



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 AM UTC

PDB ID : 8A9Z / pdb_00008a9z
Title : Tubulin-[1,2]oxazoloisoindole-2e complex
Authors : Prota, A.E.; Abel, A.-C.; Steinmetz, M.O.; Barraja, P.; Montalbano, A.; Spano, V.
Deposited on : 2022-06-29
Resolution : 2.29 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

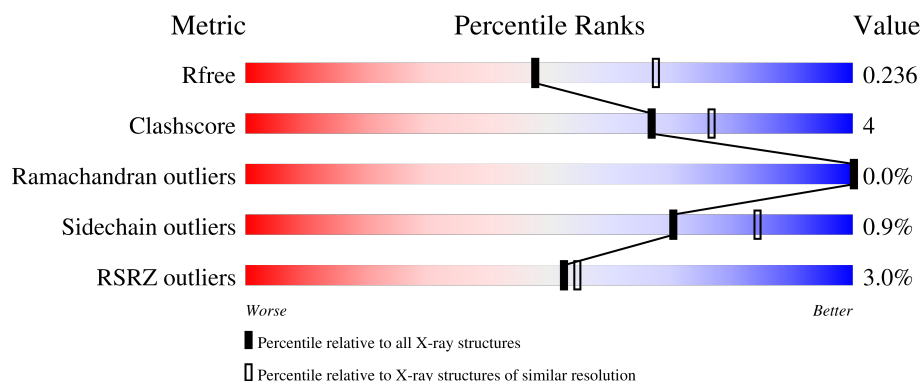
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	451	0% 86% 10% .
1	C	451	2% 88% 9% .
2	B	445	2% 87% 9% .
2	D	445	3% 84% 11% .
3	E	143	5% 81% 15% .

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Mol	Chain	Length	Quality of chain
4	F	384	5% 70% 10% 19%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	6	0
			3443	2183	583	653	24			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	1	0
			3368	2115	576	650	27			
2	D	425	Total	C	N	O	S	0	0	0
			3335	2094	569	645	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	0	0
			1009	622	182	200	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 beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	310	Total	C	N	O	S	0	0	0
			2539	1640	432	455	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

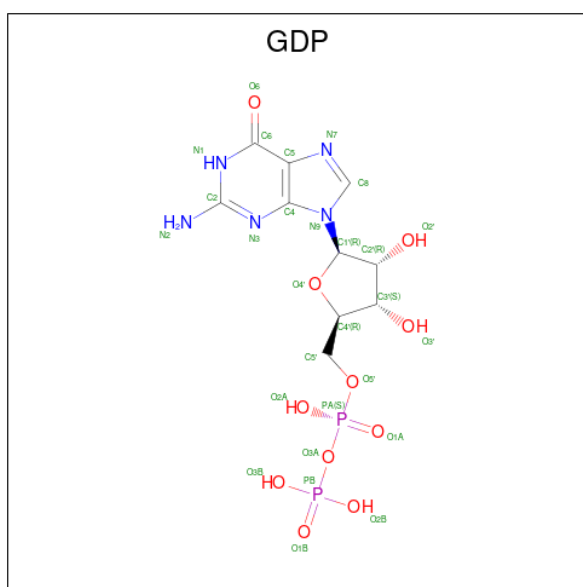
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



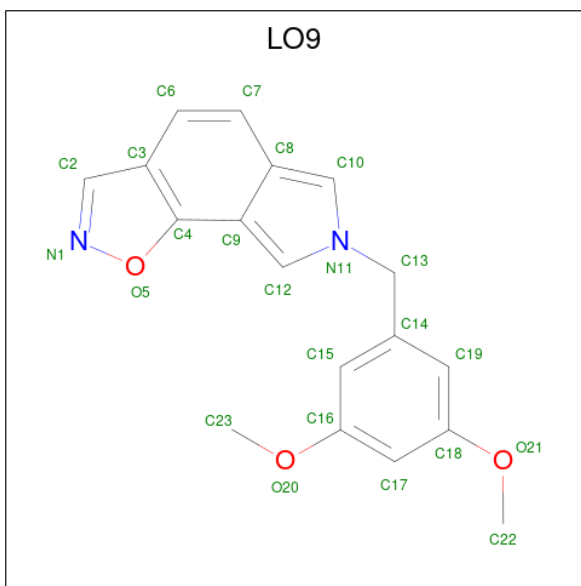
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



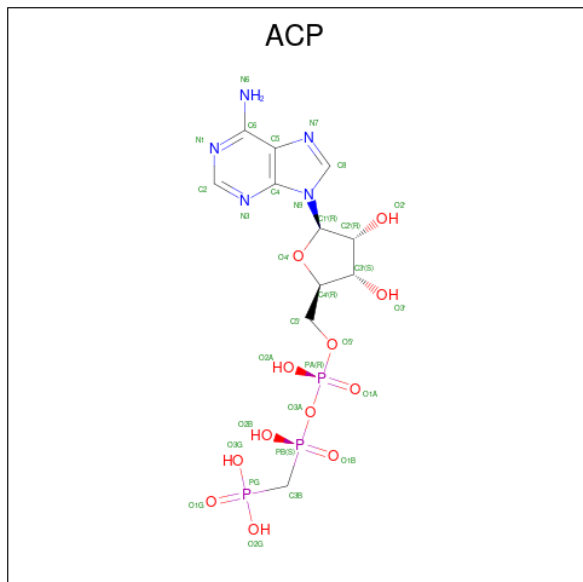
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 7-[(3,5-dimethoxyphenyl)methyl]pyrrolo[3,4-g][1,2]benzoxazole (CCD ID: LO9) (formula: $C_{18}H_{16}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O		0	0
			23	18	2	3			
10	D	1	Total	C	N	O		0	0
			23	18	2	3			

- 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	N	O	P	0	0
			31	11	5	12	3		

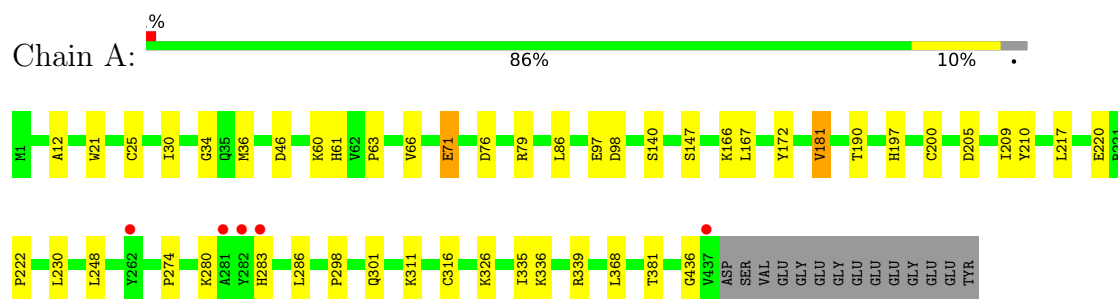
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	85	Total	O	0	0
			85	85		
12	B	90	Total	O	0	0
			90	90		
12	C	154	Total	O	0	0
			154	154		
12	D	44	Total	O	0	0
			44	44		
12	E	15	Total	O	0	0
			15	15		
12	F	49	Total	O	0	0
			49	49		

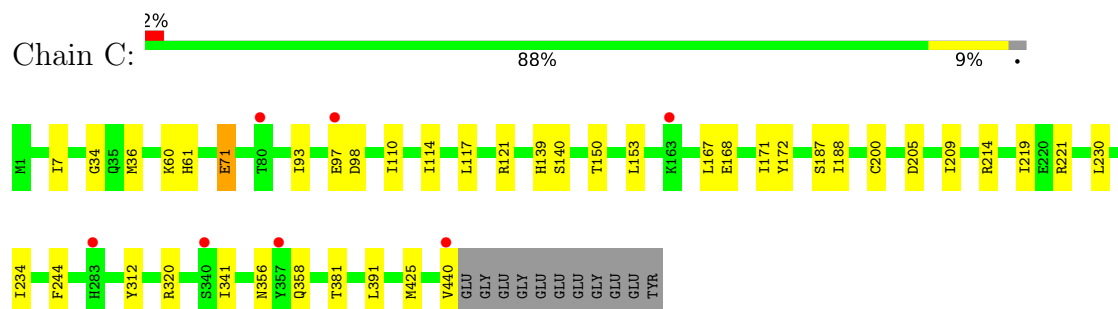
3 Residue-property plots [i](#)

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

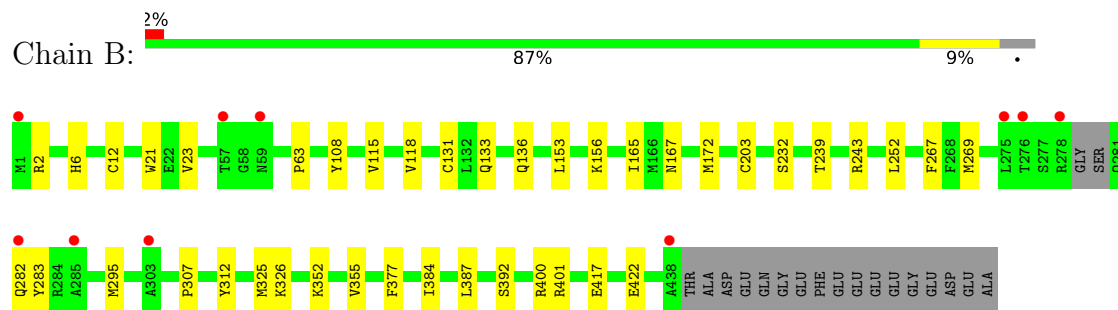
- Molecule 1: Tubulin alpha-1B chain



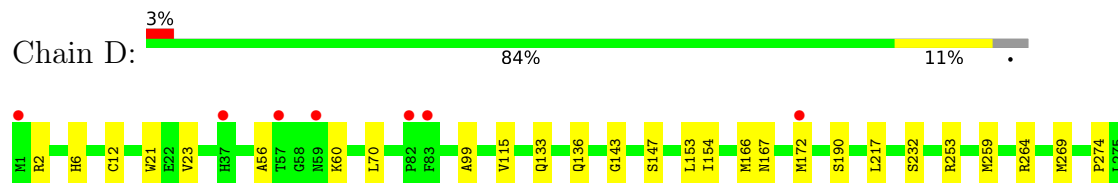
- Molecule 1: Tubulin alpha-1B chain

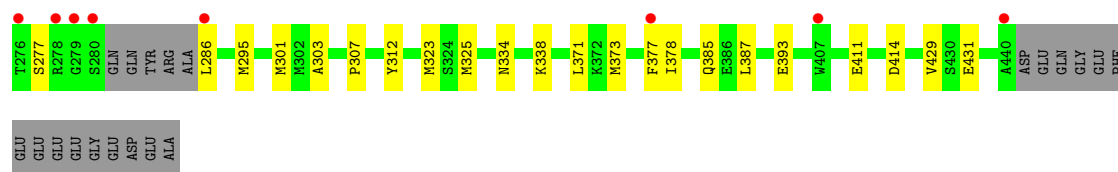


- Molecule 2: Tubulin beta-2B chain

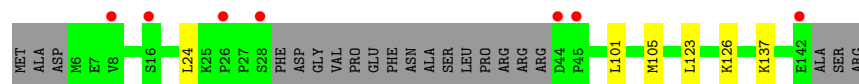
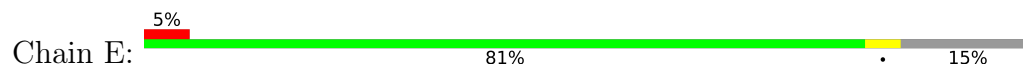


- Molecule 2: Tubulin beta-2B chain

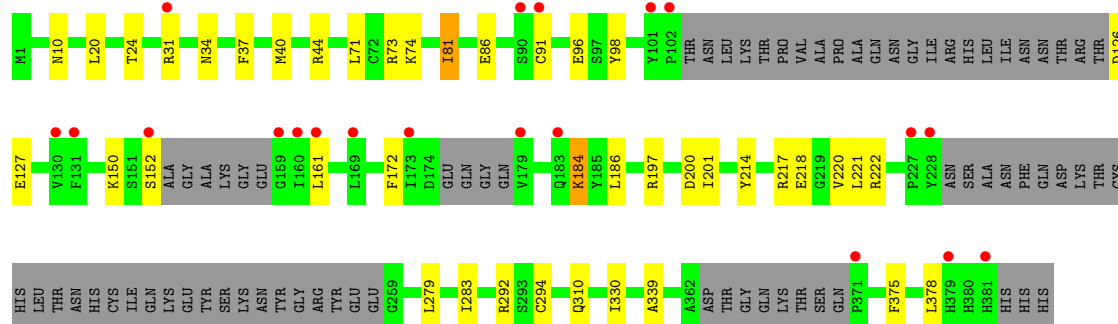




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.50Å 155.85Å 178.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 2.29 49.89 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.89-2.29) 99.8 (49.89-2.29)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.199 , 0.240 0.196 , 0.236	Depositor DCC
R_{free} test set	6539 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17786	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: CA, GDP, GTP, MG, ACP, LO9, MES

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	0.12	0/3536	0.28	0/4801
1	C	0.12	0/3515	0.30	0/4772
2	B	0.17	0/3442	0.33	0/4660
2	D	0.10	0/3408	0.25	0/4615
3	E	0.09	0/1017	0.20	0/1349
4	F	0.10	0/2597	0.27	0/3507
All	All	0.12	0/17515	0.29	0/23704

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	3443	0	3372	29	0
1	C	3437	0	3348	20	0
2	B	3368	0	3246	28	0
2	D	3335	0	3218	28	0
3	E	1009	0	1024	5	0
4	F	2539	0	2533	20	0
5	A	32	0	12	0	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
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	12	0	13	0	0
10	B	23	0	0	2	0
10	D	23	0	0	0	0
11	F	31	0	14	2	0
12	A	85	0	0	1	0
12	B	90	0	0	1	0
12	C	154	0	0	0	0
12	D	44	0	0	1	0
12	E	15	0	0	0	0
12	F	49	0	0	0	0
All	All	17786	0	16816	125	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 4.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:31:ARG:HG3	4:F:34:ASN:HB2	1.72	0.72
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.78	0.64
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.80	0.62
2:D:253:ARG:NH1	12:D:601:HOH:O	2.24	0.62
2:B:325:MET:HG3	2:B:355:VAL:HG21	1.82	0.61
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.84	0.59
4:F:330:ILE:HG21	11:F:401:ACP:H5'2	1.85	0.58
1:A:280:LYS:NZ	12:A:601:HOH:O	2.36	0.58
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.85	0.58
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.87	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.86	0.57
2:D:217:LEU:HA	2:D:277:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HE2	1:A:283:HIS:HA	1.86	0.56
4:F:74:LYS:HG3	4:F:152:SER:HB3	1.86	0.56
2:B:352:LYS:NZ	12:B:601:HOH:O	2.38	0.55
1:C:97:GLU:O	1:C:110:ILE:HG21	2.07	0.55
1:A:97:GLU:HG3	2:B:131:CYS:SG	2.48	0.54
1:A:181:VAL:HG13	10:B:505:LO9:C2	2.37	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.54
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.39	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.52
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.91	0.52
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.92	0.52
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.92	0.52
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.93	0.51
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.93	0.51
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.91	0.51
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.10	0.51
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.94	0.50
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.30	0.50
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.94	0.50
2:D:334:ASN:OD1	2:D:338:LYS:NZ	2.35	0.50
2:B:269:MET:HG2	2:B:384:ILE:HD13	1.94	0.49
2:B:136:GLN:HA	2:B:167:ASN:O	2.12	0.49
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.94	0.49
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.43	0.49
1:C:221:ARG:HG2	2:D:325:MET:CG	2.44	0.48
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.95	0.48
2:D:136:GLN:HA	2:D:167:ASN:O	2.14	0.48
2:B:352:LYS:HB2	10:B:505:LO9:C4	2.44	0.48
2:B:392:SER:OG	2:B:422[A]:GLU:OE2	2.32	0.48
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.49	0.47
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.47
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.97	0.47
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.97	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.47
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.97	0.47
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.50	0.46
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.46
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.96	0.46
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.97	0.46
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.98	0.46
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.97	0.46
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.97	0.46
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.97	0.46
2:D:301:MET:HE3	2:D:307:PRO:HG3	1.96	0.46
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.32	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.45
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.52	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.45
2:D:147:SER:OG	2:D:190:SER:OG	2.32	0.45
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.52	0.45
3:E:123:LEU:HD23	3:E:126:LYS:HD3	1.99	0.45
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.53	0.44
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.00	0.44
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.99	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
4:F:161:LEU:HD22	4:F:172:PHE:HB2	1.99	0.44
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.99	0.44
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.99	0.44
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.36	0.44
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.98	0.44
3:E:123:LEU:HA	3:E:126:LYS:HD3	1.99	0.44
4:F:81:ILE:HG23	4:F:91:CYS:SG	2.58	0.44
1:C:140:SER:HA	1:C:171:ILE:HB	2.00	0.44
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.99	0.44
2:D:323:MET:HE2	2:D:373:MET:HG2	1.99	0.44
4:F:86:GLU:H	4:F:86:GLU:CD	2.26	0.43
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.53	0.43
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.49	0.43
2:D:274:PRO:HD2	2:D:371:LEU:HD13	2.01	0.43
2:B:295:MET:CG	2:B:377:PHE:HB2	2.48	0.43
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.00	0.43
3:E:101:LEU:O	3:E:105:MET:HG2	2.19	0.43
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.85	0.43
2:B:115:VAL:HG21	2:B:156:LYS:HD2	2.01	0.43
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.54	0.43
1:A:248:LEU:HD21	1:A:316[B]:CYS:SG	2.60	0.42
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.59	0.42
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.83	0.42
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:220:VAL:HG11	4:F:339:ALA:HB2	2.01	0.42
2:B:282:GLN:H	2:B:282:GLN:CD	2.27	0.42
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.55	0.42
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.37	0.42
2:B:239:THR:O	2:B:243:ARG:HG3	2.19	0.42
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.52	0.42
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.42
4:F:126:ASP:OD1	4:F:127:GLU:N	2.53	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.02	0.42
1:A:298:PRO:HA	1:A:301:GLN:CD	2.44	0.41
2:B:2:ARG:HA	2:B:131:CYS:O	2.20	0.41
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.20	0.41
1:A:63:PRO:HD3	1:A:86:LEU:HG	2.02	0.41
2:D:23:VAL:HG21	2:D:232:SER:HB2	2.01	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.41
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.55	0.41
1:A:46:ASP:OD1	1:A:46:ASP:N	2.49	0.41
1:A:220:GLU:HB3	2:B:326:LYS:HD2	2.03	0.41
1:A:336:LYS:HG3	3:E:24:LEU:HD13	2.02	0.41
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.03	0.41
4:F:184:LYS:O	11:F:401:ACP:N6	2.51	0.41
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.03	0.41
4:F:292:ARG:HD3	4:F:378:LEU:HB3	2.02	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.03	0.41
1:A:25:CYS:HB3	1:A:30:ILE:O	2.21	0.41
1:C:214:ARG:HG2	1:C:219:ILE:O	2.21	0.41
2:D:411:GLU:HA	3:E:137:LYS:HD2	2.03	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.21	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41
2:D:259:MET:HE2	2:D:378:ILE:HG22	2.02	0.40
2:D:414:ASP:OD1	2:D:414:ASP:N	2.55	0.40

There are no symmetry-related clashes.

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	441/451 (98%)	434 (98%)	7 (2%)	0	100	100
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	423/445 (95%)	416 (98%)	7 (2%)	0	100	100
2	D	421/445 (95%)	413 (98%)	8 (2%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	298/384 (78%)	294 (99%)	3 (1%)	1 (0%)	36	46
All	All	2139/2319 (92%)	2104 (98%)	34 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	186	LEU

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	374/379 (99%)	370 (99%)	4 (1%)	65	81
1	C	371/379 (98%)	366 (99%)	5 (1%)	61	77
2	B	370/383 (97%)	369 (100%)	1 (0%)	86	93
2	D	367/383 (96%)	366 (100%)	1 (0%)	86	93
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	279/342 (82%)	273 (98%)	6 (2%)	45	65
All	All	1871/1993 (94%)	1854 (99%)	17 (1%)	70	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL

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Mol	Chain	Res	Type
1	A	71	GLU
1	A	181	VAL
1	A	381	THR
2	B	283	TYR
1	C	71	GLU
1	C	168	GLU
1	C	234	ILE
1	C	381	THR
1	C	440	VAL
2	D	393	GLU
4	F	73	ARG
4	F	81	ILE
4	F	150	LYS
4	F	184	LYS
4	F	197	ARG
4	F	310	GLN

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	11	GLN
1	A	15	GLN
1	A	176	GLN
1	A	301	GLN
1	A	393	HIS
2	B	50	ASN
2	B	331	GLN
1	C	256	GLN
1	C	393	HIS
2	D	426	ASN
3	E	12	ASN
4	F	183	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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, 9 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	B	501	6	29,30,30	1.19	3 (10%)	45,47,47	1.72	6 (13%)
5	GTP	C	501	6	33,34,34	0.90	0	50,54,54	1.58	12 (24%)
5	GTP	A	501	6	33,34,34	0.97	3 (9%)	50,54,54	1.51	8 (16%)
9	MES	B	504	-	12,12,12	0.68	0	15,16,16	0.36	0
8	GDP	D	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.68	6 (13%)
10	LO9	B	505	-	21,26,26	3.28	6 (28%)	29,37,37	3.14	11 (37%)
11	ACP	F	401	-	31,33,33	0.78	2 (6%)	47,52,52	0.83	1 (2%)
10	LO9	D	503	-	21,26,26	3.27	6 (28%)	29,37,37	3.00	10 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
8	GDP	D	501	6	-	4/16/32/32	0/3/3/3
10	LO9	B	505	-	-	3/8/8/8	0/4/4/4
11	ACP	F	401	-	-	4/19/38/38	0/3/3/3
10	LO9	D	503	-	-	3/8/8/8	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	LO9	C6-C7	11.20	1.56	1.38
10	D	503	LO9	C6-C7	11.10	1.56	1.38
10	D	503	LO9	C6-C3	6.26	1.51	1.41
10	B	505	LO9	C6-C3	6.16	1.51	1.41
10	B	505	LO9	C10-N11	4.18	1.42	1.37
10	B	505	LO9	C3-C4	-4.07	1.35	1.40
10	D	503	LO9	C10-N11	4.07	1.42	1.37
10	D	503	LO9	O5-N1	-3.94	1.37	1.42
10	B	505	LO9	O5-N1	-3.88	1.37	1.42
10	D	503	LO9	C3-C4	-3.85	1.35	1.40
11	F	401	ACP	PB-O3A	3.59	1.62	1.58
8	D	501	GDP	C5-C4	3.16	1.47	1.38
8	B	501	GDP	C5-C4	3.05	1.47	1.38
10	D	503	LO9	C12-N11	2.98	1.41	1.37
10	B	505	LO9	C12-N11	2.74	1.40	1.37
8	B	501	GDP	PA-O3A	2.44	1.62	1.59
8	B	501	GDP	C6-N1	-2.44	1.34	1.38
11	F	401	ACP	PA-O3A	2.33	1.62	1.59
8	D	501	GDP	C6-N1	-2.23	1.34	1.38
5	A	501	GTP	PA-O3A	2.12	1.61	1.59
5	A	501	GTP	C2-N3	2.08	1.38	1.33
5	A	501	GTP	PB-O3A	2.05	1.61	1.59

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	LO9	O5-N1-C2	7.90	109.12	104.98
10	D	503	LO9	O5-N1-C2	7.82	109.08	104.98
10	B	505	LO9	C13-N11-C10	7.66	134.83	125.47
10	D	503	LO9	C13-N11-C10	6.77	133.73	125.47
10	B	505	LO9	C13-N11-C12	-6.02	118.12	125.47
8	B	501	GDP	C5-C4-N3	-5.95	118.92	128.39
8	D	501	GDP	C5-C4-N3	-5.73	119.27	128.39
11	F	401	ACP	PB-O3A-PA	-5.43	114.66	132.37
8	B	501	GDP	C2-N3-C4	5.11	121.09	112.30
10	D	503	LO9	C10-N11-C12	-4.99	106.82	110.10
10	D	503	LO9	C13-N11-C12	-4.95	119.42	125.47
8	D	501	GDP	C2-N3-C4	4.86	120.68	112.30
5	A	501	GTP	C5-C4-N3	-4.72	120.87	128.39
5	C	501	GTP	C5-C4-N3	-4.65	120.99	128.39
10	B	505	LO9	C10-N11-C12	-4.65	107.04	110.10
5	C	501	GTP	C2-N3-C4	4.48	120.02	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	N9-C4-N3	4.43	134.82	125.95
10	D	503	LO9	C13-C14-C15	4.40	128.57	120.27
5	A	501	GTP	C2-N3-C4	4.40	119.88	112.30
10	B	505	LO9	C6-C7-C8	-4.33	114.97	120.94
8	D	501	GDP	N9-C4-N3	4.14	134.24	125.95
10	D	503	LO9	C6-C7-C8	-4.12	115.25	120.94
10	B	505	LO9	C13-C14-C15	4.08	127.96	120.27
10	D	503	LO9	C6-C3-C4	3.98	123.83	119.28
10	B	505	LO9	C6-C3-C4	3.84	123.67	119.28
10	D	503	LO9	C13-C14-C19	-3.75	113.20	120.27
10	B	505	LO9	C13-C14-C19	-3.65	113.39	120.27
8	D	501	GDP	C6-C5-N7	3.54	136.74	130.29
10	B	505	LO9	C14-C13-N11	3.46	119.02	112.39
8	B	501	GDP	C6-C5-N7	3.45	136.56	130.29
10	D	503	LO9	C7-C6-C3	-3.38	114.96	121.36
10	B	505	LO9	C7-C6-C3	-3.27	115.16	121.36
5	A	501	GTP	N9-C4-N3	2.89	131.73	125.95
5	C	501	GTP	N9-C8-N7	-2.87	108.07	113.40
5	C	501	GTP	C2-N1-C6	-2.74	120.15	125.11
5	C	501	GTP	N9-C4-N3	2.73	131.42	125.95
5	A	501	GTP	C2-N1-C6	-2.73	120.16	125.11
5	C	501	GTP	C8-N7-C5	2.71	109.09	104.26
8	D	501	GDP	C4-C5-N7	-2.67	106.43	110.67
5	A	501	GTP	N9-C8-N7	-2.65	108.48	113.40
10	D	503	LO9	C14-C13-N11	2.60	117.38	112.39
8	B	501	GDP	C4-C5-N7	-2.57	106.59	110.67
5	A	501	GTP	C8-N7-C5	2.51	108.73	104.26
5	C	501	GTP	O2B-PB-O3A	2.44	113.86	107.27
5	A	501	GTP	C5-C6-N1	2.38	119.31	113.25
5	C	501	GTP	C5-C6-N1	2.36	119.26	113.25
10	B	505	LO9	C9-C12-N11	-2.21	107.16	109.60
5	A	501	GTP	O6-C6-C5	-2.16	120.83	126.53
5	C	501	GTP	O6-C6-C5	-2.14	120.89	126.53
8	B	501	GDP	O6-C6-C5	-2.13	120.91	126.53
5	C	501	GTP	O3G-PG-O3B	2.10	111.67	104.64
5	C	501	GTP	O2A-PA-O3A	2.07	112.87	107.27
5	C	501	GTP	C4-C5-N7	-2.05	107.42	110.67
8	D	501	GDP	O6-C6-C5	-2.01	121.24	126.53

There are no chirality outliers.

All (32) 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	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	PA-O3A-PB-O3B
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
10	D	503	LO9	C15-C16-O20-C23
10	D	503	LO9	C17-C16-O20-C23
10	B	505	LO9	C17-C16-O20-C23
10	B	505	LO9	C15-C16-O20-C23
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O1A
10	B	505	LO9	C14-C13-N11-C12
10	D	503	LO9	C14-C13-N11-C12

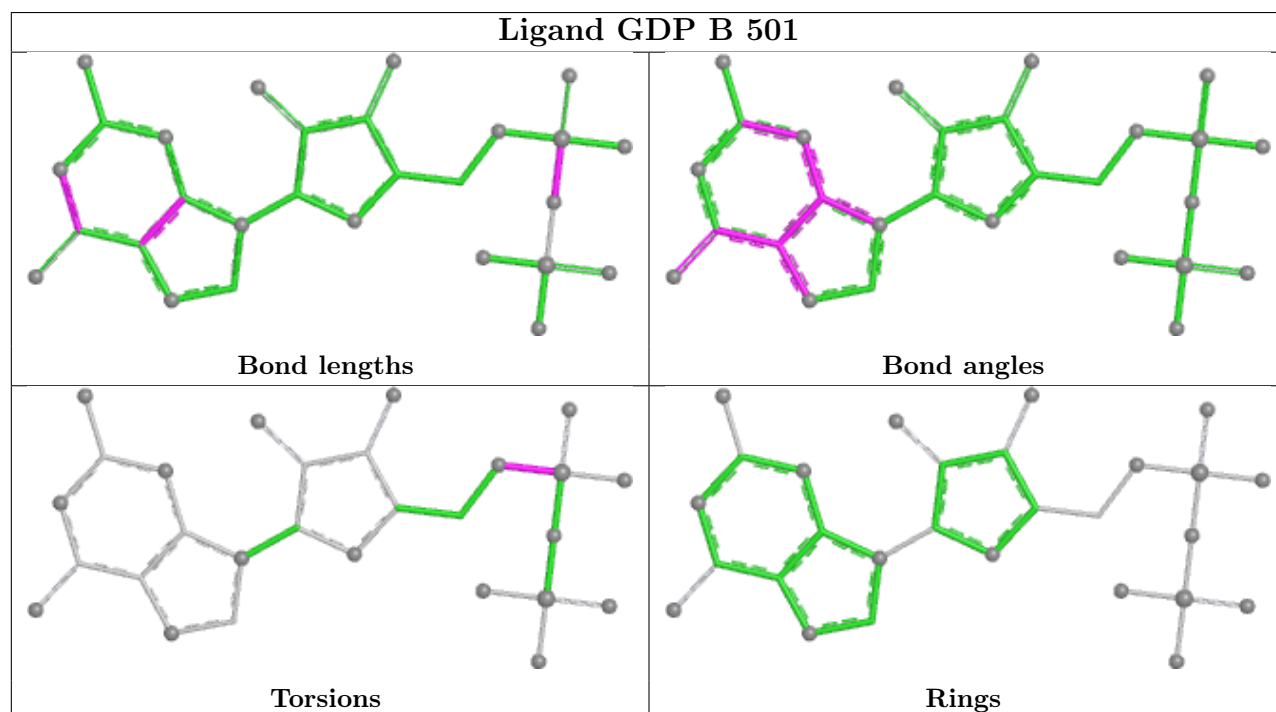
There are no ring outliers.

4 monomers are involved in 7 short contacts:

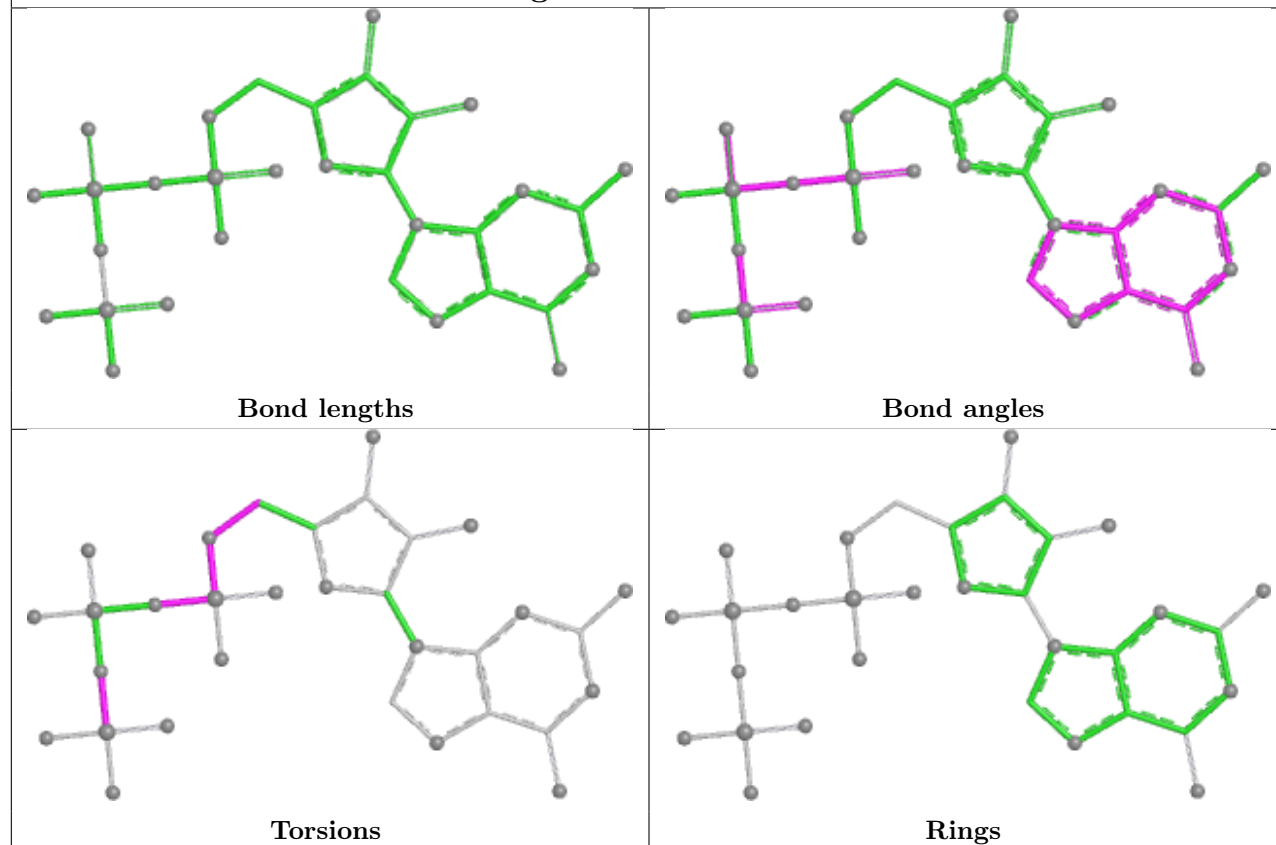
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	1	0
8	D	501	GDP	2	0
10	B	505	LO9	2	0
11	F	401	ACP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

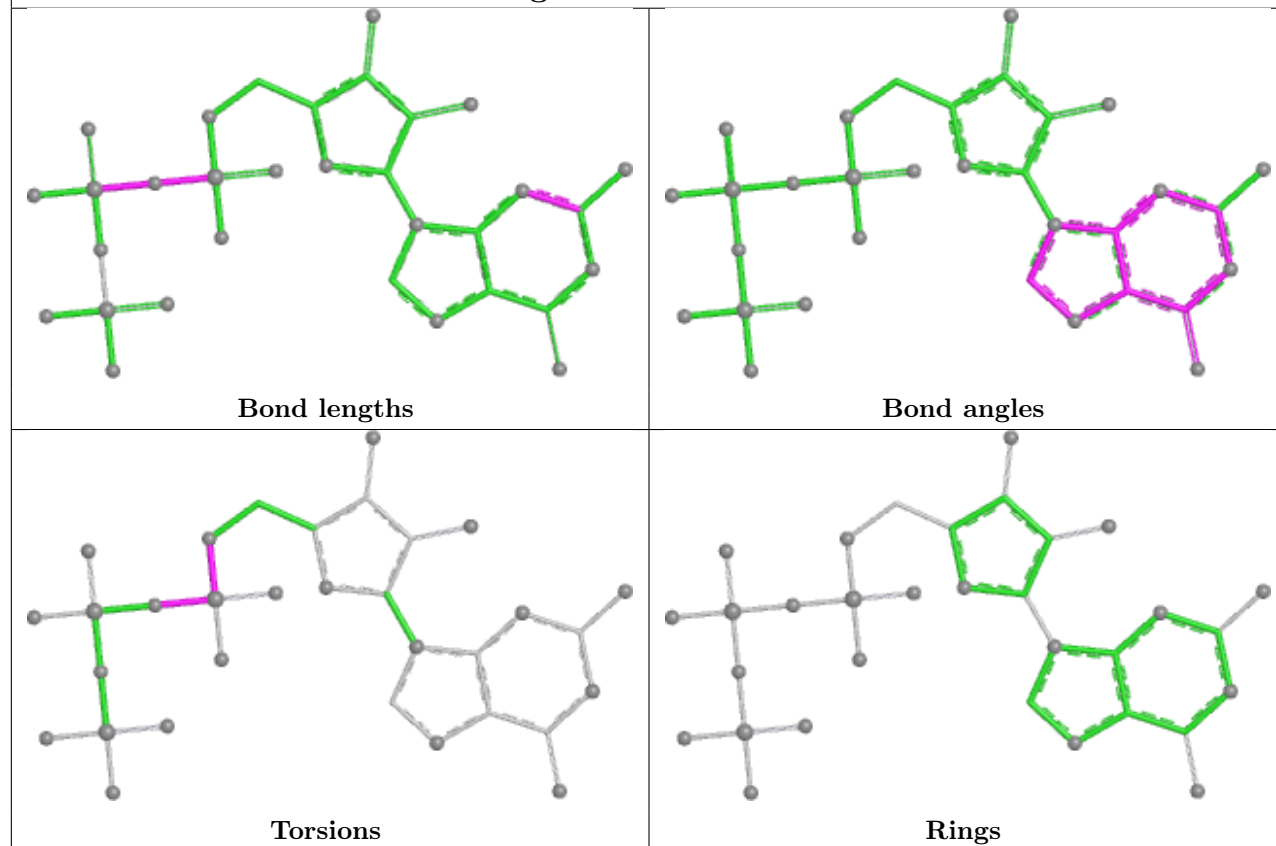
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

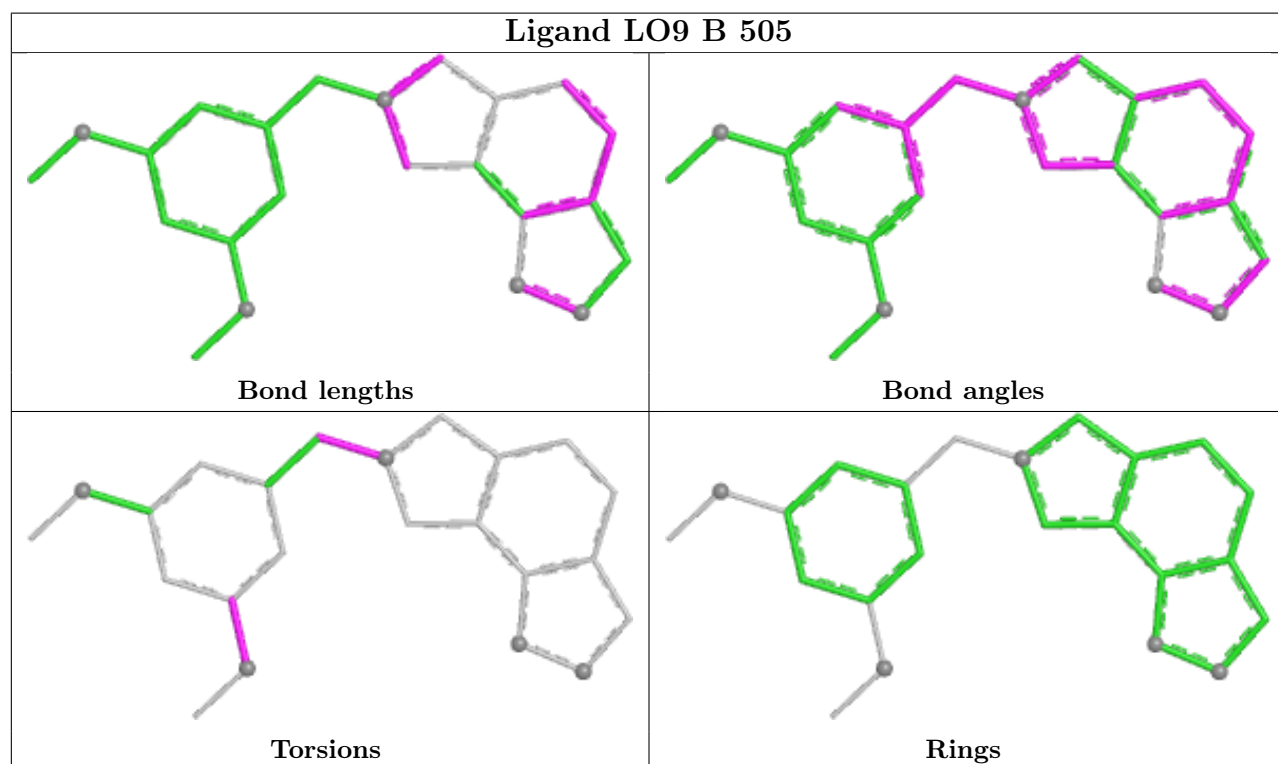
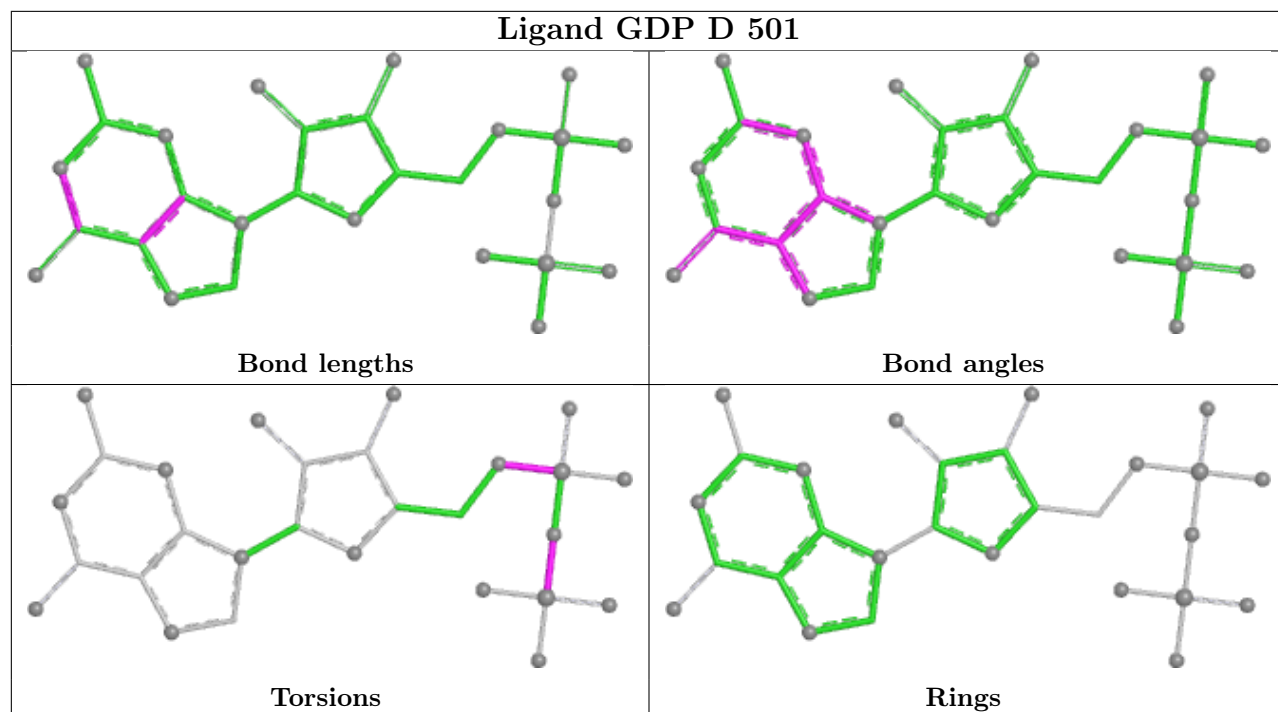


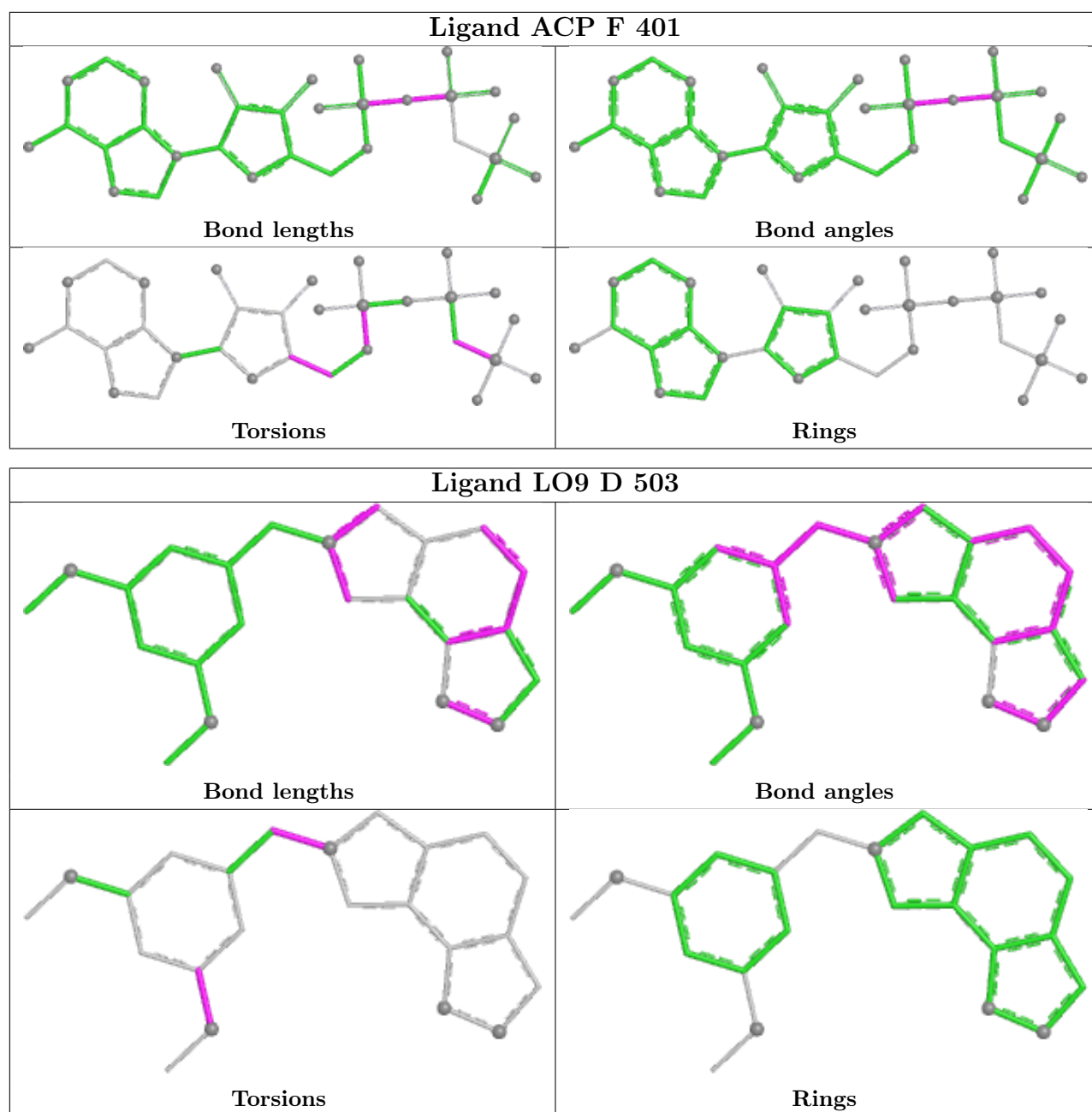
Ligand GTP C 501



Ligand GTP A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	-0.03	5 (1%) 78 79	30, 63, 95, 147	6 (1%)
1	C	440/451 (97%)	-0.22	7 (1%) 70 72	38, 51, 78, 116	0
2	B	426/445 (95%)	-0.07	10 (2%) 61 63	25, 55, 88, 139	1 (0%)
2	D	425/445 (95%)	0.25	15 (3%) 47 49	47, 73, 109, 158	1 (0%)
3	E	122/143 (85%)	0.50	7 (5%) 29 31	55, 78, 111, 139	0
4	F	310/384 (80%)	0.51	20 (6%) 25 27	56, 81, 142, 177	0
All	All	2160/2319 (93%)	0.08	64 (2%) 52 54	25, 64, 112, 177	8 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	371	PRO	4.7
4	F	159	GLY	4.4
1	C	357	TYR	3.9
1	A	437	VAL	3.8
2	D	1	MET	3.8
2	D	377	PHE	3.6
4	F	152	SER	3.6
4	F	381	HIS	3.4
4	F	173	ILE	3.4
2	D	286	LEU	3.4
2	B	285	ALA	3.4
2	D	407	TRP	3.3
4	F	102	PRO	3.2
2	B	278	ARG	3.1
4	F	160	ILE	3.1
2	D	279	GLY	3.0
1	C	163	LYS	2.9
4	F	179	VAL	2.9
1	C	80	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	2.8
4	F	91	CYS	2.8
2	D	82	PRO	2.8
1	C	440	VAL	2.8
2	B	303	ALA	2.7
4	F	101	TYR	2.7
4	F	228	TYR	2.7
2	D	280	SER	2.7
3	E	16	SER	2.7
4	F	31	ARG	2.7
2	D	276	THR	2.6
2	B	438	ALA	2.6
1	A	283	HIS	2.6
2	D	172	MET	2.5
4	F	227	PRO	2.5
1	C	340	SER	2.5
2	B	275	LEU	2.5
2	B	59	ASN	2.5
2	D	440	ALA	2.5
3	E	45	PRO	2.5
1	A	262	TYR	2.5
2	D	57	THR	2.4
3	E	28	SER	2.4
4	F	131	PHE	2.4
2	B	276	THR	2.4
4	F	161	LEU	2.4
3	E	26	PRO	2.3
2	B	1	MET	2.3
4	F	379	HIS	2.3
2	D	83	PHE	2.2
4	F	169	LEU	2.2
3	E	142	GLU	2.2
4	F	90	SER	2.2
2	D	59	ASN	2.2
2	D	278	ARG	2.2
4	F	130	VAL	2.1
2	B	57	THR	2.1
3	E	8	VAL	2.1
1	C	283	HIS	2.1
4	F	183	GLN	2.1
1	C	97	GLU	2.0
3	E	44	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	2.0
2	B	282	GLN	2.0
2	D	37	HIS	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.

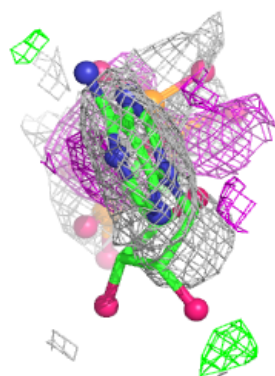
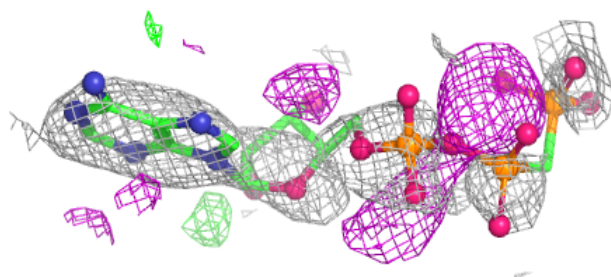
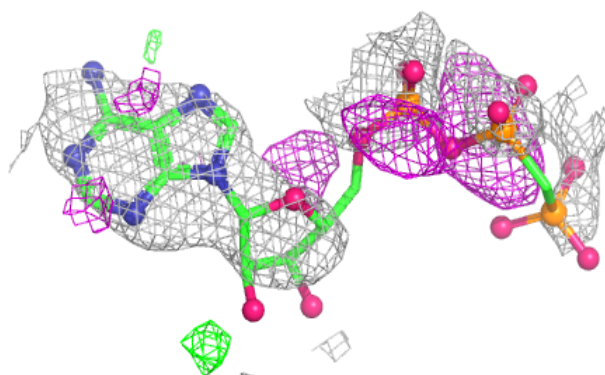
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ACP	F	401	31/31	0.65	0.14	160,174,243,250	0
7	CA	E	201	1/1	0.89	0.11	103,103,103,103	0
7	CA	B	503	1/1	0.90	0.12	99,99,99,99	0
7	CA	C	504	1/1	0.92	0.29	81,81,81,81	0
10	LO9	B	505	23/23	0.95	0.10	41,46,56,62	0
8	GDP	D	501	28/28	0.95	0.07	63,76,88,96	0
6	MG	D	502	1/1	0.96	0.08	86,86,86,86	0
10	LO9	D	503	23/23	0.96	0.10	43,47,53,54	23
9	MES	B	504	12/12	0.96	0.08	44,54,64,66	0
7	CA	A	503	1/1	0.97	0.05	91,91,91,91	0
5	GTP	A	501	32/32	0.98	0.05	39,47,55,60	0
5	GTP	C	501	32/32	0.98	0.05	37,43,52,61	0
8	GDP	B	501	28/28	0.98	0.05	40,45,52,58	0
6	MG	B	502	1/1	0.98	0.08	41,41,41,41	0
7	CA	C	503	1/1	1.00	0.04	70,70,70,70	0
6	MG	C	502	1/1	1.00	0.02	47,47,47,47	0
6	MG	A	502	1/1	1.00	0.07	51,51,51,51	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

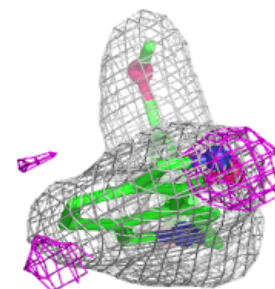
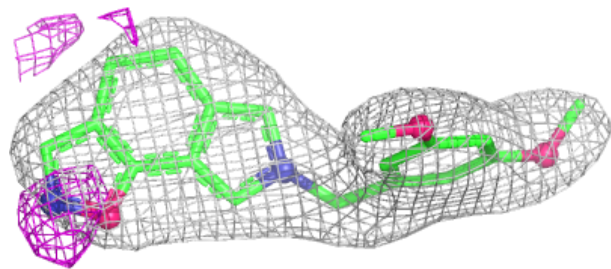
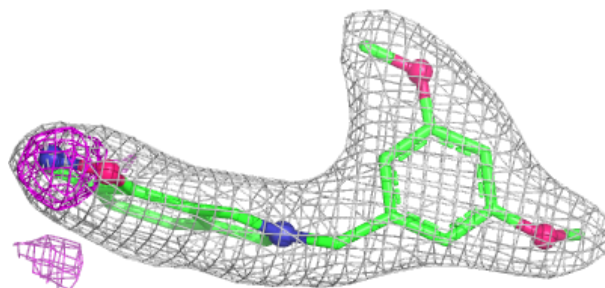
Electron density around ACP F 401:

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



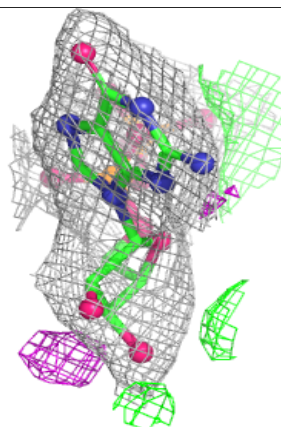
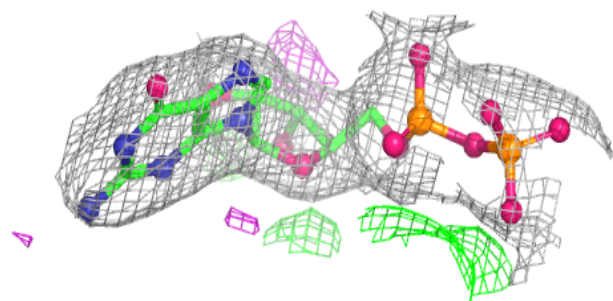
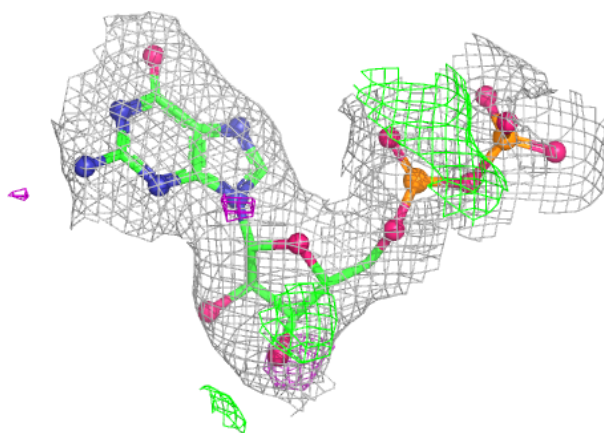
Electron density around LO9 B 505:

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

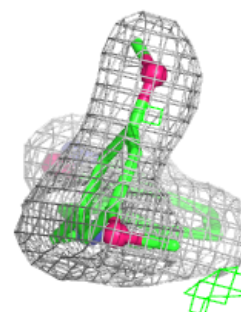
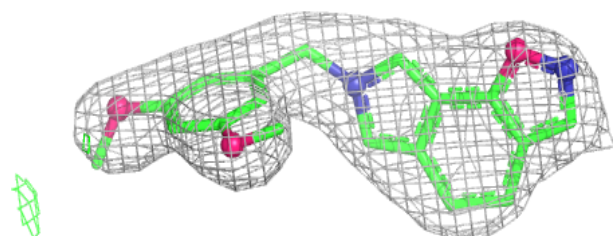
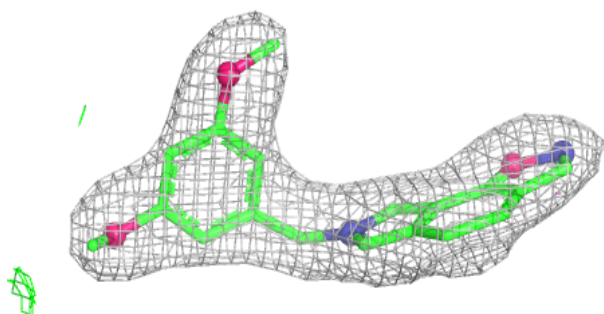


Electron density around GDP D 501:

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

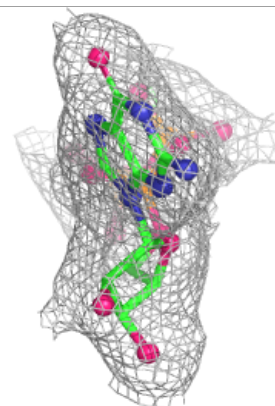
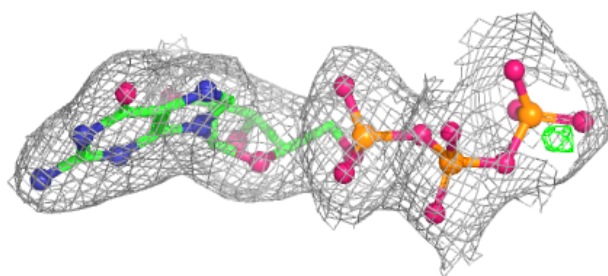
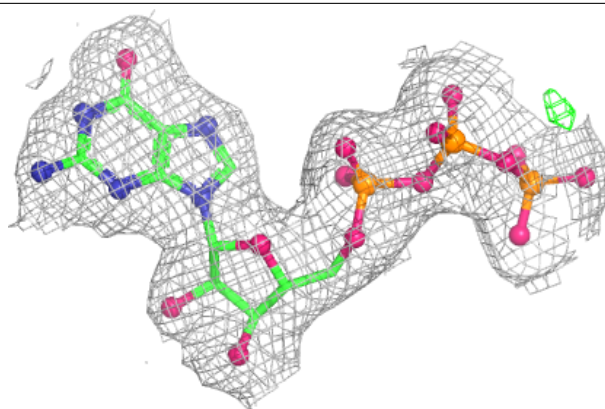
**Electron density around LO9 D 503:**

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

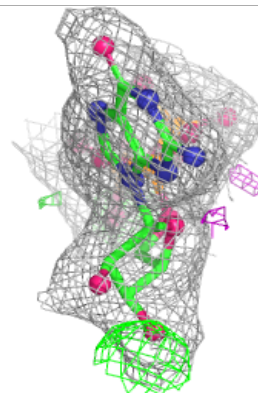
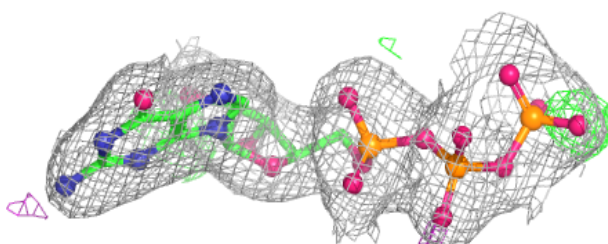
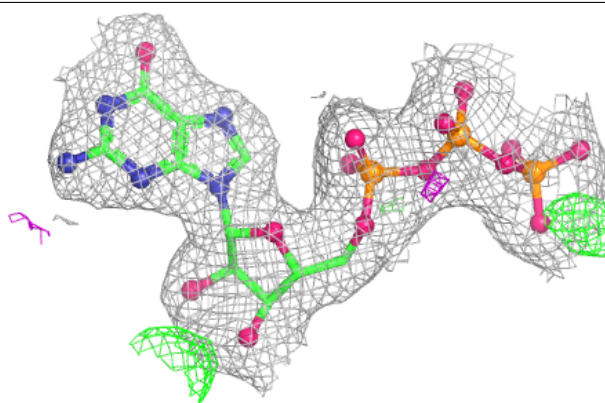


Electron density around GTP A 501:

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

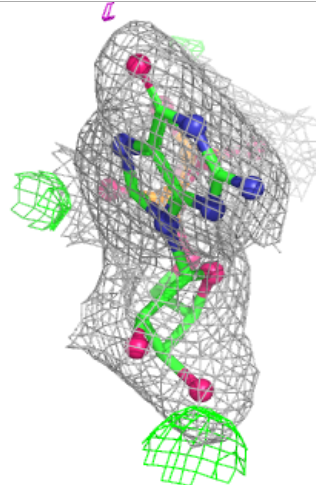
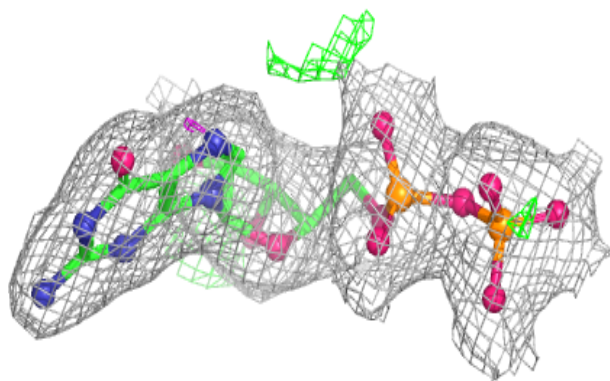
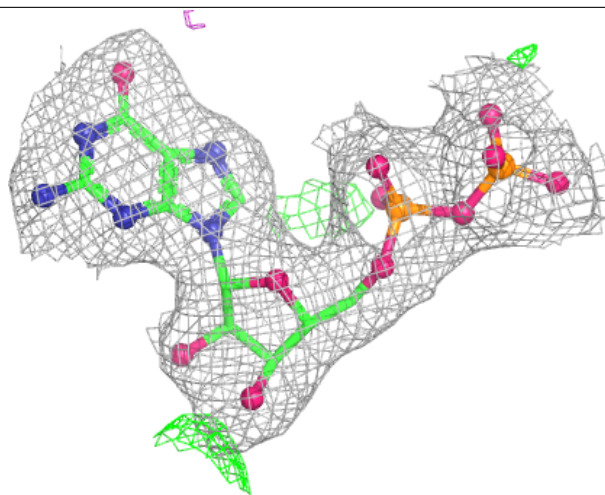
**Electron density around GTP C 501:**

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



Electron density around GDP B 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.