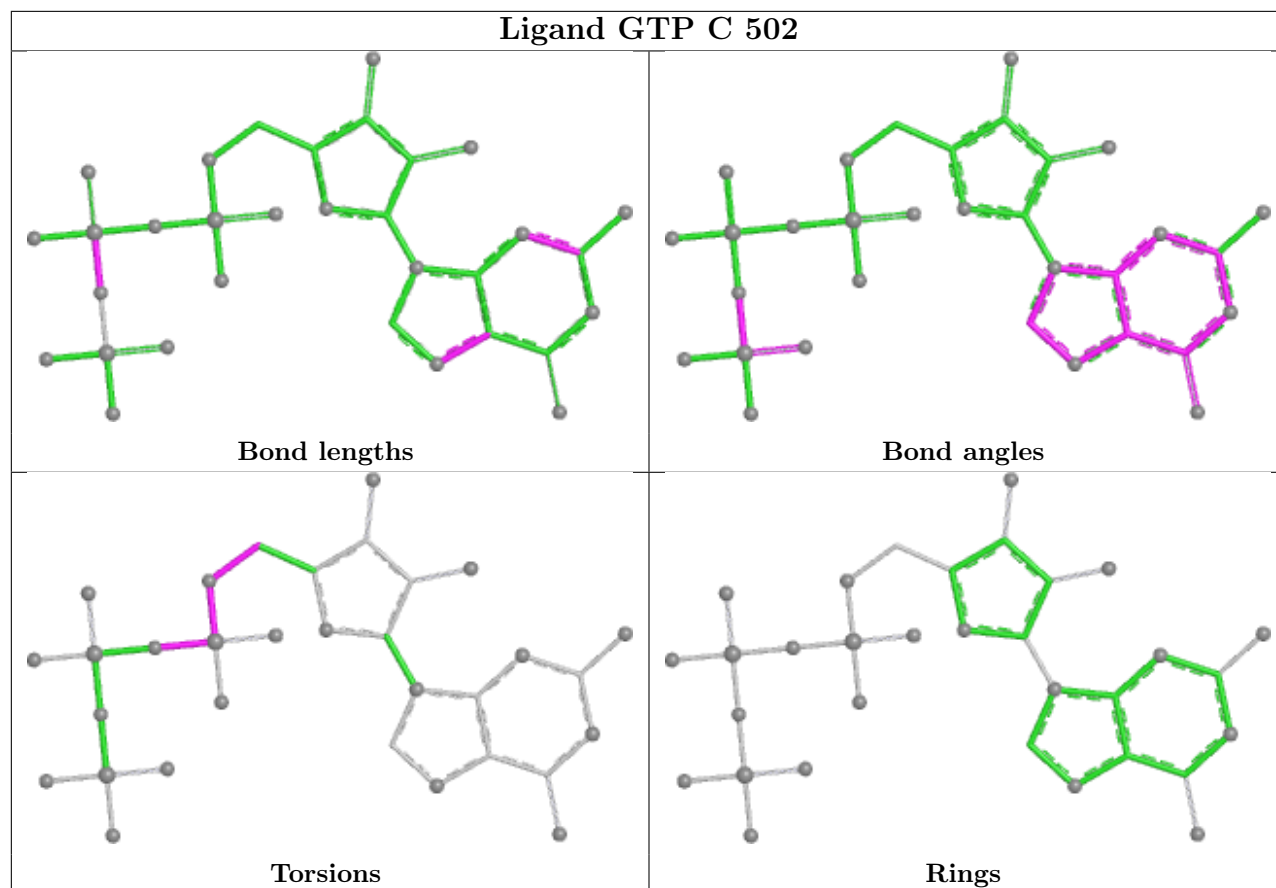
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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	438/451 (97%)	-0.52	1 (0%) 91 83	23, 55, 81, 121	3 (0%)
1	C	439/451 (97%)	-0.55	3 (0%) 84 68	22, 46, 72, 99	4 (0%)
2	B	418/431 (96%)	-0.52	0 100 100	23, 51, 83, 111	3 (0%)
2	D	426/431 (98%)	-0.32	2 (0%) 87 73	31, 62, 92, 121	1 (0%)
3	E	123/143 (86%)	-0.10	3 (2%) 59 38	32, 70, 107, 115	1 (0%)
4	F	351/384 (91%)	-0.07	3 (0%) 81 63	44, 75, 129, 143	0
All	All	2195/2291 (95%)	-0.39	12 (0%) 87 73	22, 58, 101, 143	12 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	2.9
1	C	88[A]	HIS	2.8
3	E	143	ALA	2.8
4	F	103	THR	2.7
1	C	133	GLN	2.5
3	E	12[A]	ASN	2.5
4	F	234	GLN	2.5
1	A	281	ALA	2.4
3	E	120	LEU	2.3
2	D	1	MET	2.2
4	F	237	THR	2.1
2	D	170	MET	2.1

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](#)

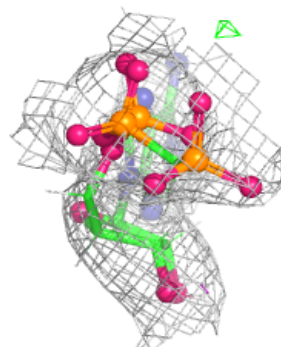
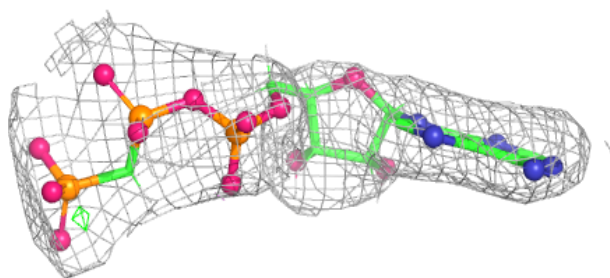
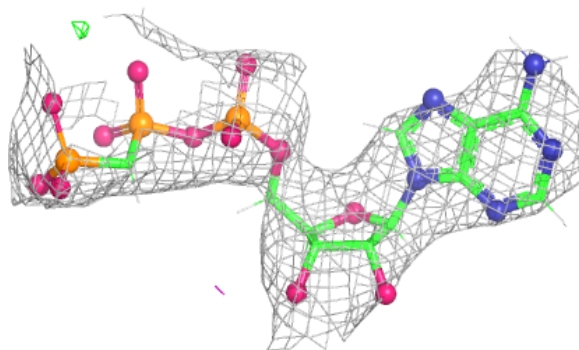
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	F	401	1/1	0.63	0.17	82,82,82,82	0
7	CA	B	503	1/1	0.75	0.10	92,92,92,92	0
7	CA	C	504	1/1	0.80	0.14	99,99,99,99	0
7	CA	B	502	1/1	0.82	0.18	86,86,86,86	0
6	MG	C	501	1/1	0.84	0.38	38,38,38,38	0
7	CA	D	502	1/1	0.89	0.09	84,84,84,84	0
11	ACP	F	402	31/31	0.92	0.09	64,92,112,121	0
10	GDP	B	505	28/28	0.94	0.09	29,48,65,78	0
5	GTP	D	503	32/32	0.95	0.08	43,54,65,70	0
7	CA	E	201	1/1	0.95	0.08	71,71,71,71	0
8	MES	B	501	12/12	0.96	0.09	39,55,65,67	0
9	W4Q	B	504	32/32	0.97	0.08	24,37,53,60	0
6	MG	D	501	1/1	0.97	0.07	41,41,41,41	0
5	GTP	A	501	32/32	0.97	0.07	33,46,59,71	0
7	CA	A	503	1/1	0.98	0.06	79,79,79,79	0
5	GTP	C	502	32/32	0.98	0.07	23,39,61,77	0
6	MG	A	502	1/1	0.99	0.10	30,30,30,30	0
6	MG	C	503	1/1	0.99	0.05	31,31,31,31	0
7	CA	C	505	1/1	0.99	0.03	74,74,74,74	0

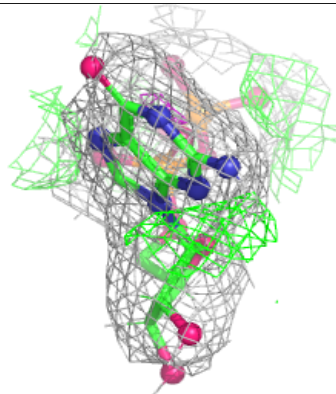
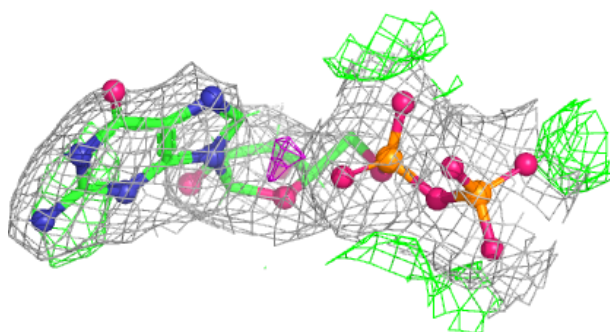
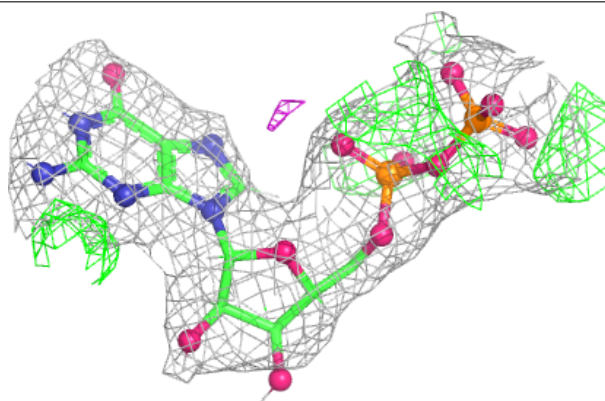
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

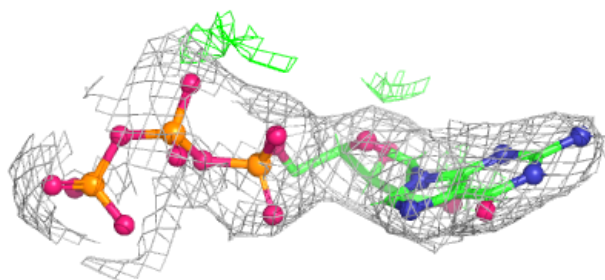
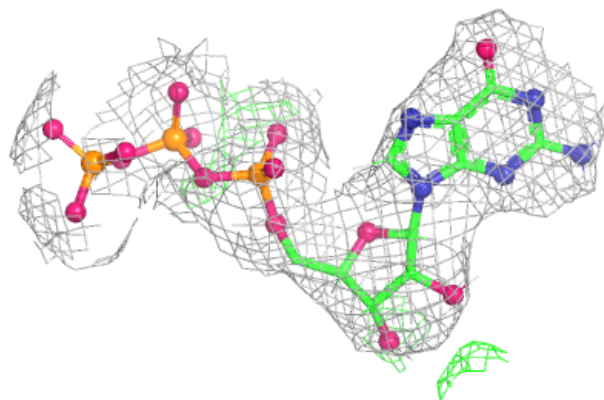
**Electron density around GDP B 505:**

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



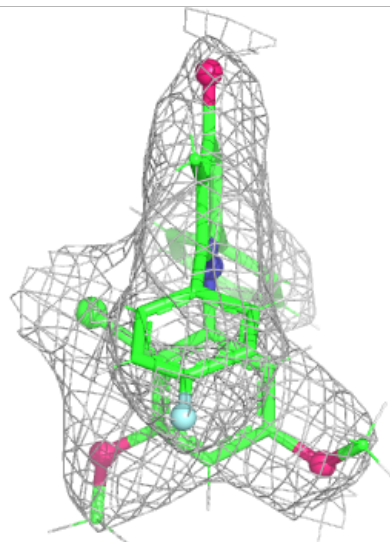
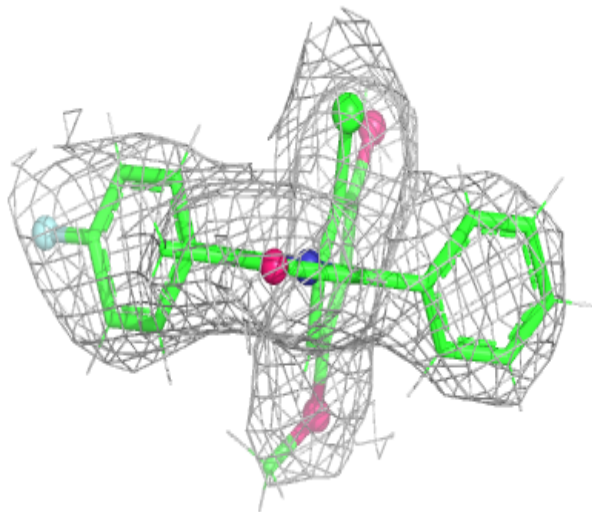
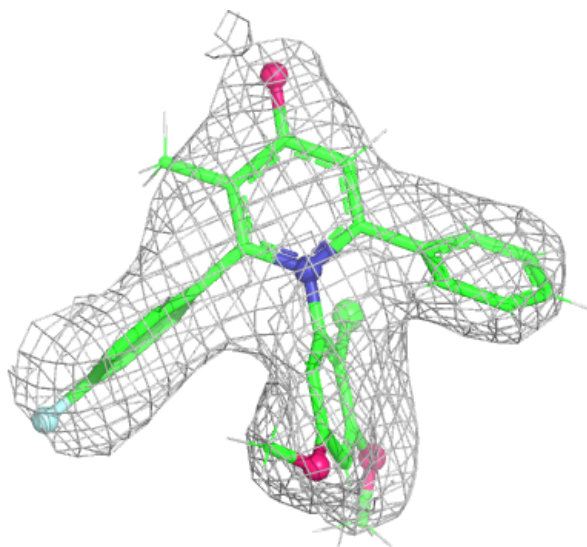
Electron density around GTP D 503:

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



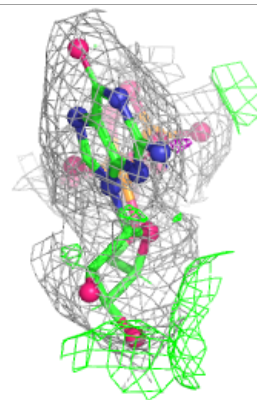
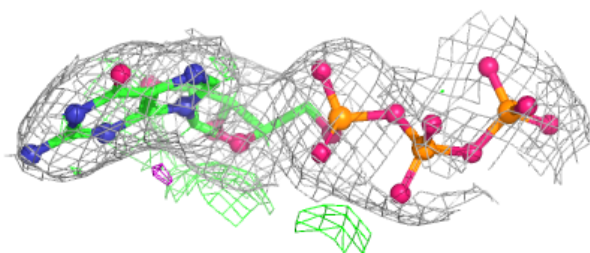
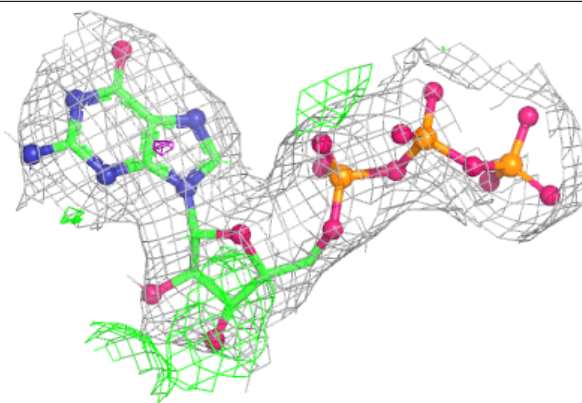
Electron density around W4Q B 504:

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

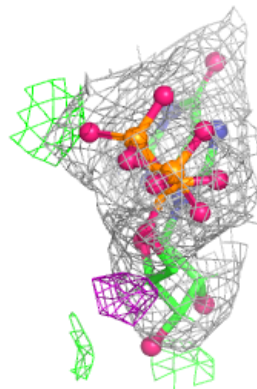
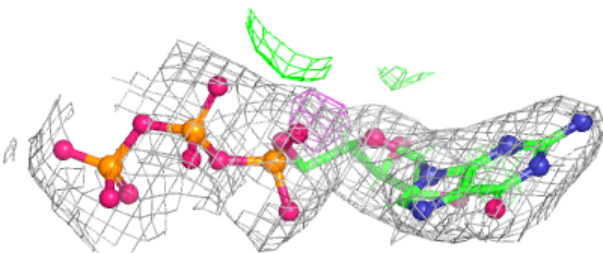
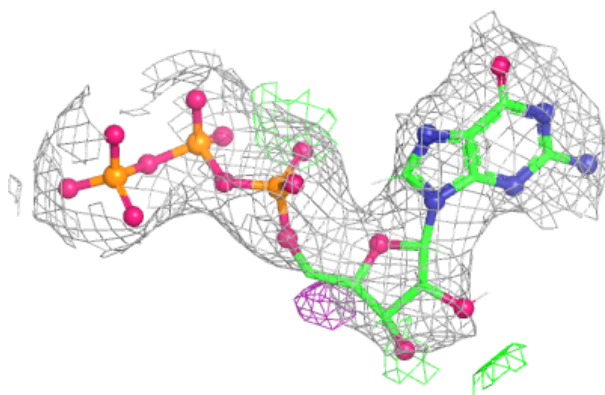


Electron density around GTP A 501:

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

**Electron density around GTP C 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.