



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:45 PM UTC

PDB ID : 5XKE / pdb_00005xke
Title : Crystal structure of T2R-TTL-Demecolcine complex
Authors : Wang, Y.; Yang, J.; Wang, T.; Chen, L.
Deposited on : 2017-05-07
Resolution : 2.60 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

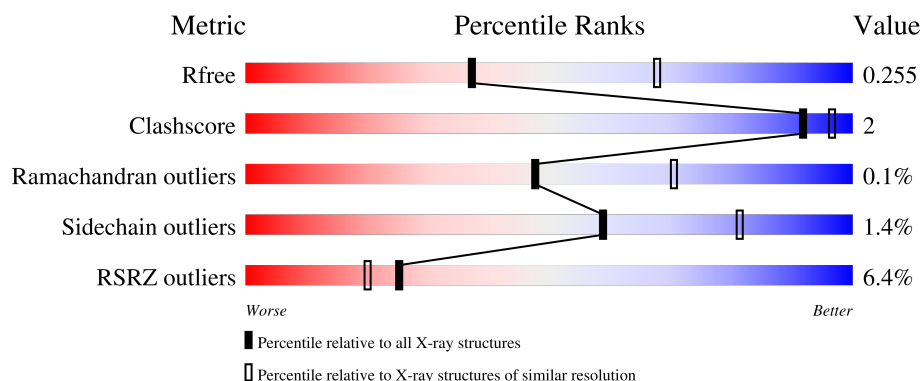
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

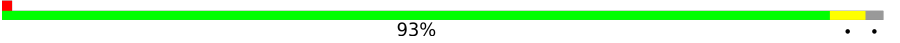
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	15% 81% 5% 13%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17729 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	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLY	GLU	conflict	UNP F2Z5B2
B	441	GLU	GLY	conflict	UNP F2Z5B2
D	440	GLY	GLU	conflict	UNP F2Z5B2
D	441	GLU	GLY	conflict	UNP F2Z5B2

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

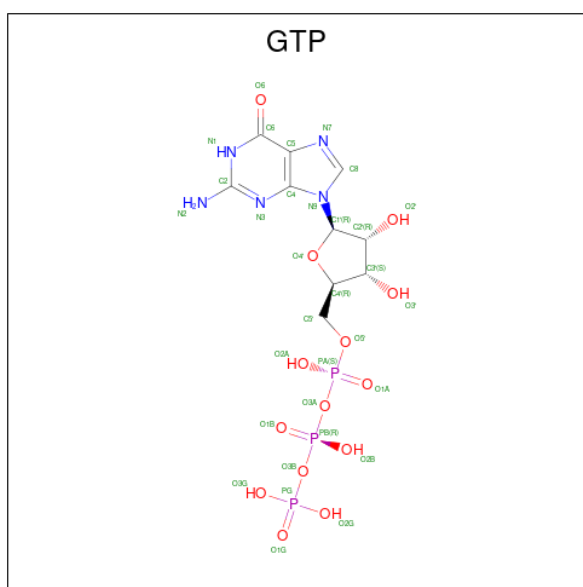
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

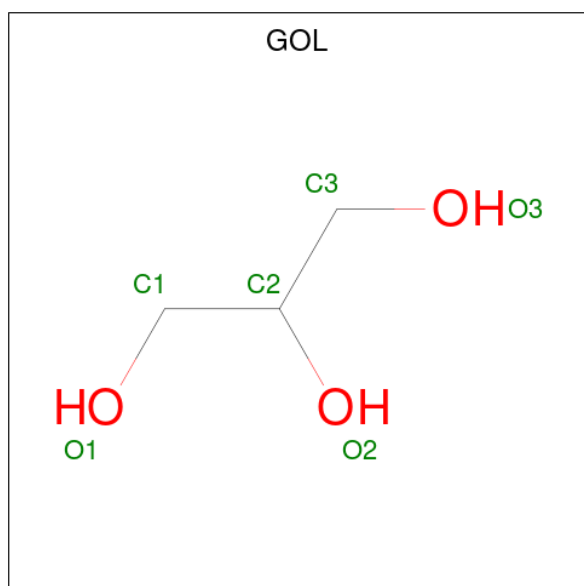
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

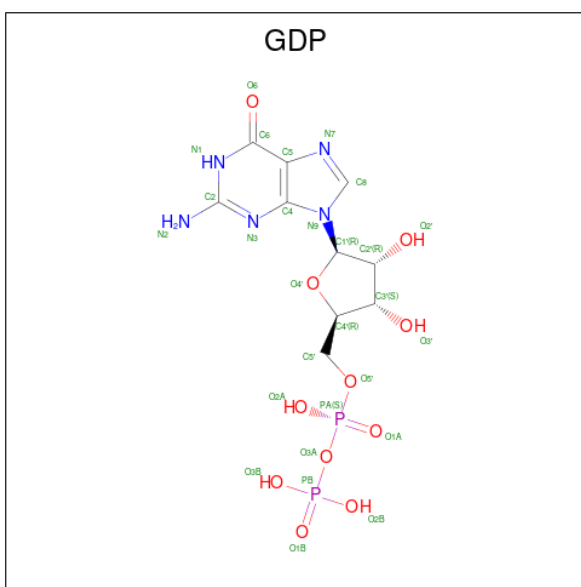
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



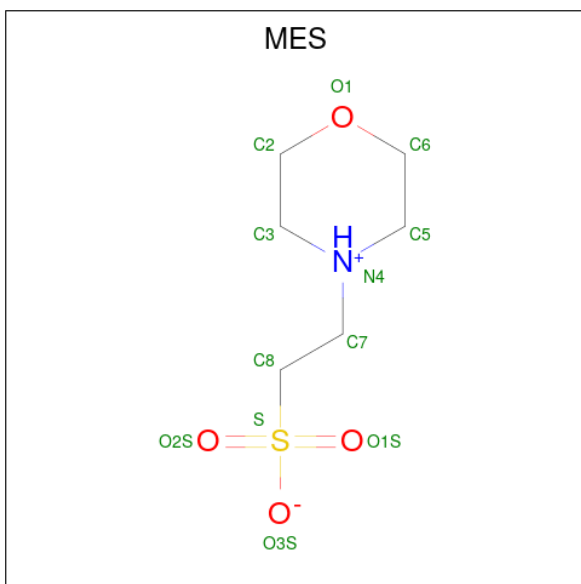
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

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



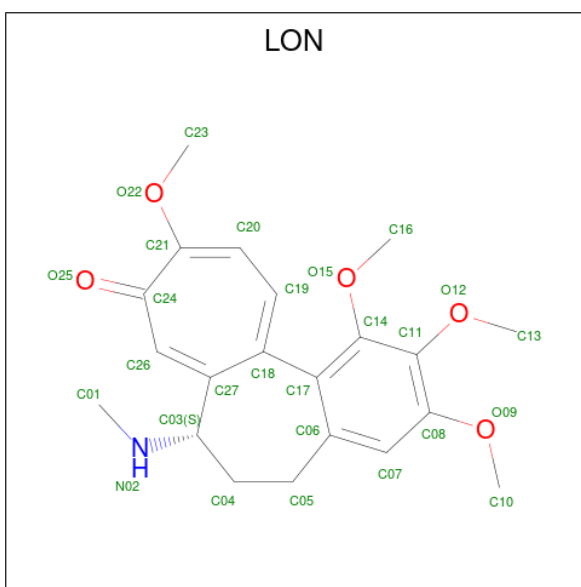
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is (7S)-1,2,3,10-tetramethoxy-7-(methylamino)-6,7-dihydro-5H-benzo[a]heptale n-9-one (CCD ID: LON) (formula: $C_{21}H_{25}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	21	1	5		
11	D	1	Total	C	N	O	0	0
			27	21	1	5		

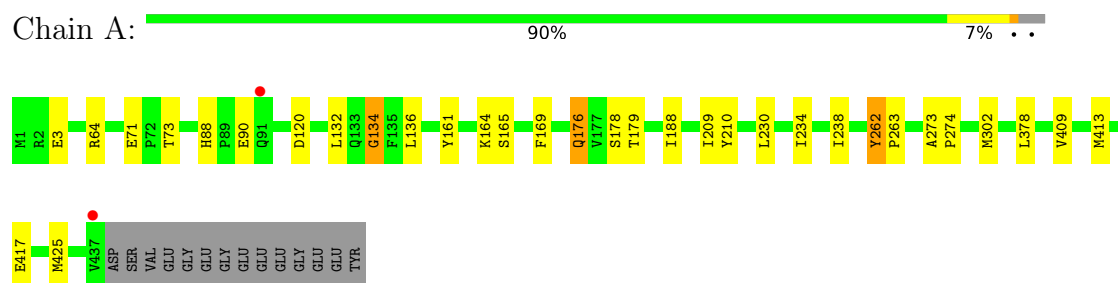
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	53	Total	O	0	0
			53	53		
12	B	55	Total	O	0	0
			55	55		
12	C	98	Total	O	0	0
			98	98		
12	D	11	Total	O	0	0
			11	11		
12	E	13	Total	O	0	0
			13	13		
12	F	22	Total	O	0	0
			22	22		

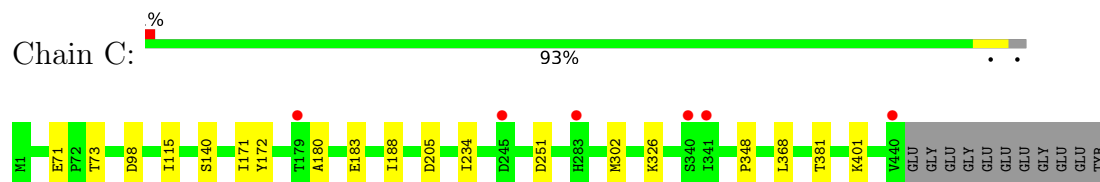
3 Residue-property plots [i](#)

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.

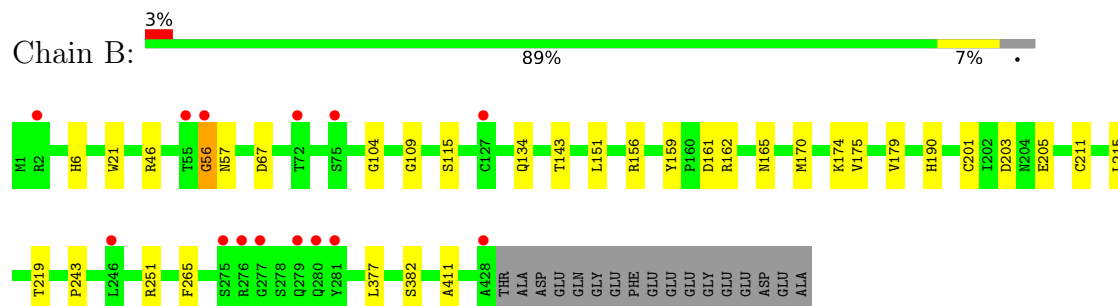
- Molecule 1: Tubulin alpha-1B chain



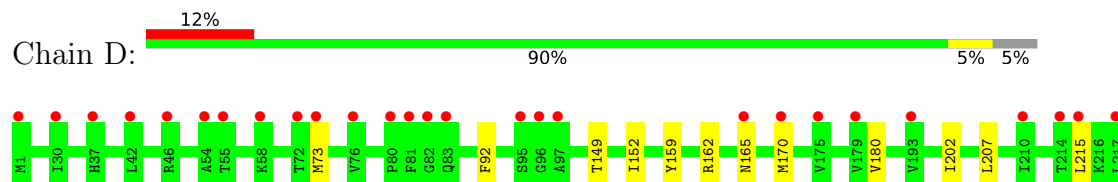
- Molecule 1: Tubulin alpha-1B chain

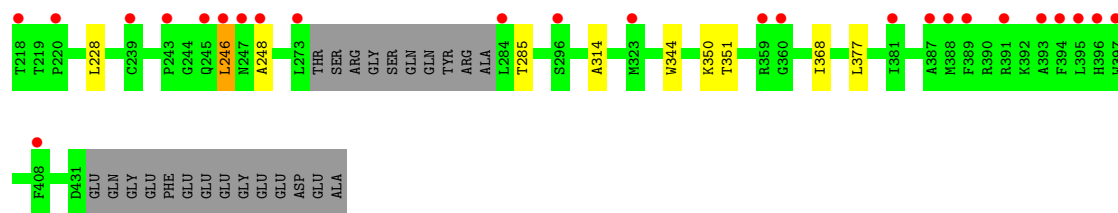


- Molecule 2: Tubulin beta chain

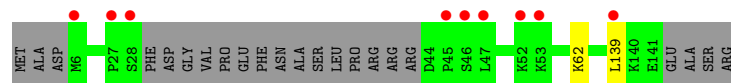
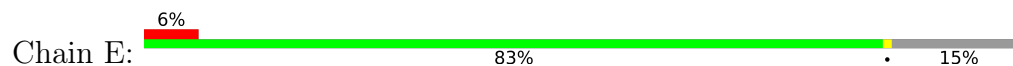


- Molecule 2: Tubulin beta chain

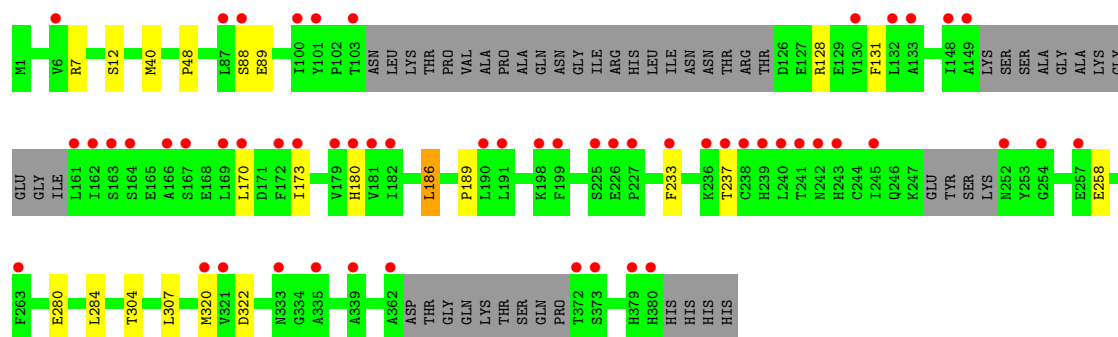
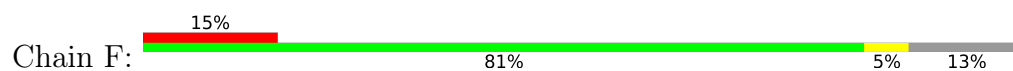




● Molecule 3: Stathmin-4



● Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.41Å 158.02Å 182.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.60) 99.6 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.221 , 0.264 (Not available) , 0.255	Depositor DCC
R_{free} test set	4629 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.9	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	0.94	EDS
Total number of atoms	17729	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, MES, GOL, LON, CA, 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	0.55	0/3494	0.97	4/4743 (0.1%)
1	C	0.53	0/3515	0.95	2/4772 (0.0%)
2	B	0.53	0/3444	0.91	0/4664
2	D	0.54	0/3382	0.94	2/4581 (0.0%)
3	E	0.50	0/1008	0.97	0/1337
4	F	0.54	0/2806	0.88	0/3791
All	All	0.53	0/17649	0.93	8/23888 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	285	THR	CA-C-N	6.49	124.33	120.24
2	D	285	THR	C-N-CA	6.49	124.33	120.24
1	C	73	THR	N-CA-C	6.02	117.84	111.28
1	A	134	GLY	N-CA-C	5.82	117.83	110.38
1	A	73	THR	N-CA-C	5.52	118.06	111.71
1	A	262	TYR	CA-C-N	5.07	125.10	119.32
1	A	262	TYR	C-N-CA	5.07	125.10	119.32
1	C	115	ILE	N-CA-C	5.06	115.28	110.42

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	3416	0	3331	15	0
1	C	3437	0	3348	8	0
2	B	3369	0	3250	18	0
2	D	3309	0	3189	10	0
3	E	1000	0	1018	0	0
4	F	2744	0	2709	8	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	2	0
11	B	27	0	0	0	0
11	D	27	0	0	1	0
12	A	53	0	0	0	0
12	B	55	0	0	0	0
12	C	98	0	0	0	0
12	D	11	0	0	0	0
12	E	13	0	0	0	0
12	F	22	0	0	0	0
All	All	17729	0	16914	56	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 2.

All (56) 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)
2:B:190:HIS:HD2	2:B:411:ALA:HA	1.61	0.63
2:D:246:LEU:HD22	2:D:248:ALA:HB2	1.81	0.62
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.87	0.56
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.88	0.54
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.53
2:B:156:ARG:HG3	10:B:503:MES:H62	1.93	0.51
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.93	0.50
2:B:46:ARG:HH21	2:B:243:PRO:HA	1.75	0.50
2:D:350:LYS:HG3	11:D:503:LON:C24	2.42	0.50
2:B:161:ASP:O	2:B:251:ARG:NH2	2.45	0.49
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.93	0.49
2:D:149:THR:HA	2:D:152:ILE:HD12	1.93	0.49
4:F:189:PRO:HA	4:F:322:ASP:HA	1.94	0.49
2:B:134:GLN:HA	2:B:165:ASN:O	2.12	0.49
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48
2:B:56:GLY:N	2:B:57:ASN:HA	2.30	0.47
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.96	0.47
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.97	0.47
1:A:88:HIS:HD2	1:A:90:GLU:H	1.62	0.47
4:F:128:ARG:HA	4:F:131:PHE:HB3	1.96	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.47
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.97	0.47
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.50	0.46
2:D:159:TYR:HB3	2:D:162:ARG:HG3	1.96	0.46
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.97	0.46
2:B:170:MET:HB2	2:B:203:ASP:HA	1.98	0.45
1:A:409:VAL:HA	1:A:413:MET:O	2.17	0.45
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.99	0.44
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.99	0.44
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.00	0.44
2:B:104:GLY:O	2:B:109:GLY:HA3	2.17	0.44
2:B:219:THR:HG21	1:C:326:LYS:HA	2.00	0.44
2:B:211:CYS:HA	2:B:215:LEU:HB2	2.00	0.44
1:A:273:ALA:HA	1:A:274:PRO:HA	1.81	0.44
2:D:314:ALA:HB3	2:D:368:ILE:HB	2.00	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.17	0.43
1:A:176:GLN:HG2	1:A:210:TYR:CE2	2.54	0.43
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.58	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HD3	2.01	0.43
2:B:156:ARG:CZ	10:B:503:MES:H21	2.49	0.43
2:B:159:TYR:HB3	2:B:162:ARG:HG3	2.01	0.43
2:B:67:ASP:HA	2:B:143:THR:HG21	2.02	0.42
4:F:40:MET:HE1	4:F:48:PRO:HD2	2.01	0.42
1:A:132:LEU:HD23	1:A:164:LYS:HE3	2.02	0.41
2:D:202:ILE:HG22	2:D:207:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.41
4:F:88:SER:HA	4:F:89:GLU:HA	1.72	0.41
1:C:234:ILE:HD13	1:C:302:MET:SD	2.60	0.41
4:F:280:GLU:HA	4:F:284:LEU:HB3	2.03	0.41
4:F:186:LEU:HD13	4:F:320:MET:HG2	2.03	0.40
2:D:215:LEU:HD11	2:D:228:LEU:HD21	2.03	0.40
1:A:136:LEU:HD23	1:A:169:PHE:HE2	1.85	0.40
1:A:209:ILE:HD11	1:A:302:MET:SD	2.62	0.40
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.91	0.40
1:C:140:SER:HA	1:C:171:ILE:HB	2.03	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	435/451 (96%)	427 (98%)	7 (2%)	1 (0%)	43	66
1	C	438/451 (97%)	430 (98%)	8 (2%)	0	100	100
2	B	426/445 (96%)	418 (98%)	7 (2%)	1 (0%)	43	66
2	D	417/445 (94%)	408 (98%)	9 (2%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	324/384 (84%)	318 (98%)	6 (2%)	0	100	100
All	All	2157/2319 (93%)	2118 (98%)	37 (2%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
2	B	56	GLY

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	368/379 (97%)	363 (99%)	5 (1%)	59	81
1	C	371/379 (98%)	367 (99%)	4 (1%)	65	84
2	B	370/383 (97%)	366 (99%)	4 (1%)	65	84
2	D	364/383 (95%)	360 (99%)	4 (1%)	65	84
3	E	109/127 (86%)	107 (98%)	2 (2%)	51	76
4	F	301/342 (88%)	293 (97%)	8 (3%)	39	67
All	All	1883/1993 (94%)	1856 (99%)	27 (1%)	59	81

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	120	ASP
1	A	176	GLN
1	A	179	THR
1	A	234	ILE
2	B	115	SER
2	B	151	LEU
2	B	175	VAL
2	B	382	SER
1	C	188	ILE
1	C	251	ASP
1	C	368	LEU
1	C	381	THR
2	D	165	ASN
2	D	180	VAL
2	D	246	LEU
2	D	351	THR
3	E	62	LYS
3	E	139	LEU
4	F	12	SER
4	F	170	LEU
4	F	173	ILE

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Mol	Chain	Res	Type
4	F	180	HIS
4	F	186	LEU
4	F	233	PHE
4	F	237	THR
4	F	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	88	HIS
1	A	176	GLN
1	A	329	ASN
1	A	342	GLN
1	A	372	GLN
2	B	8	GLN
2	B	14	ASN
2	B	134	GLN
2	B	329	GLN
2	B	332	ASN
2	B	347	ASN
2	B	375	GLN
1	C	15	GLN
1	C	293	ASN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	43	GLN
2	D	347	ASN
2	D	426	GLN
3	E	90	ASN
4	F	136	ASN
4	F	212	ASN
4	F	229	ASN
4	F	333	ASN
4	F	380	HIS

5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 6 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$
10	MES	B	503	-	12,12,12	2.31	1 (8%)	15,16,16	1.45	2 (13%)
11	LON	D	503	-	29,29,29	3.38	14 (48%)	41,41,41	3.80	14 (34%)
5	GTP	A	501	6	33,34,34	1.33	5 (15%)	50,54,54	1.68	6 (12%)
5	GTP	C	501	6	33,34,34	1.29	5 (15%)	50,54,54	1.64	5 (10%)
9	GDP	B	501	6	29,30,30	1.21	4 (13%)	45,47,47	1.73	6 (13%)
8	GOL	A	504	-	5,5,5	0.24	0	5,5,5	0.40	0
11	LON	B	504	-	29,29,29	3.42	14 (48%)	41,41,41	3.77	14 (34%)
5	GTP	D	501	6	33,34,34	1.20	3 (9%)	50,54,54	1.69	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	503	-	-	2/6/14/14	0/1/1/1
11	LON	D	503	-	-	4/8/23/23	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
8	GOL	A	504	-	-	4/4/4/4	-
11	LON	B	504	-	-	4/8/23/23	0/3/3/3
5	GTP	D	501	6	-	3/22/38/38	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.54	1.67	1.77
11	B	504	LON	C17-C06	-7.39	1.26	1.41
11	D	503	LON	C17-C06	-7.26	1.26	1.41
11	B	504	LON	C17-C18	-6.01	1.43	1.50
11	B	504	LON	C07-C06	6.00	1.48	1.39
11	D	503	LON	C17-C14	5.84	1.53	1.40
11	D	503	LON	C07-C06	5.83	1.48	1.39
11	D	503	LON	C17-C18	-5.75	1.43	1.50
11	B	504	LON	C03-C27	5.66	1.62	1.53
11	B	504	LON	C17-C14	5.64	1.53	1.40
11	D	503	LON	C03-C27	5.45	1.61	1.53
11	D	503	LON	C04-C03	4.96	1.61	1.53
11	B	504	LON	C04-C03	4.70	1.61	1.53
11	B	504	LON	C03-N02	-4.45	1.37	1.46
11	D	503	LON	C03-N02	-4.34	1.37	1.46
11	B	504	LON	O09-C08	4.28	1.44	1.37
11	B	504	LON	C26-C27	4.12	1.44	1.36
11	D	503	LON	O09-C08	4.08	1.43	1.37
11	D	503	LON	C26-C27	4.07	1.44	1.36
11	D	503	LON	O15-C14	3.74	1.45	1.38
11	B	504	LON	O15-C14	3.67	1.45	1.38
11	D	503	LON	O22-C21	3.47	1.43	1.36
5	D	501	GTP	C5-C4	3.40	1.48	1.38
11	B	504	LON	O22-C21	3.38	1.42	1.36
5	A	501	GTP	C5-C4	3.31	1.47	1.38
9	B	501	GDP	C5-C4	3.27	1.47	1.38
5	C	501	GTP	C5-C4	3.23	1.47	1.38
11	D	503	LON	O12-C11	3.16	1.44	1.38
11	B	504	LON	C18-C27	-2.98	1.39	1.43
5	C	501	GTP	PA-O3A	2.94	1.62	1.59
11	D	503	LON	C18-C27	-2.88	1.39	1.43
11	B	504	LON	C21-C24	2.87	1.51	1.47
11	B	504	LON	O12-C11	2.81	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	PB-O3B	2.77	1.62	1.59
5	A	501	GTP	PA-O3A	2.77	1.62	1.59
5	C	501	GTP	PB-O3B	2.56	1.62	1.59
9	B	501	GDP	PA-O3A	2.54	1.62	1.59
11	D	503	LON	C21-C24	2.53	1.50	1.47
5	A	501	GTP	PB-O3A	2.49	1.62	1.59
5	D	501	GTP	C5-N7	-2.15	1.34	1.39
9	B	501	GDP	C6-N1	-2.09	1.34	1.38
5	C	501	GTP	C5-N7	-2.08	1.34	1.39
5	D	501	GTP	C6-N1	-2.08	1.35	1.38
9	B	501	GDP	C5-N7	-2.06	1.34	1.39
5	C	501	GTP	C6-N1	-2.05	1.35	1.38
5	A	501	GTP	C5-N7	-2.04	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	503	LON	C17-C18-C19	-14.49	93.43	116.95
11	B	504	LON	C17-C18-C19	-14.02	94.19	116.95
11	B	504	LON	C17-C18-C27	10.61	127.31	118.62
11	D	503	LON	C17-C18-C27	9.74	126.60	118.62
11	D	503	LON	C14-C17-C18	-8.64	112.20	121.33
11	B	504	LON	C14-C17-C18	-8.15	112.72	121.33
11	D	503	LON	C06-C17-C18	7.77	128.83	120.20
11	B	504	LON	C06-C17-C18	7.55	128.58	120.20
11	B	504	LON	O22-C21-C20	-6.36	113.06	122.29
5	D	501	GTP	C5-C4-N3	-6.09	118.70	128.39
5	A	501	GTP	C5-C4-N3	-5.85	119.08	128.39
11	D	503	LON	O22-C21-C20	-5.84	113.82	122.29
9	B	501	GDP	C5-C4-N3	-5.73	119.26	128.39
5	C	501	GTP	C5-C4-N3	-5.56	119.55	128.39
11	D	503	LON	O22-C21-C24	5.52	114.67	109.60
11	B	504	LON	O22-C21-C24	5.44	114.60	109.60
5	D	501	GTP	C2-N3-C4	5.11	121.10	112.30
9	B	501	GDP	C2-N3-C4	5.02	120.94	112.30
5	A	501	GTP	C2-N3-C4	4.96	120.85	112.30
5	C	501	GTP	C2-N3-C4	4.90	120.73	112.30
5	D	501	GTP	N9-C4-N3	4.67	135.29	125.95
9	B	501	GDP	N9-C4-N3	4.40	134.76	125.95
5	A	501	GTP	N9-C4-N3	4.35	134.66	125.95
5	C	501	GTP	N9-C4-N3	4.17	134.29	125.95
11	D	503	LON	C03-C27-C18	-3.86	111.85	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C6-C5-N7	3.51	136.68	130.29
5	A	501	GTP	C6-C5-N7	3.47	136.61	130.29
11	D	503	LON	C03-C27-C26	-3.44	114.02	117.06
9	B	501	GDP	C6-C5-N7	3.43	136.53	130.29
5	D	501	GTP	C6-C5-N7	3.22	136.15	130.29
11	B	504	LON	C27-C03-N02	-3.15	111.43	114.37
11	D	503	LON	O09-C08-C11	3.01	120.30	115.14
11	B	504	LON	O09-C08-C11	3.00	120.28	115.14
11	B	504	LON	C27-C26-C24	-2.81	129.20	134.20
11	D	503	LON	O09-C08-C07	-2.68	119.47	124.08
11	D	503	LON	C05-C04-C03	2.67	115.36	112.13
11	B	504	LON	C03-C27-C18	-2.65	112.95	115.37
5	A	501	GTP	C4-C5-N7	-2.65	106.48	110.67
11	B	504	LON	C05-C04-C03	2.65	115.33	112.13
10	B	503	MES	O1S-S-C8	2.64	110.72	106.73
5	C	501	GTP	C4-C5-N7	-2.58	106.58	110.67
10	B	503	MES	C5-N4-C3	2.55	114.34	108.84
5	D	501	GTP	C4-C5-N7	-2.40	106.87	110.67
9	B	501	GDP	C4-C5-N7	-2.36	106.93	110.67
11	B	504	LON	C03-C27-C26	-2.28	115.05	117.06
11	B	504	LON	C20-C19-C18	-2.28	126.59	131.06
11	D	503	LON	C19-C18-C27	2.25	126.96	124.67
11	B	504	LON	O09-C08-C07	-2.25	120.20	124.08
9	B	501	GDP	O6-C6-C5	-2.24	120.62	126.53
5	A	501	GTP	O6-C6-C5	-2.18	120.78	126.53
5	D	501	GTP	O6-C6-C5	-2.13	120.90	126.53
11	D	503	LON	C27-C26-C24	-2.12	130.42	134.20
11	D	503	LON	C27-C03-N02	-2.10	112.41	114.37

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	B	503	MES	C8-C7-N4-C5
11	B	504	LON	C20-C21-O22-C23
11	B	504	LON	C24-C21-O22-C23
11	D	503	LON	C20-C21-O22-C23
11	D	503	LON	C24-C21-O22-C23
11	B	504	LON	C11-C08-O09-C10
11	D	503	LON	C11-C08-O09-C10
11	D	503	LON	C07-C08-O09-C10
11	B	504	LON	C07-C08-O09-C10
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	C1-C2-C3-O3
8	A	504	GOL	O2-C2-C3-O3
8	A	504	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A

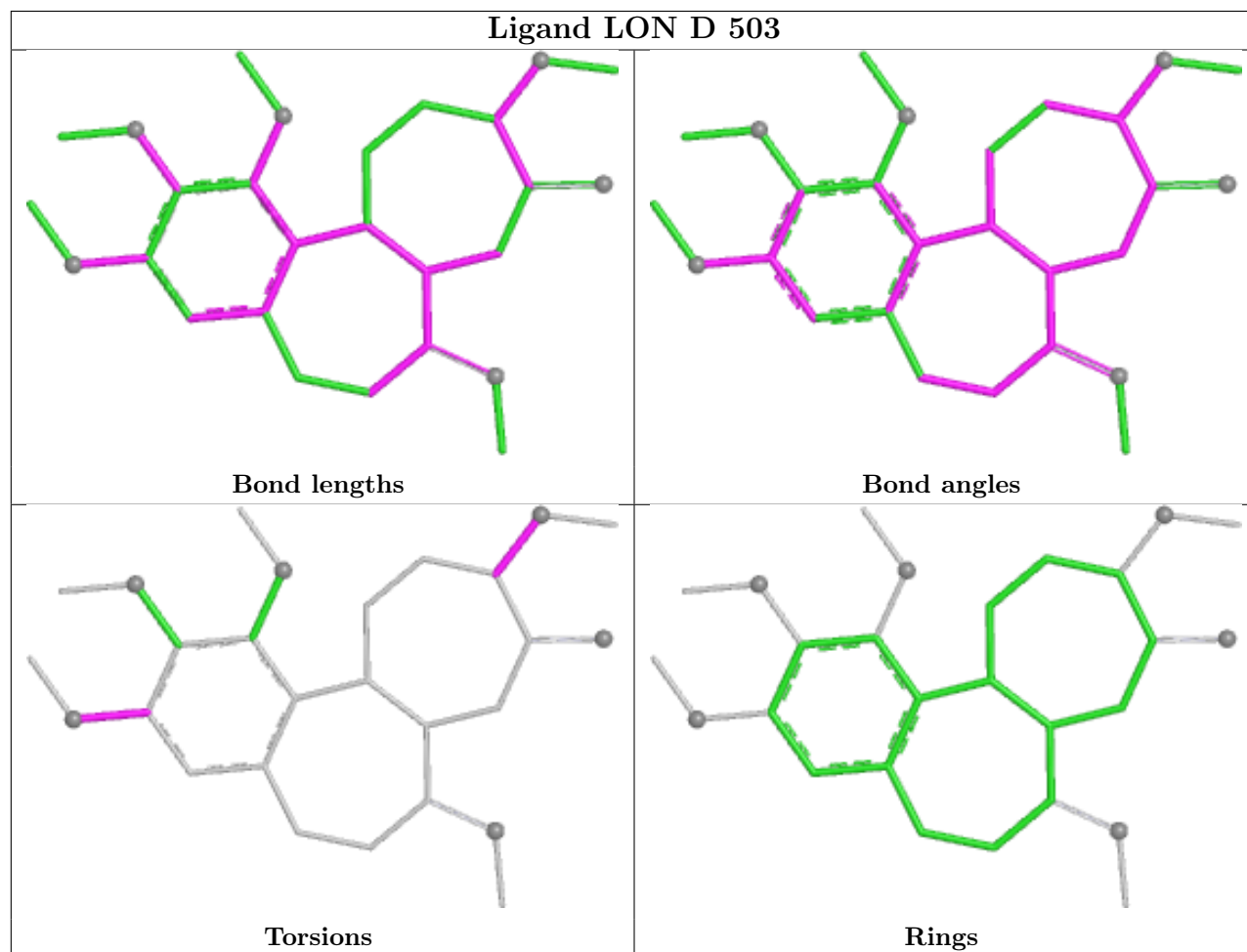
There are no ring outliers.

2 monomers are involved in 3 short contacts:

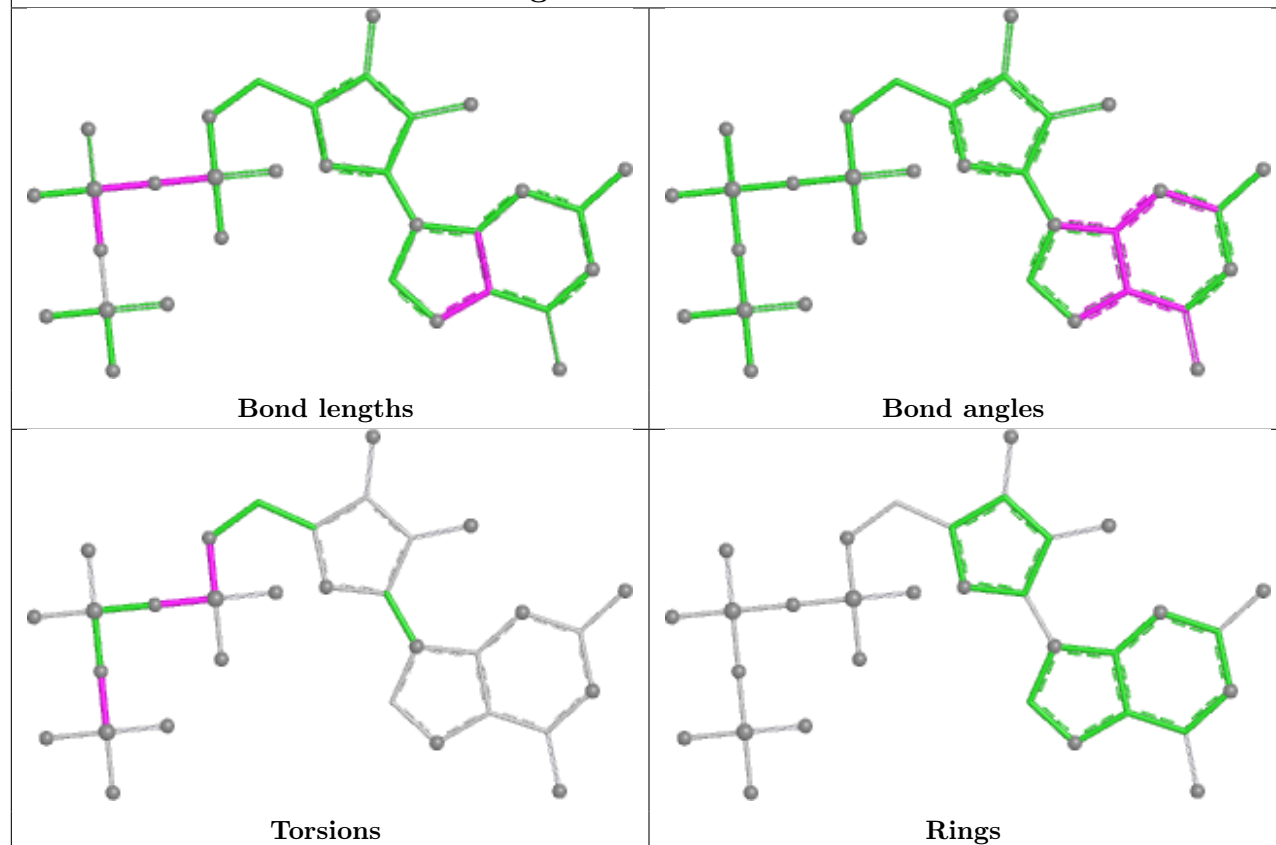
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	2	0
11	D	503	LON	1	0

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

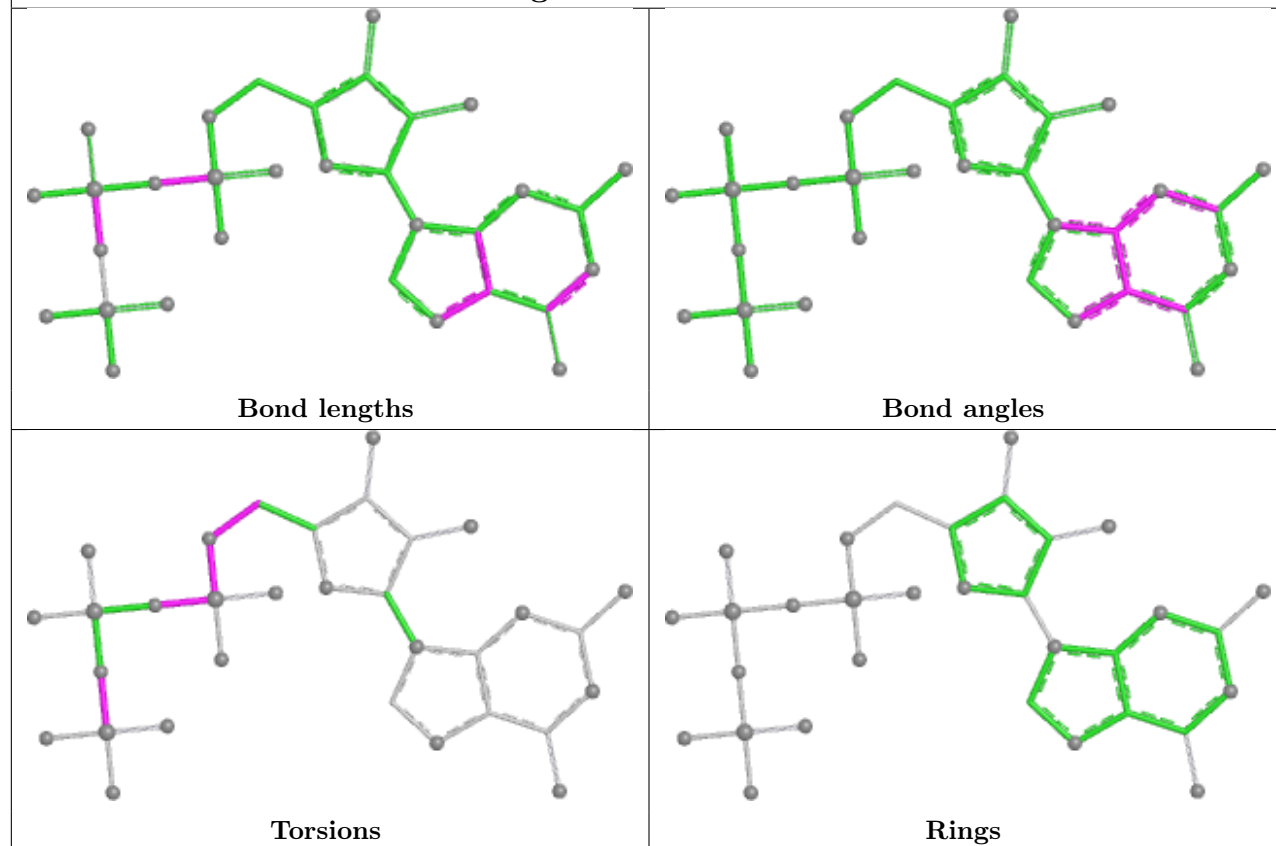
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

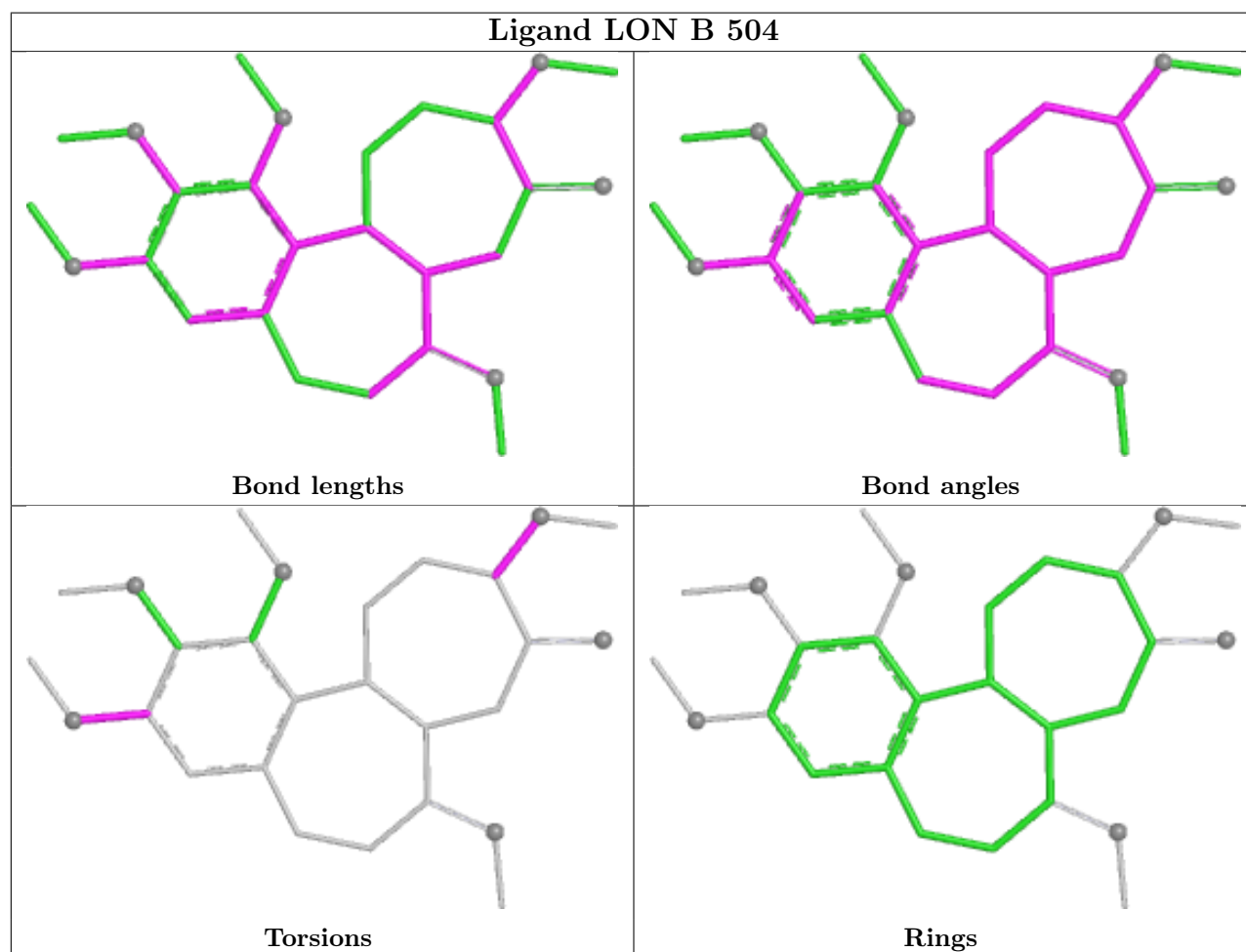
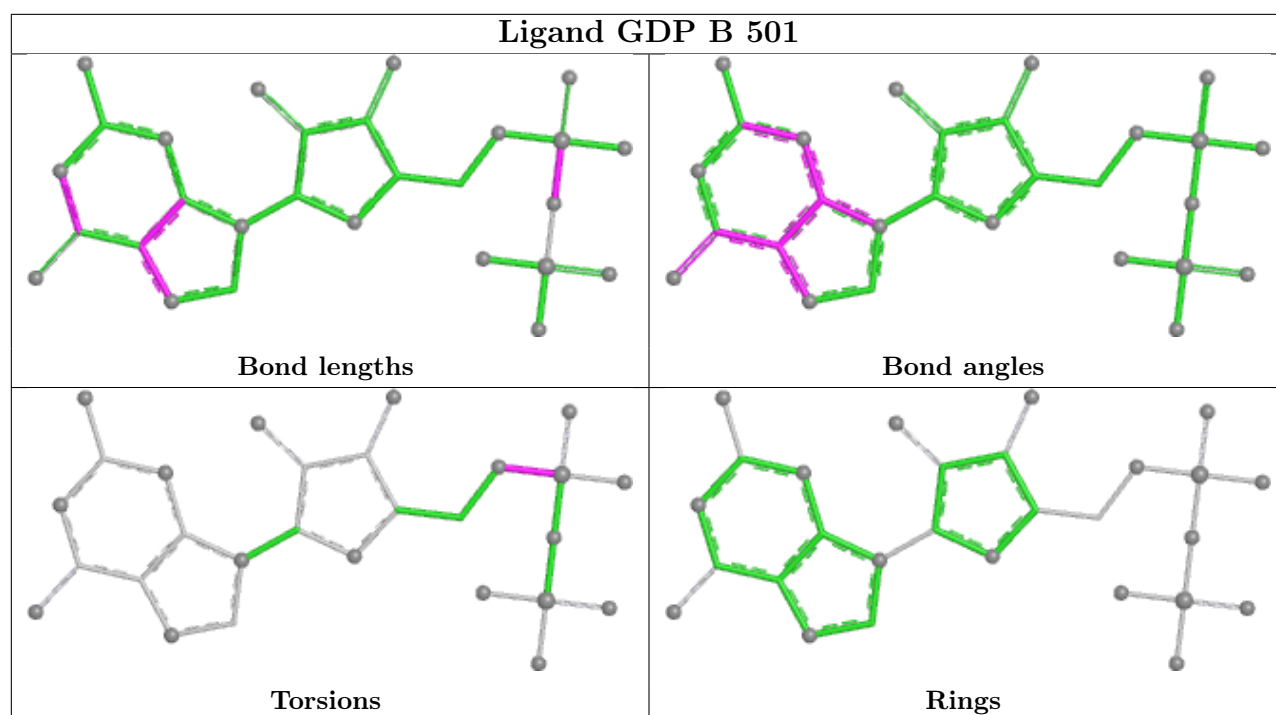


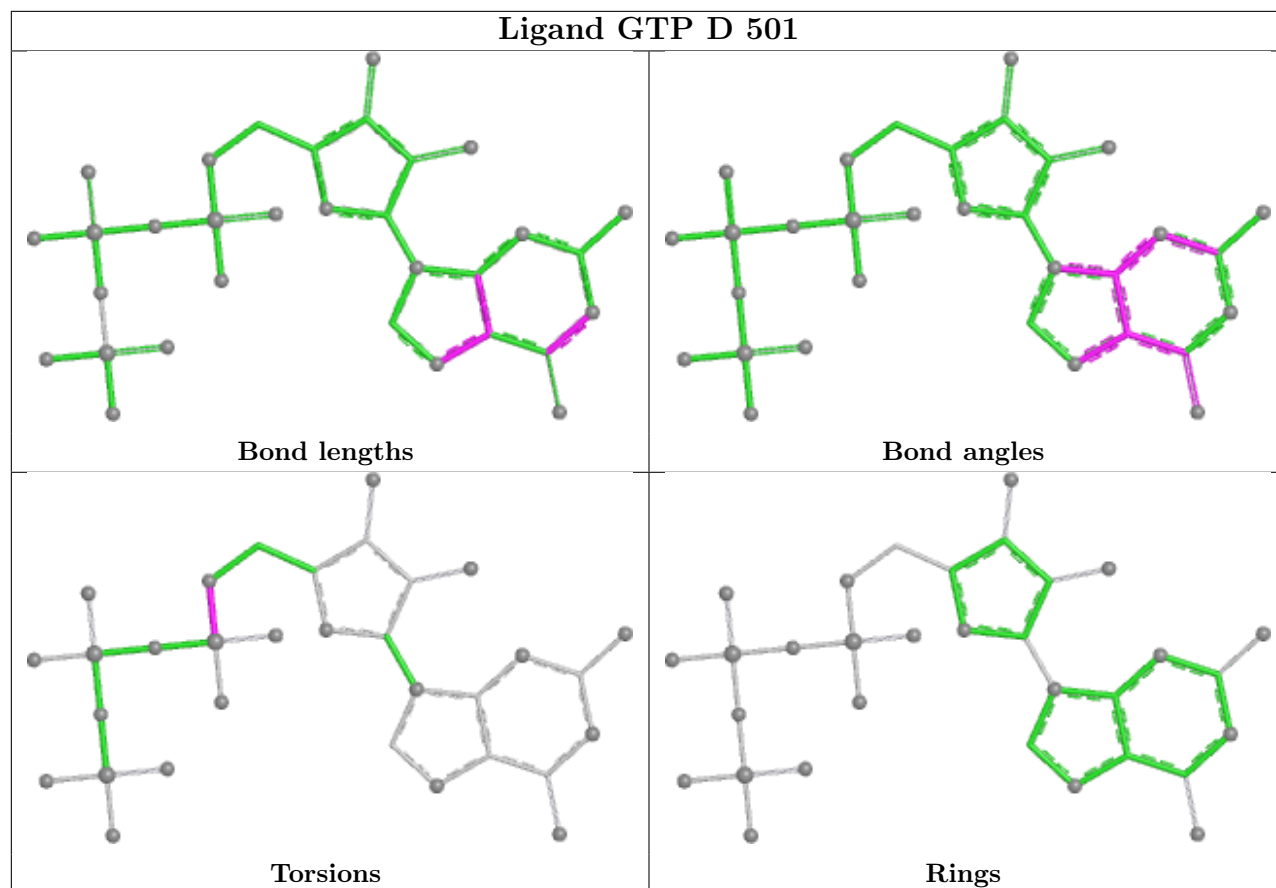
Ligand GTP A 501



Ligand GTP C 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%)	0.13	2 (0%) 87 85	31, 50, 74, 88	0
1	C	440/451 (97%)	-0.15	6 (1%) 73 69	25, 41, 64, 77	0
2	B	428/445 (96%)	0.23	14 (3%) 49 43	29, 49, 89, 121	0
2	D	421/445 (94%)	0.98	52 (12%) 8 6	41, 72, 109, 127	0
3	E	121/143 (84%)	0.84	9 (7%) 20 16	41, 67, 99, 117	0
4	F	334/384 (86%)	1.04	56 (16%) 4 3	40, 75, 138, 151	0
All	All	2181/2319 (94%)	0.44	139 (6%) 25 20	25, 56, 107, 151	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	5.5
4	F	241	THR	5.3
2	D	247	ASN	4.8
2	B	246	LEU	4.6
4	F	180	HIS	4.5
4	F	240	LEU	4.3
2	D	72	THR	4.3
2	D	1	MET	4.1
2	D	214	THR	3.9
4	F	237	THR	3.9
4	F	169	LEU	3.9
4	F	132	LEU	3.8
4	F	149	ALA	3.8
2	D	73	MET	3.7
4	F	233	PHE	3.7
2	D	80	PRO	3.7
2	D	394	PHE	3.7
3	E	46	SER	3.6
2	D	246	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	245	ILE	3.6
2	B	55	THR	3.5
4	F	182	ILE	3.4
4	F	199	PHE	3.3
2	D	245	GLN	3.3
2	D	393	ALA	3.3
4	F	133	ALA	3.2
3	E	28	SER	3.2
4	F	181	VAL	3.2
1	C	340	SER	3.1
4	F	88	SER	3.1
1	A	437	VAL	3.1
4	F	103	THR	3.1
4	F	242	ASN	3.1
4	F	254	GLY	3.1
4	F	164	SER	3.1
2	D	284	LEU	3.0
2	B	276	ARG	3.0
4	F	170	LEU	3.0
2	D	37	HIS	3.0
4	F	226	GLU	3.0
4	F	239	HIS	3.0
4	F	333	ASN	2.9
2	D	179	VAL	2.9
2	D	42	LEU	2.9
2	B	56	GLY	2.9
4	F	130	VAL	2.9
4	F	191	LEU	2.9
4	F	243	HIS	2.9
4	F	252	ASN	2.9
2	D	55	THR	2.9
3	E	139	LEU	2.9
4	F	162	ILE	2.9
2	D	58	LYS	2.8
3	E	6	MET	2.8
4	F	380	HIS	2.8
2	D	360	GLY	2.7
4	F	263	PHE	2.7
3	E	27	PRO	2.7
2	D	54	ALA	2.7
4	F	166	ALA	2.7
2	D	96	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	163	SER	2.7
4	F	179	VAL	2.7
2	B	281	TYR	2.6
2	D	170	MET	2.6
4	F	362	ALA	2.6
4	F	148	ILE	2.6
2	D	81	PHE	2.6
2	D	220	PRO	2.6
2	B	72	THR	2.6
4	F	372	THR	2.6
2	B	277	GLY	2.6
2	D	217	LEU	2.5
2	D	273	LEU	2.5
4	F	87	LEU	2.5
2	D	218	THR	2.5
4	F	173	ILE	2.5
4	F	320	MET	2.5
2	D	210	ILE	2.4
4	F	172	PHE	2.4
2	D	76	VAL	2.4
2	B	428	ALA	2.4
2	D	248	ALA	2.4
1	C	179	THR	2.4
2	D	397	TRP	2.4
2	D	239	CYS	2.3
2	D	82	GLY	2.3
2	B	2	ARG	2.3
2	D	395	LEU	2.3
3	E	45	PRO	2.3
2	D	387	ALA	2.3
2	D	396	HIS	2.3
4	F	257	GLU	2.3
4	F	373	SER	2.3
2	B	279	GLN	2.3
2	D	175	VAL	2.3
2	D	389	PHE	2.3
2	D	165	ASN	2.3
2	D	46	ARG	2.3
4	F	167	SER	2.3
4	F	321	VAL	2.3
4	F	339	ALA	2.2
1	C	440	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	193	VAL	2.2
2	D	83	GLN	2.2
3	E	47	LEU	2.2
3	E	53	LYS	2.2
2	D	215	LEU	2.2
1	C	245	ASP	2.2
2	D	296	SER	2.2
2	D	30	ILE	2.2
2	D	97	ALA	2.1
2	D	359	ARG	2.1
2	B	280	GLN	2.1
2	D	388	MET	2.1
4	F	6	VAL	2.1
4	F	335	ALA	2.1
4	F	198	LYS	2.1
4	F	236	LYS	2.1
1	C	283	HIS	2.1
4	F	100	ILE	2.1
2	D	408	PHE	2.1
1	C	341	ILE	2.1
2	B	275	SER	2.1
4	F	225	SER	2.1
4	F	227	PRO	2.1
2	D	323	MET	2.1
2	B	127	CYS	2.1
4	F	238	CYS	2.1
4	F	379	HIS	2.1
4	F	101	TYR	2.1
2	D	95	SER	2.0
3	E	52	LYS	2.0
2	D	243	PRO	2.0
1	A	91	GLN	2.0
4	F	190	LEU	2.0
2	D	391	ARG	2.0
2	B	75	SER	2.0
2	D	381	ILE	2.0

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

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](#)

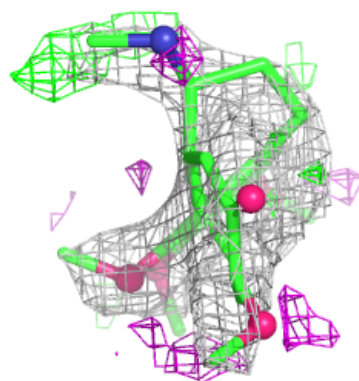
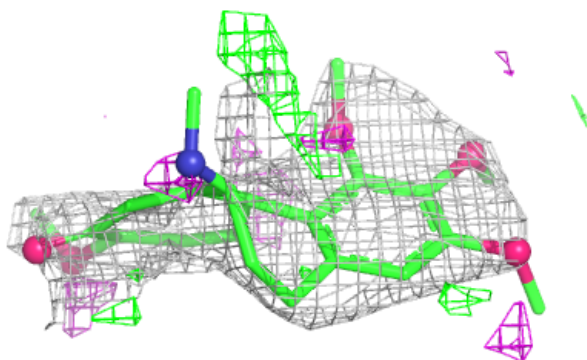
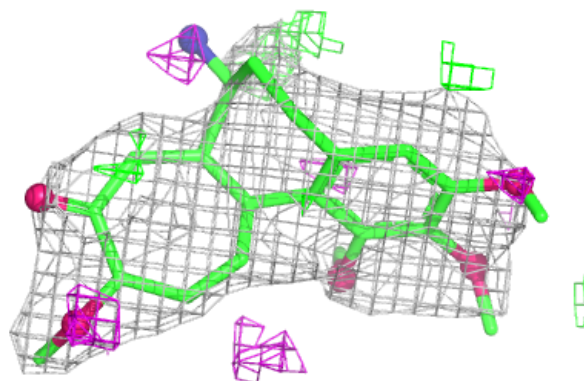
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	502	1/1	0.79	0.21	77,77,77,77	0
10	MES	B	503	12/12	0.81	0.19	73,79,86,87	0
11	LON	D	503	27/27	0.84	0.23	92,97,102,104	0
8	GOL	A	504	6/6	0.86	0.15	75,77,78,79	0
7	CA	C	503	1/1	0.89	0.09	69,69,69,69	0
5	GTP	D	501	32/32	0.89	0.11	61,66,77,79	0
11	LON	B	504	27/27	0.90	0.14	55,57,60,62	0
7	CA	A	503	1/1	0.91	0.11	72,72,72,72	0
5	GTP	A	501	32/32	0.97	0.06	34,36,37,38	0
9	GDP	B	501	28/28	0.98	0.05	30,35,36,38	0
5	GTP	C	501	32/32	0.98	0.05	30,32,33,35	0
6	MG	C	502	1/1	0.99	0.03	34,34,34,34	0
6	MG	A	502	1/1	0.99	0.02	33,33,33,33	0
6	MG	B	502	1/1	0.99	0.03	28,28,28,28	0

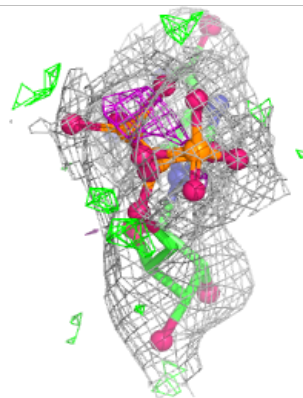
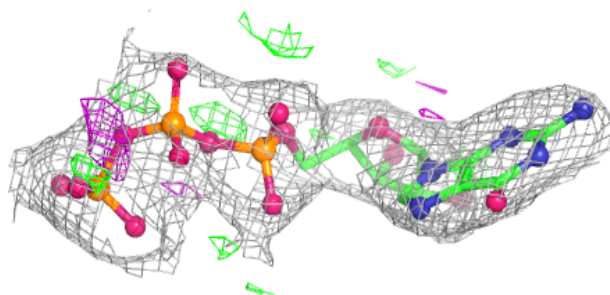
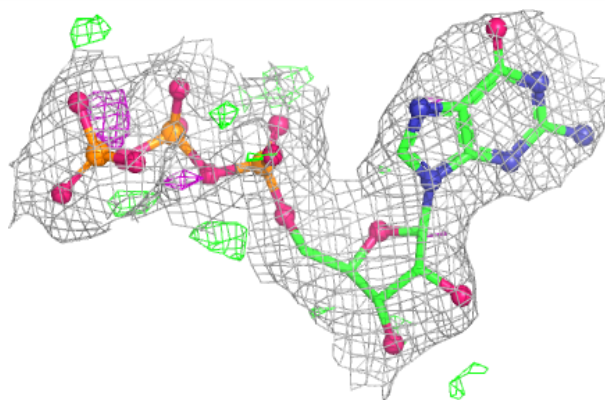
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LON 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)

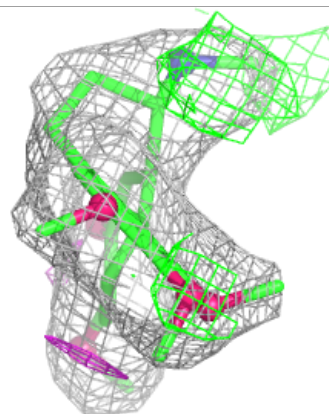
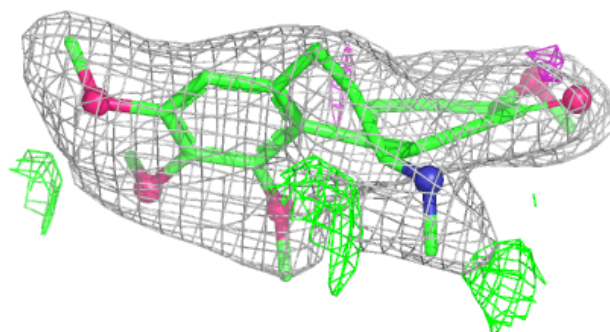
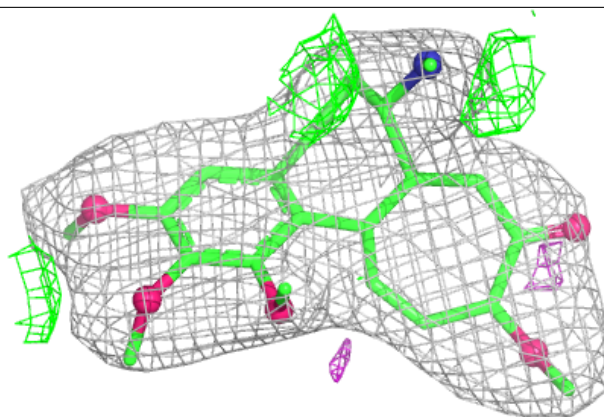
**Electron density around GTP D 501:**

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

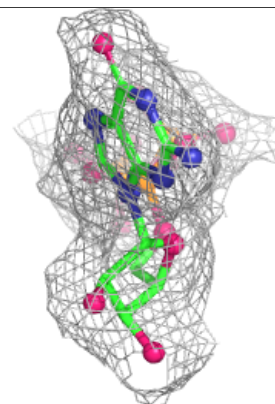
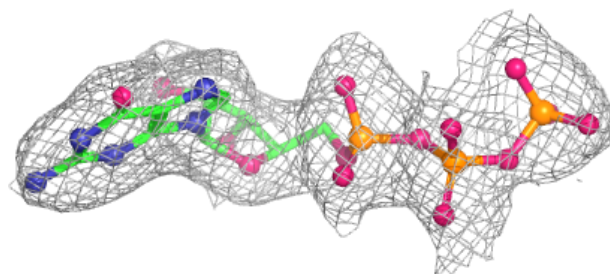
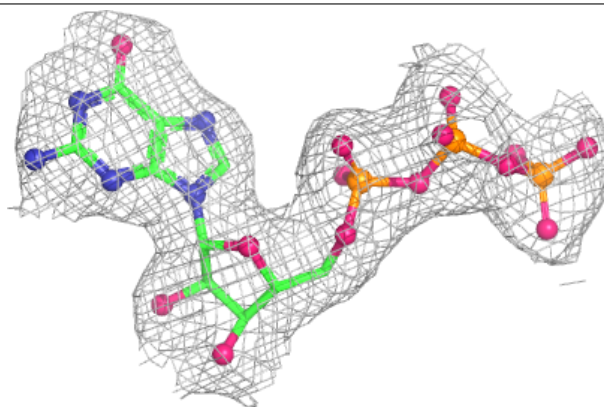


Electron density around LON B 504:

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

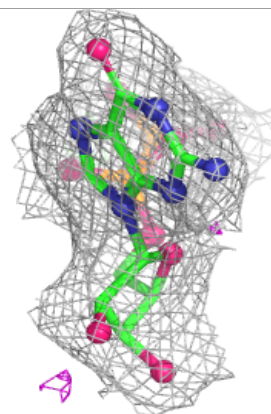
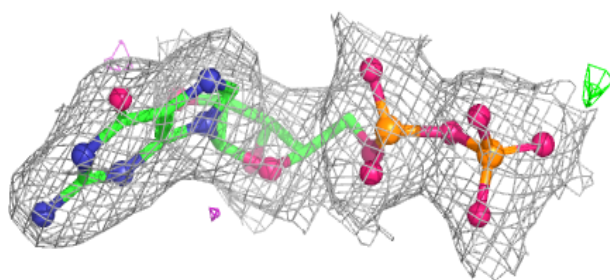
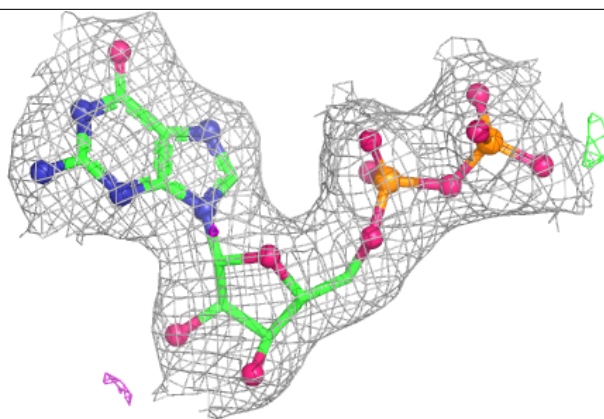
**Electron density around GTP A 501:**

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

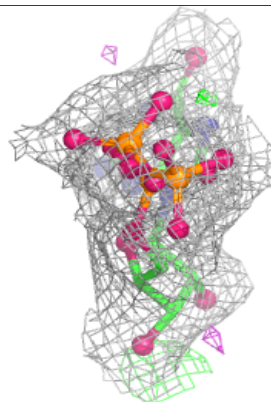
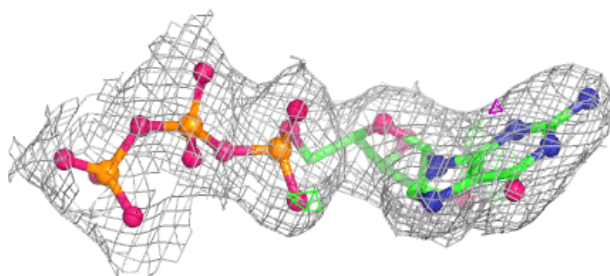
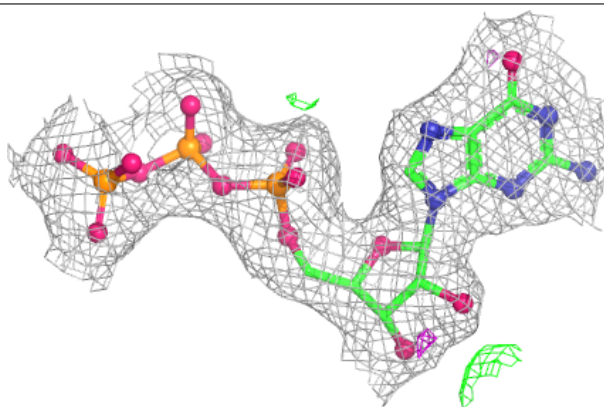


Electron density around GDP B 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.