



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:08 PM UTC

PDB ID : 8JJB / pdb_00008jjb
Title : Crystal structure of T2R-TTL-Y61 complex
Authors : Yang, J.
Deposited on : 2023-05-30
Resolution : 2.68 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

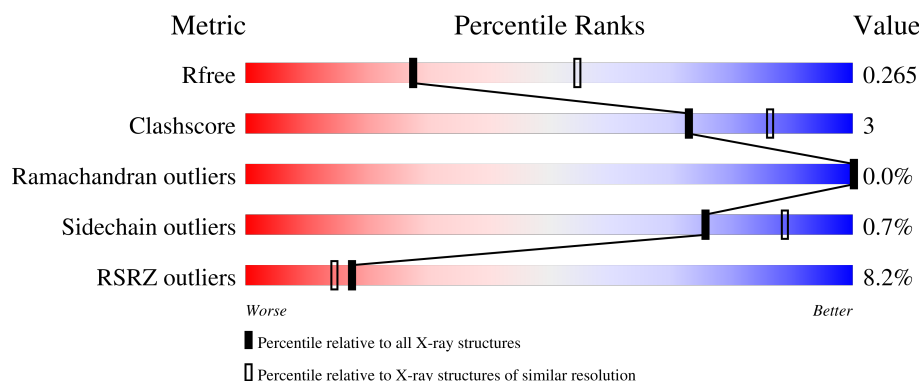
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	189	

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Mol	Chain	Length	Quality of chain
4	F	380	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a red segment at the beginning labeled '19%', a large green segment labeled '83%', a yellow segment labeled '9%', and a small grey segment at the end labeled '8%'.

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34306 atoms, of which 16750 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	2	0
			6760	2171	3330	583	653	23			
1	C	440	Total	C	H	N	O	S	0	5	0
			6749	2178	3314	578	656	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	1	0
			6490	2095	3157	569	644	25			
2	D	423	Total	C	H	N	O	S	0	1	0
			6386	2063	3108	551	637	27			

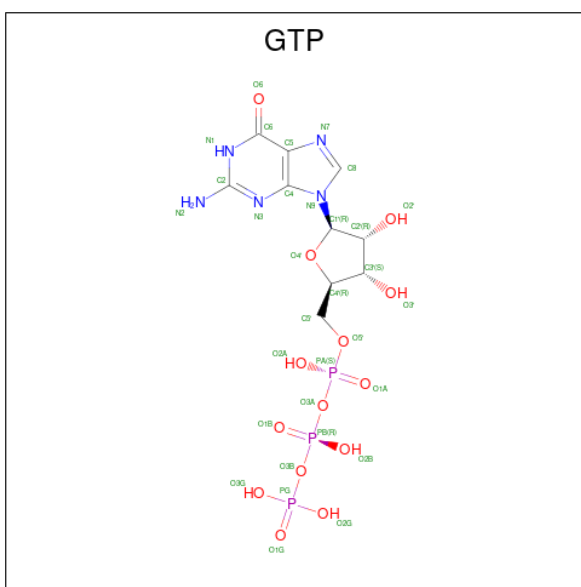
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	2	0
			2045	627	1028	185	200	5			

- Molecule 4 is a protein called TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	349	Total	C	H	N	O	S	0	0	0
			5506	1795	2709	477	511	14			

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



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

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

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

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

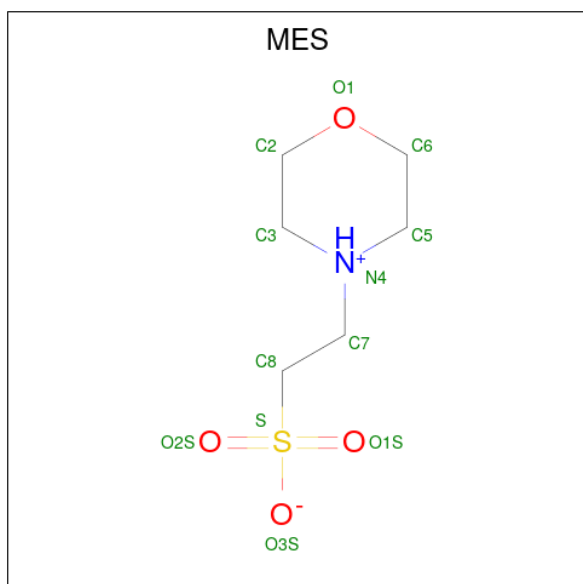
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca		
			1	1	1	0

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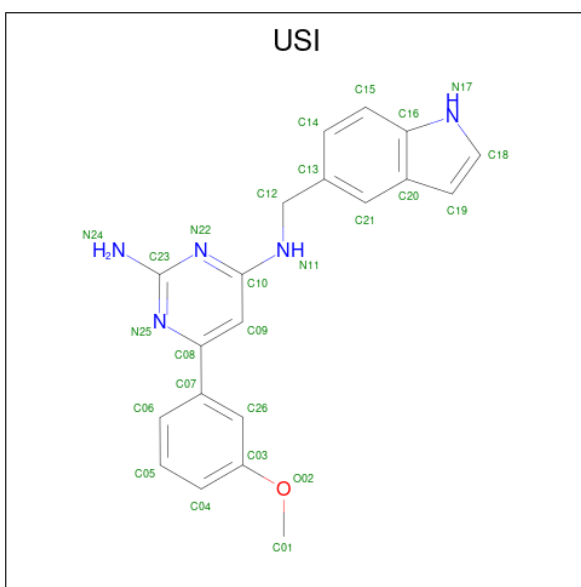
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	2	0
			2	2		
7	C	1	Total	Ca	1	0
			1	1		
7	D	1	Total	Ca	1	0
			1	1		
7	E	1	Total	Ca	1	0
			1	1		

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



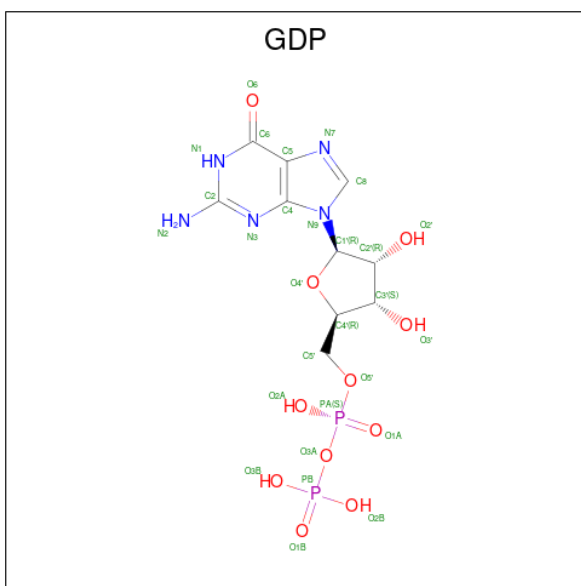
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	24	0
			24	6	12	1	4	1		

- Molecule 9 is {N}4-(1 {H}-indol-5-ylmethyl)-6-(3-methoxyphenyl)pyrimidine-2,4-diamine (CCD ID: USI) (formula: $C_{20}H_{19}N_5O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			45	20	19	5	1		
9	D	1	Total	C	H	N	O	0	0
			45	20	19	5	1		

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

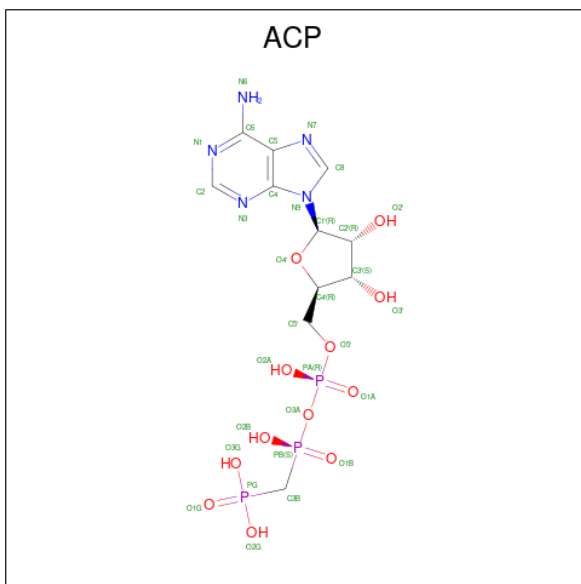


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	P	38	0
			38	10	10	5	11	2		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total Cl 1 1	1	0

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



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

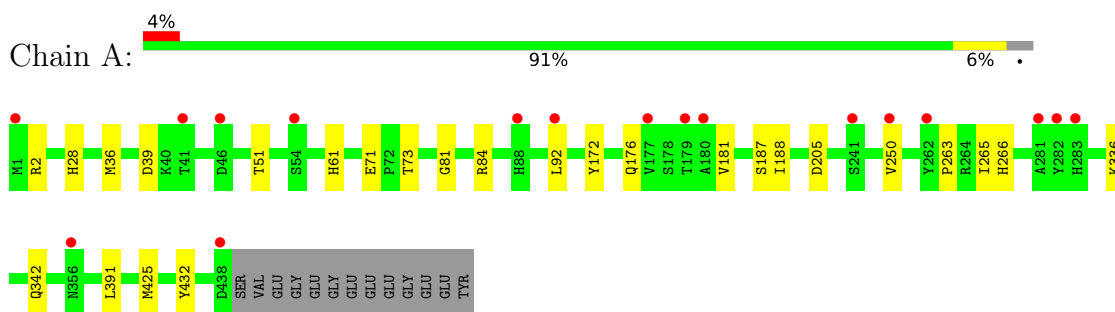
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	4	Total O 4 4	0	0
13	B	9	Total O 9 9	0	0
13	C	9	Total O 9 9	0	0
13	D	3	Total O 3 3	0	0
13	E	3	Total O 3 3	0	0
13	F	7	Total O 7 7	0	0

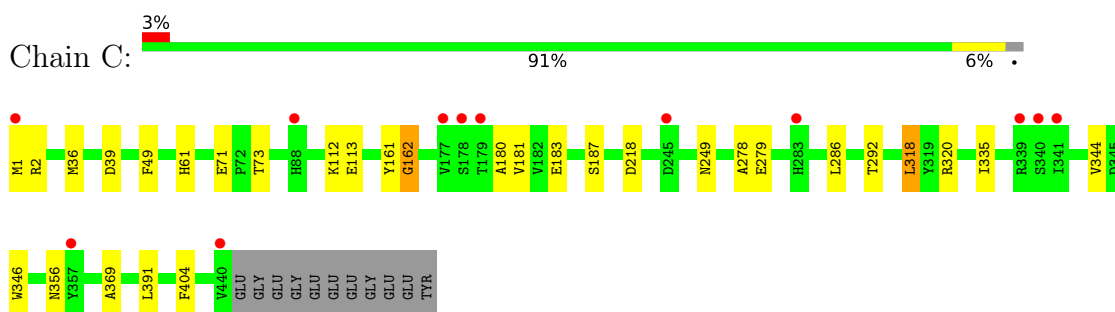
3 Residue-property plots [i](#)

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.

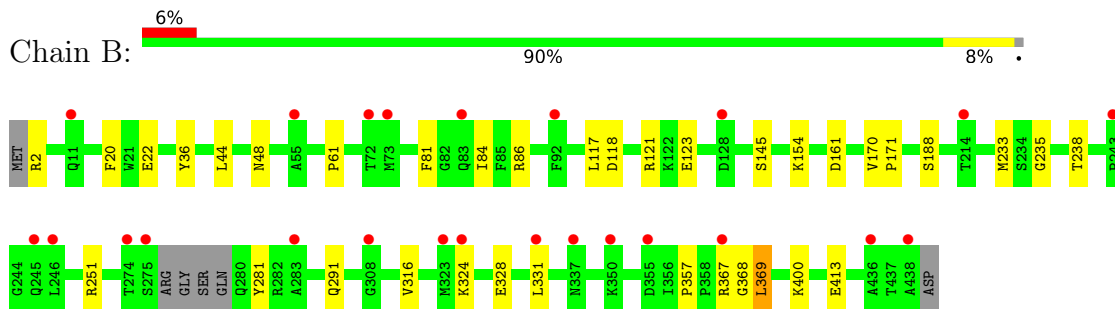
- Molecule 1: Tubulin alpha-1B chain



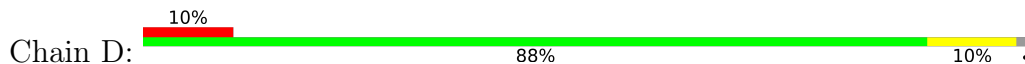
- Molecule 1: Tubulin alpha-1B chain

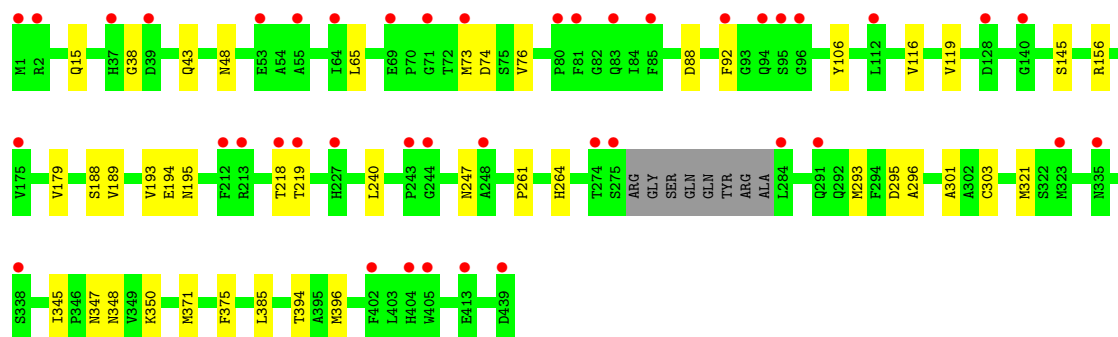


- Molecule 2: Tubulin beta chain

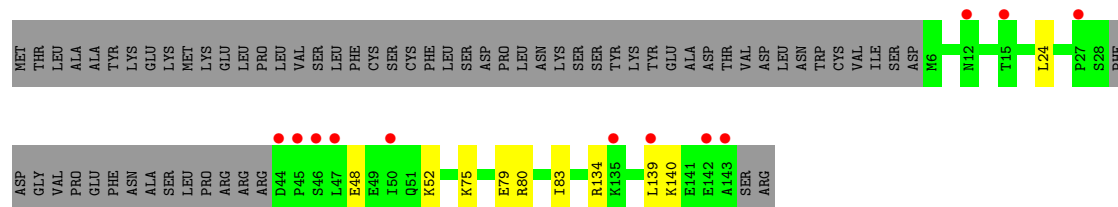


- Molecule 2: Tubulin beta chain

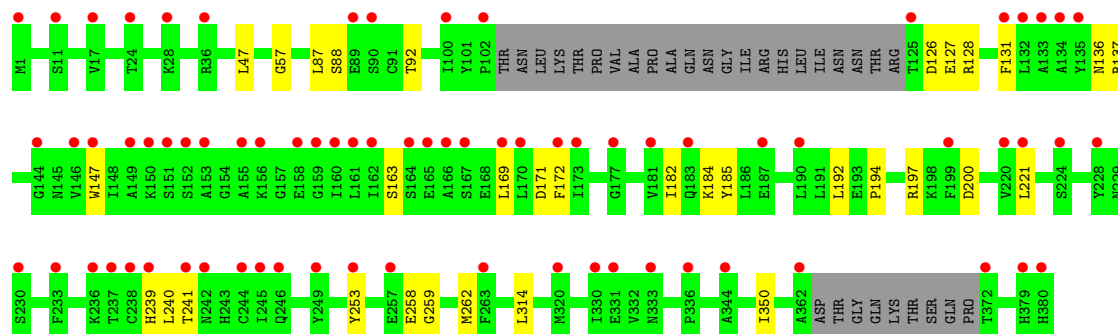
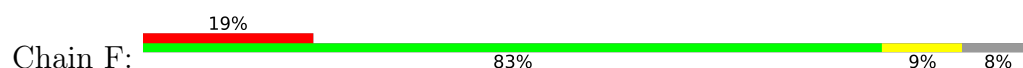




• Molecule 3: Stathmin-4



• Molecule 4: TTL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.29Å 157.91Å 181.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.68 48.06 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.06-2.68) 99.7 (48.06-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.227 , 0.260 0.232 , 0.265	Depositor DCC
R_{free} test set	1280 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.4	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	0.93	EDS
Total number of atoms	34306	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, USI, ACP, CA, CL, MES, GDP, 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	0.12	0/3511	0.31	0/4767
1	C	0.12	0/3526	0.31	0/4795
2	B	0.15	0/3410	0.33	0/4623
2	D	0.12	0/3352	0.29	0/4548
3	E	0.10	0/1028	0.25	0/1365
4	F	0.10	0/2862	0.27	0/3873
All	All	0.12	0/17689	0.30	0/23971

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	3430	3330	3341	16	0
1	C	3435	3314	3327	21	0
2	B	3333	3157	3198	21	0
2	D	3278	3108	3138	26	0
3	E	1017	1028	1031	7	0
4	F	2797	2709	2724	23	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
5	D	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	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	26	19	0	0	0
9	D	26	19	0	1	0
10	B	28	10	12	0	0
11	D	1	0	0	0	0
12	F	31	14	14	0	0
13	A	4	0	0	0	0
13	B	9	0	0	2	0
13	C	9	0	0	0	0
13	D	3	0	0	0	0
13	E	3	0	0	0	0
13	F	7	0	0	0	0
All	All	17556	16750	16833	109	0

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

All (109) 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:200:ASP:OD1	4:F:241:THR:OG1	2.02	0.77
2:D:145:SER:HG	2:D:188:SER:HG	1.38	0.72
1:C:36:MET:HE3	1:C:39:ASP:HB2	1.69	0.72
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.23	0.71
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.75	0.68
1:A:263:PRO:O	1:A:266:HIS:ND1	2.20	0.67
2:D:73:MET:SD	2:D:92:PHE:CB	2.82	0.67
2:D:179:VAL:O	2:D:396:MET:HE1	1.95	0.66
2:D:156:ARG:NH1	2:D:195:ASN:OD1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:126:ASP:OD1	4:F:128:ARG:N	2.34	0.60
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.37	0.59
2:B:2:ARG:N	13:B:601:HOH:O	2.35	0.58
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.86	0.58
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.38	0.57
2:D:189:VAL:O	2:D:193:VAL:HG23	2.04	0.56
2:D:156:ARG:NH1	2:D:194:GLU:O	2.39	0.56
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.40	0.55
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.36	0.55
2:D:218:THR:O	2:D:219:THR:OG1	2.24	0.55
2:B:235:GLY:O	2:B:238:THR:HG22	2.08	0.54
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.89	0.54
2:D:48:ASN:N	2:D:48:ASN:OD1	2.42	0.53
4:F:126:ASP:OD1	4:F:127:GLU:N	2.42	0.53
2:B:324:LYS:NZ	2:B:328:GLU:OE1	2.41	0.53
2:D:347:ASN:O	2:D:350:LYS:NZ	2.42	0.53
4:F:194:PRO:O	4:F:197:ARG:NH1	2.42	0.52
2:B:48:ASN:OD1	2:B:48:ASN:N	2.42	0.52
4:F:163:SER:CB	4:F:169:LEU:HD21	2.40	0.51
1:C:279:GLU:N	1:C:279:GLU:OE1	2.43	0.51
3:E:139:LEU:C	3:E:139:LEU:HD12	2.36	0.51
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.93	0.51
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.45	0.51
1:A:81:GLY:O	1:A:84:ARG:HD3	2.12	0.50
2:B:118:ASP:OD1	2:B:121:ARG:NH2	2.44	0.50
2:D:88:ASP:OD1	2:D:88:ASP:N	2.43	0.50
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.94	0.50
4:F:136:ASN:OD1	4:F:137:ARG:N	2.45	0.49
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.23	0.49
1:A:187:SER:CB	1:A:391:LEU:HD21	2.42	0.49
4:F:47:LEU:C	4:F:47:LEU:HD23	2.39	0.48
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.96	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.47
4:F:240:LEU:HD12	4:F:240:LEU:N	2.28	0.47
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.44	0.47
2:B:368:GLY:O	2:B:369:LEU:HD13	2.14	0.47
3:E:48:GLU:O	3:E:52:LYS:N	2.46	0.47
1:A:250:VAL:HG12	1:A:250:VAL:O	2.14	0.47
1:C:161:TYR:O	1:C:162:GLY:C	2.58	0.47
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.44	0.47
4:F:171:ASP:OD1	4:F:172:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:TYR:O	3:E:134:ARG:NH1	2.48	0.47
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.97	0.46
4:F:184:LYS:NZ	4:F:185:TYR:O	2.48	0.46
2:D:385:LEU:C	2:D:385:LEU:HD23	2.40	0.46
4:F:182:ILE:HG22	4:F:182:ILE:O	2.15	0.46
4:F:185:TYR:OH	4:F:239:HIS:ND1	2.40	0.46
2:B:145:SER:HG	2:B:188:SER:HG	1.63	0.46
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.29	0.46
2:D:65:LEU:HD12	2:D:65:LEU:N	2.32	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.45
4:F:87:LEU:O	4:F:88:SER:OG	2.23	0.45
2:B:20:PHE:HB2	2:B:233:MET:HE3	1.99	0.45
1:A:181:VAL:HG22	1:A:181:VAL:O	2.17	0.44
2:B:161:ASP:O	2:B:251:ARG:NH2	2.50	0.44
1:C:71:GLU:OE2	2:D:247:ASN:ND2	2.47	0.44
4:F:314:LEU:HD13	4:F:350:ILE:HD11	1.99	0.44
2:D:321:MET:HB3	2:D:371:MET:HE2	1.99	0.44
1:C:318:LEU:HD12	1:C:318:LEU:N	2.32	0.44
1:A:28:HIS:O	1:A:36:MET:HE3	2.17	0.44
2:B:331:LEU:HD13	4:F:57:GLY:HA3	1.99	0.44
2:D:38:GLY:HA3	2:D:43:GLN:OE1	2.18	0.43
1:C:181[B]:VAL:HG21	1:C:404:PHE:CZ	2.53	0.43
2:D:65:LEU:HD23	2:D:76:VAL:HG11	2.00	0.43
4:F:163:SER:HB3	4:F:169:LEU:HD11	2.00	0.43
1:C:36:MET:HE2	1:C:61:HIS:NE2	2.33	0.43
4:F:192:LEU:HD23	4:F:262:MET:HE1	2.01	0.43
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.54	0.43
2:B:170:VAL:HG13	2:B:171:PRO:HD2	2.00	0.43
2:B:81:PHE:O	2:B:84:ILE:HG22	2.19	0.43
1:C:1:MET:O	1:C:2:ARG:HB2	2.18	0.43
2:D:301:ALA:O	2:D:303:CYS:N	2.52	0.43
1:C:181[A]:VAL:HG21	1:C:404:PHE:CZ	2.54	0.42
1:A:92:LEU:HD12	1:A:92:LEU:N	2.35	0.42
1:A:336:LYS:HD2	3:E:24:LEU:HD13	2.00	0.42
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.01	0.42
4:F:147:TRP:CE3	4:F:184:LYS:HA	2.54	0.42
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.50	0.42
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.02	0.42
2:B:117:LEU:HD11	2:B:154:LYS:HB3	2.01	0.42
2:D:240:LEU:HD12	9:D:504:USI:C05	2.50	0.42
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.50	0.42
2:D:261:PRO:O	2:D:264:HIS:ND1	2.46	0.42
2:B:2:ARG:N	13:B:604:HOH:O	2.53	0.41
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.20	0.41
1:A:342:GLN:N	1:A:342:GLN:OE1	2.52	0.41
2:B:357:PRO:HB2	2:B:369:LEU:O	2.21	0.41
1:C:181[B]:VAL:HG13	2:D:350:LYS:NZ	2.36	0.41
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.02	0.41
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.55	0.41
2:B:86:ARG:NH1	2:B:123:GLU:OE2	2.54	0.41
2:D:116:VAL:O	2:D:119:VAL:HG12	2.21	0.41
2:B:238:THR:CG2	2:B:316:VAL:HG11	2.51	0.41
2:B:400:LYS:NZ	2:B:413:GLU:OE1	2.45	0.41
1:C:187:SER:CB	1:C:391:LEU:HD21	2.51	0.41
2:D:293:MET:CG	2:D:375:PHE:HB2	2.51	0.41
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.40	0.40
3:E:139:LEU:HD12	3:E:140:LYS:N	2.36	0.40
2:D:295:ASP:OD1	2:D:296:ALA:N	2.53	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	438/451 (97%)	428 (98%)	10 (2%)	0	100	100
1	C	443/451 (98%)	429 (97%)	13 (3%)	1 (0%)	43	65
2	B	422/431 (98%)	409 (97%)	13 (3%)	0	100	100
2	D	420/431 (97%)	407 (97%)	13 (3%)	0	100	100
3	E	121/189 (64%)	118 (98%)	3 (2%)	0	100	100
4	F	343/380 (90%)	333 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2187/2333 (94%)	2124 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/379 (98%)	369 (100%)	1 (0%)	86	94
1	C	370/379 (98%)	367 (99%)	3 (1%)	73	87
2	B	363/370 (98%)	359 (99%)	4 (1%)	65	83
2	D	356/370 (96%)	353 (99%)	3 (1%)	73	87
3	E	110/171 (64%)	110 (100%)	0	100	100
4	F	298/338 (88%)	296 (99%)	2 (1%)	76	89
All	All	1867/2007 (93%)	1854 (99%)	13 (1%)	76	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
2	B	281	TYR
2	B	291	GLN
2	B	367	ARG
2	B	369	LEU
1	C	218	ASP
1	C	286	LEU
1	C	318	LEU
2	D	15	GLN
2	D	74	ASP
2	D	394	THR

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Mol	Chain	Res	Type
4	F	92	THR
4	F	258	GLU

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	283	HIS
1	A	285	GLN
1	A	393	HIS
2	B	8	GLN
2	B	134	GLN
2	B	347	ASN
1	C	393	HIS
2	D	329	GLN
4	F	26	GLN
4	F	196	HIS
4	F	260	ASN
4	F	289	HIS

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 20 ligands modelled in this entry, 12 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
9	USI	D	504	-	29,29,29	1.64	5 (17%)	39,40,40	1.87	13 (33%)
9	USI	B	505	-	29,29,29	1.50	5 (17%)	39,40,40	1.69	11 (28%)
8	MES	B	502	-	12,12,12	2.32	1 (8%)	15,16,16	1.69	2 (13%)
12	ACP	F	402	6	31,33,33	1.61	8 (25%)	47,52,52	1.92	13 (27%)
5	GTP	A	501	6	33,34,34	0.90	1 (3%)	50,54,54	1.66	11 (22%)
5	GTP	D	503	6	33,34,34	1.01	4 (12%)	50,54,54	1.61	8 (16%)
10	GDP	B	506	6	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
5	GTP	C	501	6	33,34,34	0.93	1 (3%)	50,54,54	1.61	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	USI	D	504	-	-	3/11/11/11	0/4/4/4
9	USI	B	505	-	-	4/11/11/11	0/4/4/4
8	MES	B	502	-	-	1/6/14/14	0/1/1/1
12	ACP	F	402	6	-	8/19/38/38	0/3/3/3
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
5	GTP	D	503	6	-	9/22/38/38	0/3/3/3
10	GDP	B	506	6	-	0/16/32/32	0/3/3/3
5	GTP	C	501	6	-	1/22/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	MES	C8-S	-7.75	1.66	1.77
9	D	504	USI	C10-N11	4.72	1.43	1.36
12	F	402	ACP	C5-C4	4.55	1.47	1.39
9	B	505	USI	C10-N11	4.11	1.42	1.36
9	D	504	USI	C23-N24	3.34	1.40	1.33
9	D	504	USI	C18-C19	3.29	1.42	1.36
9	B	505	USI	C18-C19	3.24	1.42	1.36
10	B	506	GDP	C5-C4	3.10	1.47	1.38
9	B	505	USI	C23-N24	3.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	PG-O3G	2.92	1.61	1.55
9	D	504	USI	C23-N22	2.90	1.40	1.35
12	F	402	ACP	PG-O2G	2.88	1.61	1.55
9	B	505	USI	C23-N22	2.78	1.40	1.35
9	D	504	USI	C23-N25	2.69	1.40	1.35
12	F	402	ACP	C5-C6	2.64	1.48	1.41
10	B	506	GDP	C6-N1	-2.41	1.34	1.38
12	F	402	ACP	C8-N7	2.35	1.36	1.31
12	F	402	ACP	PB-O3A	2.29	1.60	1.58
12	F	402	ACP	C5-N7	-2.29	1.34	1.39
9	B	505	USI	C23-N25	2.26	1.39	1.35
5	D	503	GTP	C2-N3	2.26	1.38	1.33
5	C	501	GTP	C2-N3	2.22	1.38	1.33
5	A	501	GTP	C2-N3	2.16	1.38	1.33
5	D	503	GTP	PA-O3A	2.16	1.61	1.59
5	D	503	GTP	PB-O3A	2.15	1.61	1.59
10	B	506	GDP	C5-N7	-2.10	1.34	1.39
12	F	402	ACP	PB-O2B	2.06	1.61	1.56
5	D	503	GTP	PB-O3B	2.04	1.61	1.59

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	506	GDP	C5-C4-N3	-6.07	118.73	128.39
12	F	402	ACP	C5-C4-N3	-5.71	118.85	126.72
9	B	505	USI	C21-C20-C16	5.58	122.58	119.13
9	D	504	USI	C21-C20-C16	5.38	122.46	119.13
5	C	501	GTP	C5-C4-N3	-5.24	120.05	128.39
5	D	503	GTP	C5-C4-N3	-5.17	120.16	128.39
5	A	501	GTP	C5-C4-N3	-5.02	120.41	128.39
10	B	506	GDP	C2-N3-C4	5.01	120.93	112.30
5	C	501	GTP	C2-N3-C4	4.79	120.55	112.30
5	A	501	GTP	C2-N3-C4	4.73	120.44	112.30
5	D	503	GTP	C2-N3-C4	4.70	120.39	112.30
12	F	402	ACP	N3-C4-N9	4.66	135.10	127.17
10	B	506	GDP	N9-C4-N3	4.53	135.01	125.95
8	B	502	MES	C5-N4-C3	4.18	117.85	108.84
12	F	402	ACP	PB-O3A-PA	-3.95	119.48	132.37
12	F	402	ACP	C2-N3-C4	3.82	121.17	111.83
12	F	402	ACP	N3-C2-N1	-3.70	122.97	128.58
9	D	504	USI	N11-C10-N22	3.51	122.19	116.42
9	B	505	USI	C15-C16-C20	-3.50	118.96	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	504	USI	C08-N25-C23	-3.48	114.30	116.35
5	C	501	GTP	N9-C4-N3	3.41	132.78	125.95
9	D	504	USI	C15-C16-C20	-3.41	119.05	122.13
12	F	402	ACP	C4-C5-N7	-3.37	106.73	110.58
5	D	503	GTP	N9-C4-N3	3.35	132.65	125.95
10	B	506	GDP	C6-C5-N7	3.23	136.17	130.29
5	A	501	GTP	N9-C4-N3	3.14	132.24	125.95
12	F	402	ACP	C4-N9-C8	3.09	108.99	105.74
5	D	503	GTP	C2-N1-C6	-2.96	119.74	125.11
9	D	504	USI	C16-N17-C18	2.94	111.06	108.91
5	C	501	GTP	C2-N1-C6	-2.92	119.81	125.11
9	D	504	USI	C15-C14-C13	2.91	124.82	121.00
9	B	505	USI	C16-N17-C18	2.91	111.04	108.91
5	A	501	GTP	C2-N1-C6	-2.87	119.91	125.11
9	B	505	USI	C15-C14-C13	2.77	124.64	121.00
9	B	505	USI	C08-N25-C23	-2.74	114.73	116.35
9	D	504	USI	C20-C21-C13	-2.70	119.08	122.22
12	F	402	ACP	C5-N7-C8	2.70	107.69	103.45
5	A	501	GTP	N9-C8-N7	-2.66	108.47	113.40
9	B	505	USI	C20-C21-C13	-2.66	119.13	122.22
5	D	503	GTP	N9-C8-N7	-2.58	108.62	113.40
5	C	501	GTP	N9-C8-N7	-2.55	108.67	113.40
5	A	501	GTP	C8-N7-C5	2.54	108.79	104.26
10	B	506	GDP	C4-C5-N7	-2.54	106.65	110.67
5	D	503	GTP	C5-C6-N1	2.54	119.71	113.25
5	D	503	GTP	C8-N7-C5	2.52	108.75	104.26
5	C	501	GTP	C8-N7-C5	2.52	108.75	104.26
9	D	504	USI	C09-C10-N11	-2.52	116.70	120.79
5	A	501	GTP	C5-C6-N1	2.50	119.62	113.25
5	C	501	GTP	C5-C6-N1	2.50	119.61	113.25
9	D	504	USI	C12-N11-C10	2.47	127.96	123.04
9	D	504	USI	C06-C07-C08	-2.42	117.45	121.28
10	B	506	GDP	C3'-C2'-C1'	2.42	106.04	101.46
9	D	504	USI	C26-C07-C08	2.41	123.96	120.59
5	D	503	GTP	O6-C6-C5	-2.41	120.18	126.53
12	F	402	ACP	N9-C8-N7	-2.39	110.55	113.94
5	C	501	GTP	O6-C6-C5	-2.36	120.30	126.53
5	A	501	GTP	O6-C6-C5	-2.35	120.33	126.53
9	B	505	USI	C19-C18-N17	-2.34	107.54	110.25
9	D	504	USI	C19-C18-N17	-2.33	107.55	110.25
12	F	402	ACP	C3'-C2'-C1'	2.32	105.86	101.46
9	B	505	USI	N11-C10-N22	2.24	120.10	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O3G-PG-O3B	2.24	112.14	104.64
12	F	402	ACP	C2'-C1'-N9	-2.22	107.80	113.30
5	A	501	GTP	O2B-PB-O3A	2.20	113.23	107.27
5	A	501	GTP	O3G-PG-O3B	2.18	111.96	104.64
5	A	501	GTP	O2G-PG-O3B	2.13	111.79	104.64
8	B	502	MES	C7-N4-C5	2.13	116.91	111.24
9	D	504	USI	C20-C16-N17	2.11	109.23	107.53
10	B	506	GDP	O6-C6-C5	-2.10	120.98	126.53
5	C	501	GTP	O2A-PA-O3A	2.09	112.94	107.27
12	F	402	ACP	C6-C5-N7	2.09	136.13	132.09
9	B	505	USI	C06-C07-C08	-2.08	117.99	121.28
12	F	402	ACP	C2-N1-C6	2.06	122.12	118.73
9	B	505	USI	C20-C16-N17	2.01	109.15	107.53
9	B	505	USI	C26-C07-C08	2.00	123.39	120.59

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	D	503	GTP	PB-O3B-PG-O3G
5	D	503	GTP	C5'-O5'-PA-O3A
5	D	503	GTP	C5'-O5'-PA-O2A
9	B	505	USI	C09-C10-N11-C12
9	B	505	USI	N22-C10-N11-C12
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O2B
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O3A
9	B	505	USI	C04-C03-O02-C01
9	B	505	USI	C26-C03-O02-C01
9	D	504	USI	C04-C03-O02-C01
9	D	504	USI	C13-C12-N11-C10
9	D	504	USI	C26-C03-O02-C01
8	B	502	MES	C8-C7-N4-C3
12	F	402	ACP	C3'-C4'-C5'-O5'
5	D	503	GTP	PG-O3B-PB-O1B
12	F	402	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C4'-C5'-O5'-PA
5	D	503	GTP	C4'-C5'-O5'-PA
5	D	503	GTP	PB-O3B-PG-O2G
5	D	503	GTP	PG-O3B-PB-O2B
5	D	503	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PG-O3B-PB-O2B
5	D	503	GTP	PA-O3A-PB-O2B

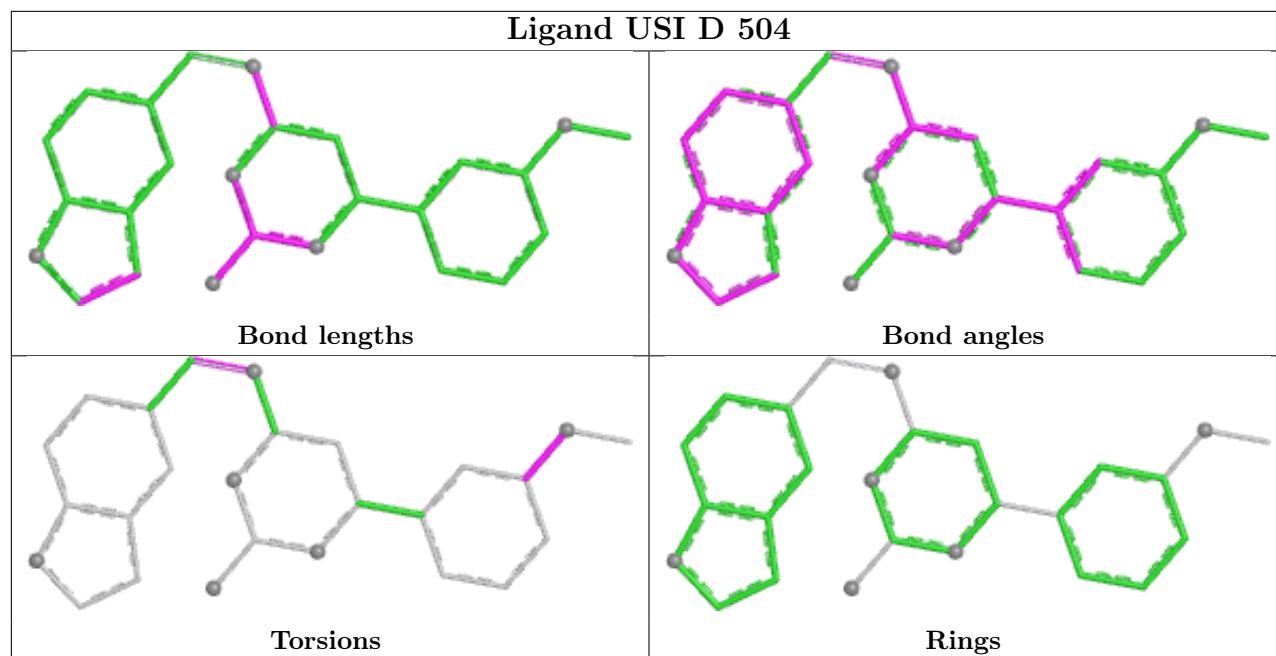
There are no ring outliers.

1 monomer is involved in 1 short contact:

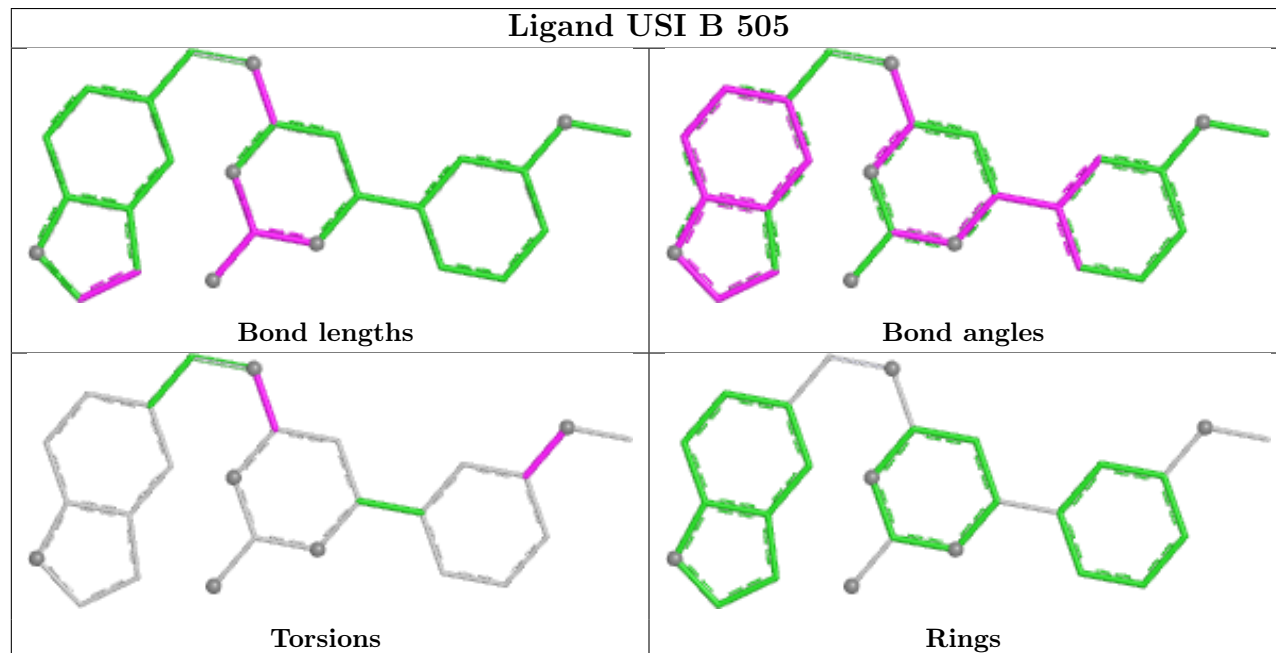
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	504	USI	1	0

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.

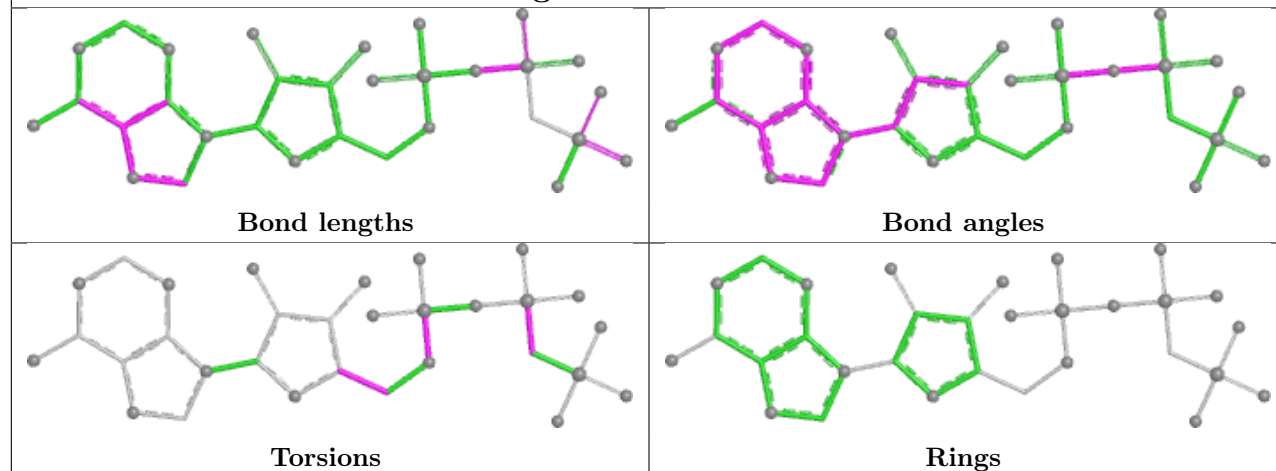
Ligand USI D 504



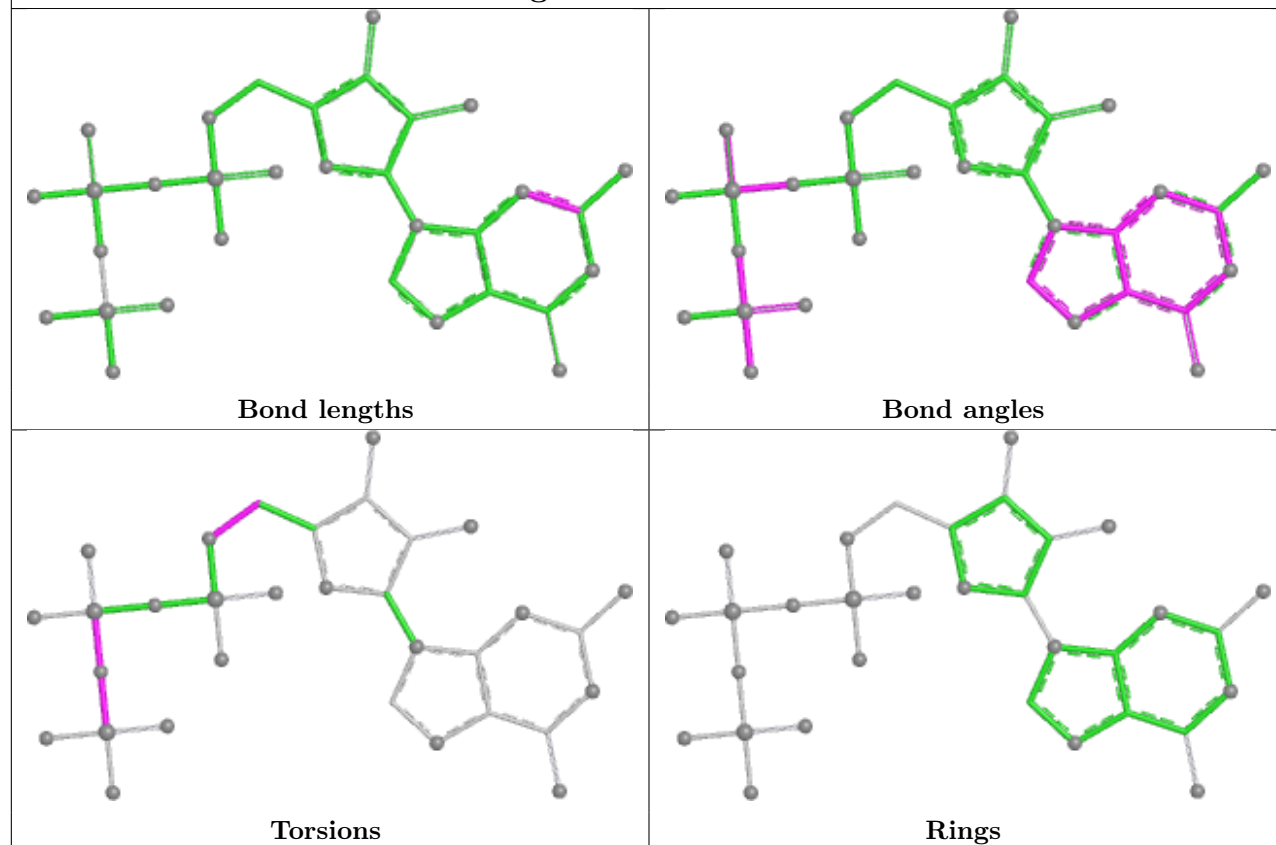
Ligand USI B 505

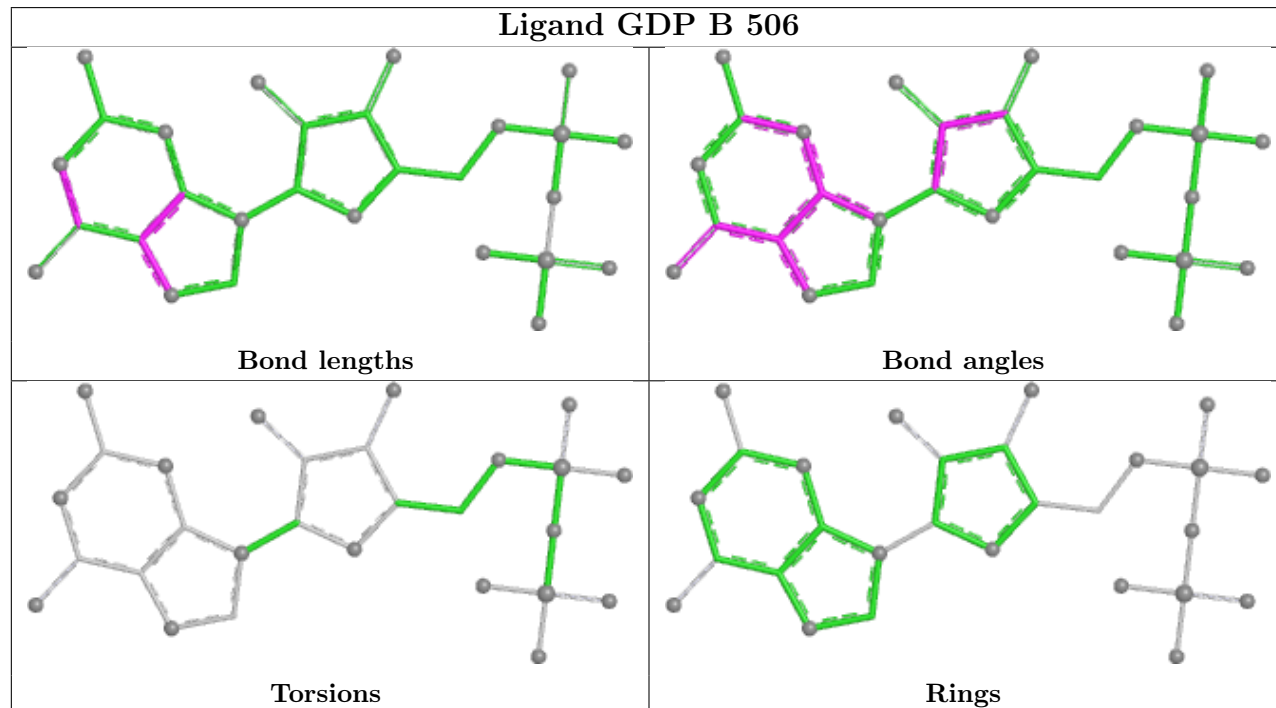
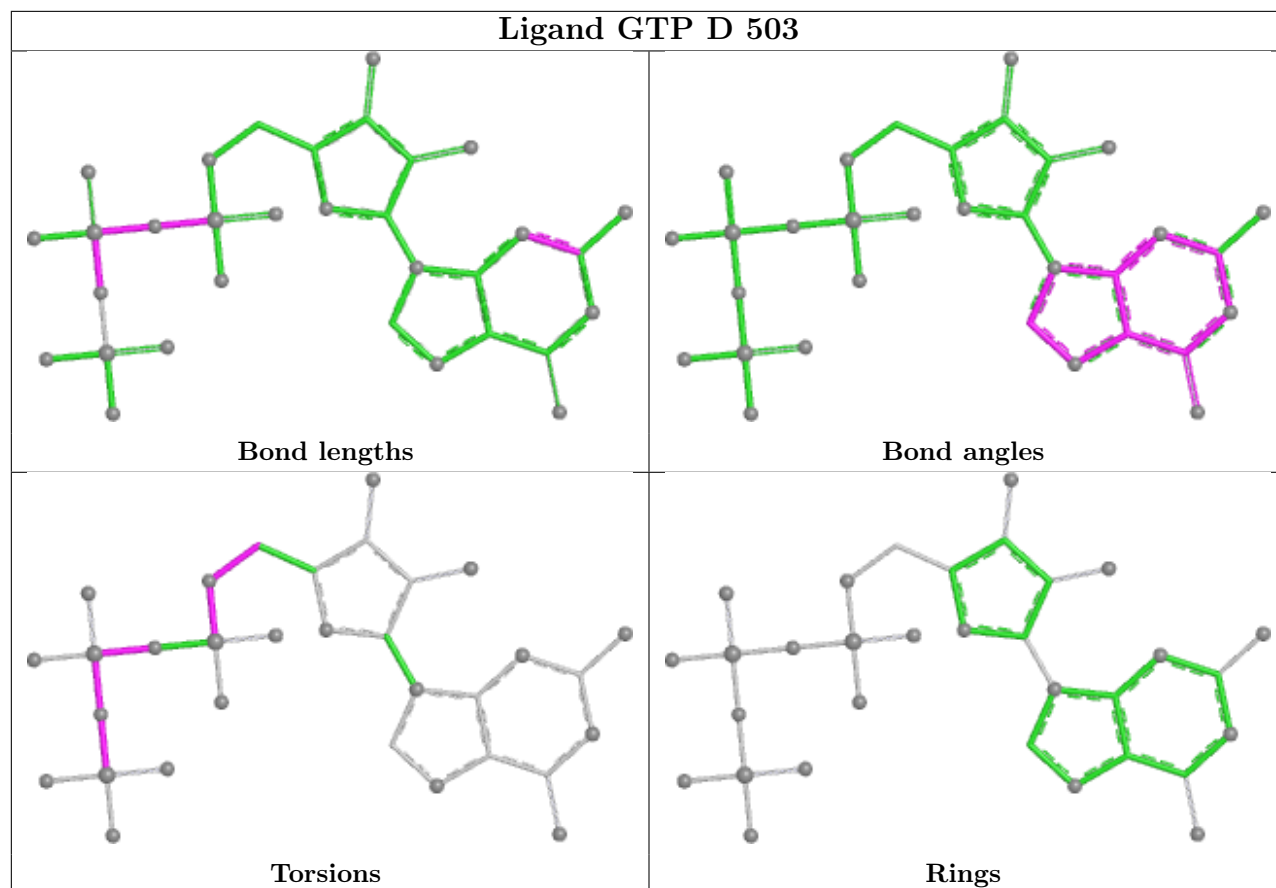


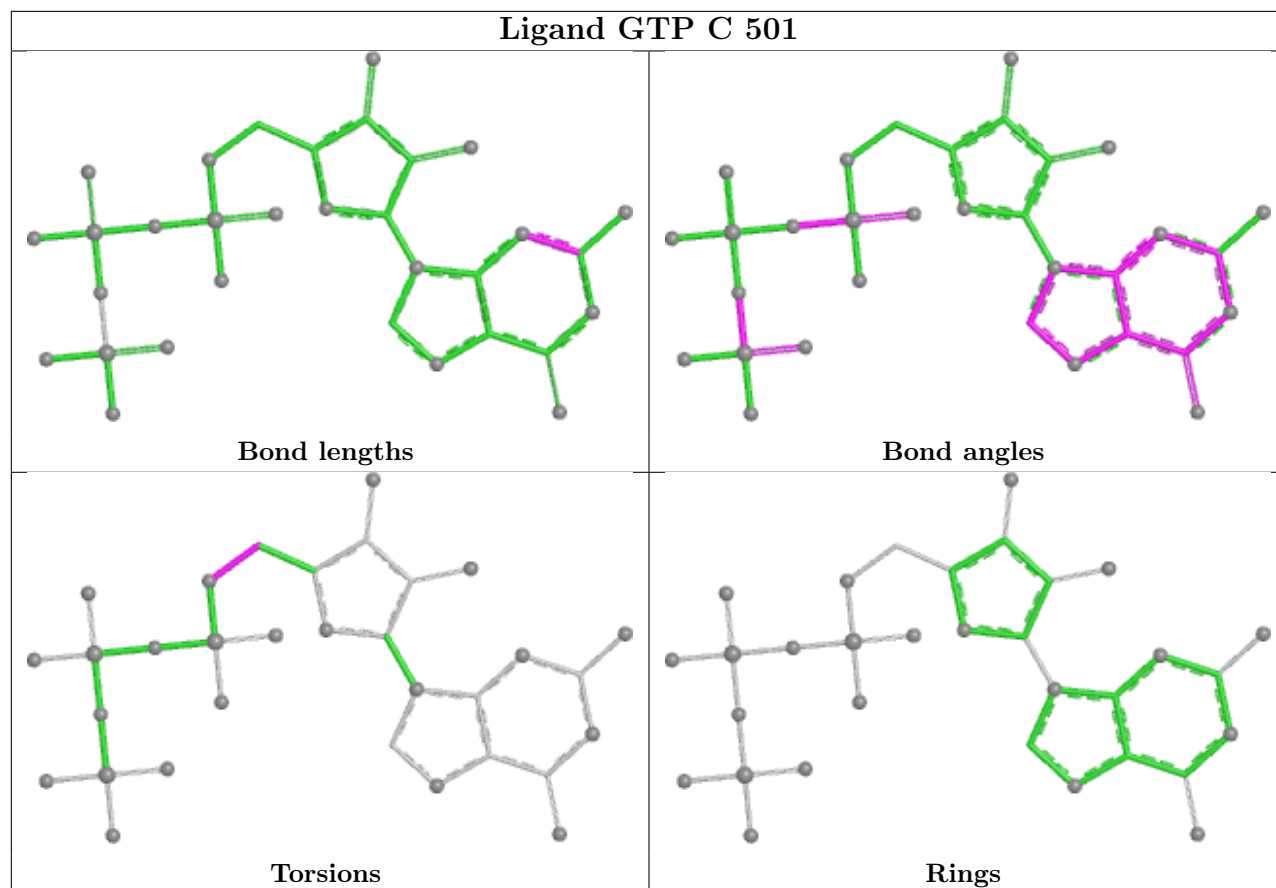
Ligand ACP F 402



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	438/451 (97%)	0.39	17 (3%)	43	38	29, 65, 99, 148	2 (0%)
1	C	440/451 (97%)	0.06	12 (2%)	56	52	25, 54, 88, 125	5 (1%)
2	B	425/431 (98%)	0.42	24 (5%)	30	26	34, 66, 111, 147	1 (0%)
2	D	423/431 (98%)	0.78	42 (9%)	13	10	46, 82, 118, 158	1 (0%)
3	E	123/189 (65%)	0.76	12 (9%)	13	11	36, 84, 125, 143	2 (1%)
4	F	349/380 (91%)	1.16	74 (21%)	2	2	58, 98, 161, 200	0
All	All	2198/2333 (94%)	0.55	181 (8%)	17	14	25, 72, 128, 200	11 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	73	MET	6.8
1	C	179	THR	6.7
2	D	55	ALA	6.0
1	A	179	THR	5.9
4	F	150	LYS	5.3
4	F	169	LEU	5.2
4	F	159	GLY	5.1
2	D	275	SER	5.1
4	F	233	PHE	4.5
4	F	173	ILE	4.0
2	B	246	LEU	3.9
1	C	178	SER	3.9
2	D	95	SER	3.9
1	A	281	ALA	3.9
4	F	166	ALA	3.9
2	D	53	GLU	3.8
4	F	161	LEU	3.8
3	E	143	ALA	3.8
2	B	367	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	350	LYS	3.8
1	C	88[A]	HIS	3.7
1	A	41	THR	3.7
1	A	46	ASP	3.6
2	B	438	ALA	3.5
2	B	331	LEU	3.5
4	F	144	GLY	3.5
1	A	180	ALA	3.5
4	F	249	TYR	3.4
4	F	181	VAL	3.4
4	F	362	ALA	3.4
2	B	55	ALA	3.4
2	B	283	ALA	3.4
1	A	262	TYR	3.3
4	F	242	ASN	3.3
4	F	183	GLN	3.3
2	D	140	GLY	3.3
2	D	92	PHE	3.3
3	E	139	LEU	3.2
2	D	37	HIS	3.2
4	F	164	SER	3.2
4	F	320	MET	3.2
4	F	239	HIS	3.2
1	A	282	TYR	3.2
4	F	125	THR	3.1
4	F	263	PHE	3.1
1	C	283	HIS	3.1
4	F	244	CYS	3.1
3	E	46	SER	3.1
3	E	142	GLU	3.0
4	F	149	ALA	3.0
4	F	333	ASN	3.0
2	D	1	MET	3.0
2	B	274	THR	3.0
4	F	372	THR	3.0
1	C	177	VAL	2.9
4	F	153	ALA	2.9
4	F	1	MET	2.9
3	E	44	ASP	2.9
2	D	80	PRO	2.9
1	A	177	VAL	2.9
2	D	404	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	439	ASP	2.8
1	C	440	VAL	2.8
2	D	85	PHE	2.8
4	F	89	GLU	2.8
4	F	379	HIS	2.8
4	F	131	PHE	2.8
2	D	2	ARG	2.8
4	F	221	LEU	2.7
2	B	308	GLY	2.7
4	F	155	ALA	2.7
3	E	45	PRO	2.7
1	C	357	TYR	2.7
2	D	405	TRP	2.7
4	F	224	SER	2.7
1	A	250	VAL	2.7
1	A	438	ASP	2.7
2	D	112	LEU	2.7
2	B	337	ASN	2.7
2	D	413	GLU	2.7
3	E	12[A]	ASN	2.7
2	D	291	GLN	2.6
3	E	50	ILE	2.6
2	B	436	ALA	2.6
2	D	402	PHE	2.6
4	F	162	ILE	2.6
4	F	228	TYR	2.6
2	D	96	GLY	2.6
4	F	134	ALA	2.6
4	F	190	LEU	2.5
4	F	100	ILE	2.5
4	F	36	ARG	2.5
4	F	170	LEU	2.5
1	C	1	MET	2.5
2	D	219	THR	2.5
2	D	128	ASP	2.5
4	F	156	LYS	2.5
4	F	172	PHE	2.5
2	D	218	THR	2.5
2	B	324	LYS	2.5
1	A	241	SER	2.5
4	F	132	LEU	2.5
4	F	160	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	71	GLY	2.5
2	B	275	SER	2.4
1	C	245	ASP	2.4
4	F	177	GLY	2.4
2	B	245	GLN	2.4
2	D	94	GLN	2.4
1	C	339	ARG	2.4
2	D	274	THR	2.4
2	B	128	ASP	2.4
4	F	158	GLU	2.4
2	D	248	ALA	2.4
1	A	88	HIS	2.4
2	D	338	SER	2.4
4	F	165	GLU	2.4
1	A	1	MET	2.4
4	F	28	LYS	2.4
2	D	244	GLY	2.4
4	F	133	ALA	2.4
2	D	284	LEU	2.4
4	F	241	THR	2.4
2	B	73	MET	2.4
2	D	212	PHE	2.4
4	F	199	PHE	2.4
2	B	214	THR	2.3
3	E	15	THR	2.3
2	D	39	ASP	2.3
4	F	90	SER	2.3
4	F	102	PRO	2.3
4	F	336	PRO	2.3
2	D	175	VAL	2.3
4	F	253	TYR	2.3
4	F	187	GLU	2.3
4	F	238	CYS	2.3
2	D	69	GLU	2.3
4	F	151	SER	2.3
1	A	283	HIS	2.3
1	C	340	SER	2.3
4	F	167	SER	2.3
4	F	246	GLN	2.2
3	E	47	LEU	2.2
4	F	146	VAL	2.2
2	B	72	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	24	THR	2.2
1	A	356	ASN	2.2
2	B	11	GLN	2.2
4	F	11	SER	2.2
2	B	323	MET	2.2
2	D	323	MET	2.2
4	F	237	THR	2.2
4	F	230	SER	2.2
2	B	83	GLN	2.2
1	A	54	SER	2.2
2	D	64	ILE	2.2
3	E	27	PRO	2.1
2	B	355	ASP	2.1
4	F	330	ILE	2.1
4	F	257	GLU	2.1
2	D	335	ASN	2.1
2	D	213	ARG	2.1
3	E	135	LYS	2.1
2	D	227	HIS	2.1
4	F	220	VAL	2.1
2	B	92	PHE	2.1
1	A	92	LEU	2.1
4	F	152	SER	2.0
2	B	243	PRO	2.0
2	D	83	GLN	2.0
1	C	341	ILE	2.0
4	F	17	VAL	2.0
2	D	81	PHE	2.0
4	F	331	GLU	2.0
4	F	236	LYS	2.0
4	F	344	ALA	2.0
4	F	147	TRP	2.0
2	D	243	PRO	2.0
4	F	380	HIS	2.0
4	F	245	ILE	2.0
4	F	135	TYR	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](#)

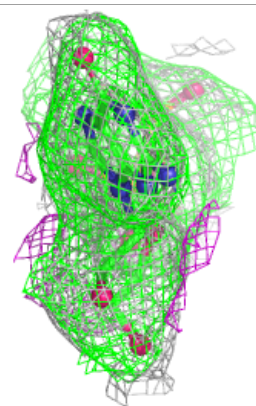
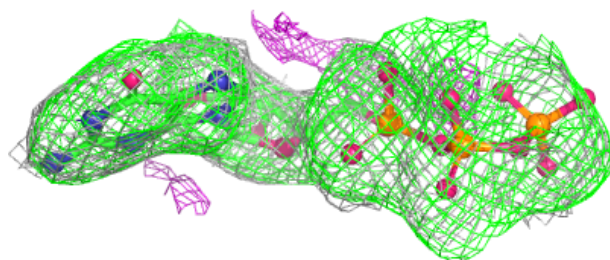
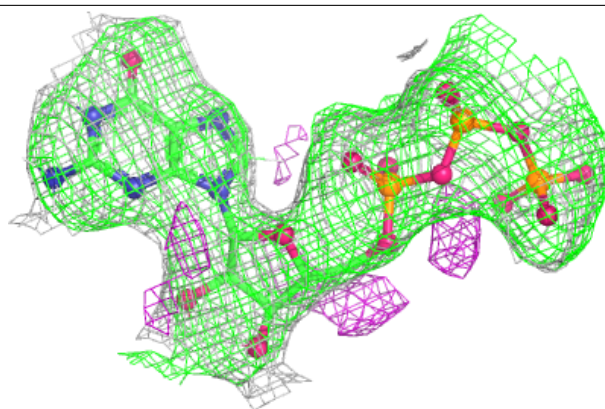
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	GTP	A	501	32/32	-	-	47,51,67,71	42
5	GTP	C	501	32/32	-	-	39,45,62,65	42
5	GTP	D	503	32/32	-	-	67,82,95,99	42
6	MG	A	502	1/1	-	-	54,54,54,54	1
6	MG	B	501	1/1	-	-	58,58,58,58	1
6	MG	C	502	1/1	-	-	43,43,43,43	1
6	MG	D	501	1/1	-	-	94,94,94,94	1
6	MG	F	401	1/1	-	-	112,112,112,112	1
7	CA	A	503	1/1	-	-	84,84,84,84	1
7	CA	B	503	1/1	-	-	70,70,70,70	1
7	CA	B	504	1/1	-	-	76,76,76,76	1
7	CA	C	503	1/1	-	-	66,66,66,66	1
7	CA	D	502	1/1	-	-	74,74,74,74	1
7	CA	E	201	1/1	-	-	75,75,75,75	1
8	MES	B	502	12/12	-	-	48,52,61,61	24
9	USI	D	504	26/26	0.88	0.16	55,76,101,109	0
9	USI	B	505	26/26	0.92	0.16	48,73,117,140	0
10	GDP	B	506	28/28	-	-	46,53,64,65	38
11	CL	D	505	1/1	-	-	61,61,61,61	1
12	ACP	F	402	31/31	-	-	96,108,133,142	45

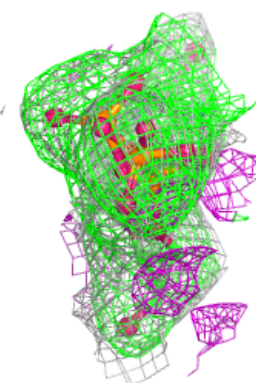
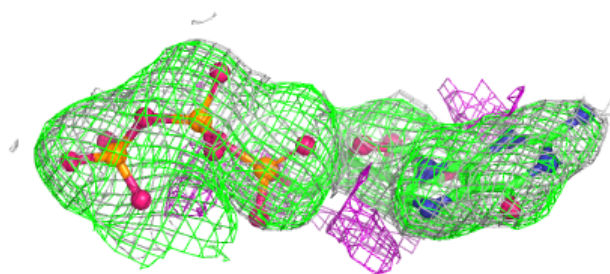
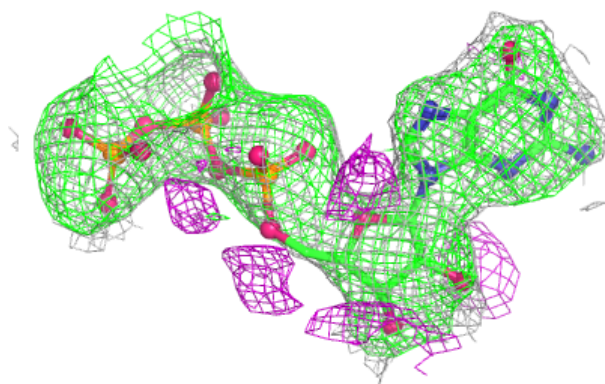
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

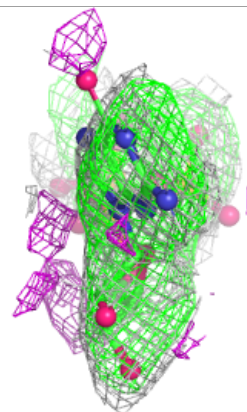
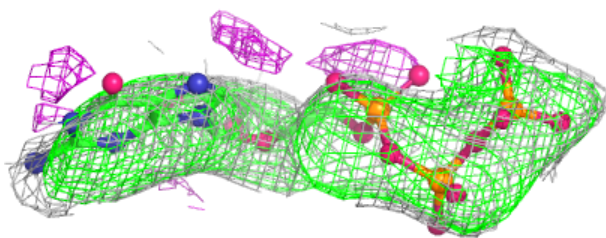
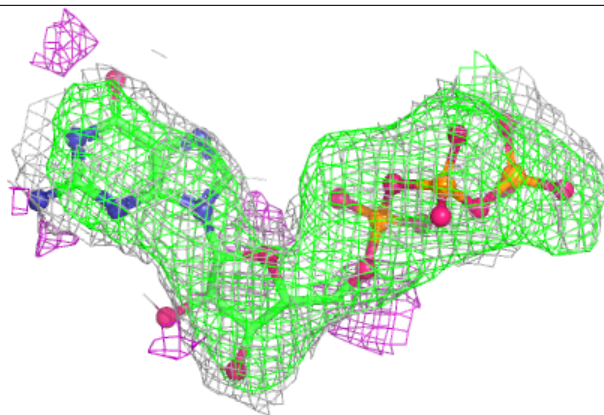
**Electron density around GTP C 501:**

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

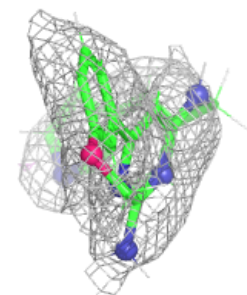
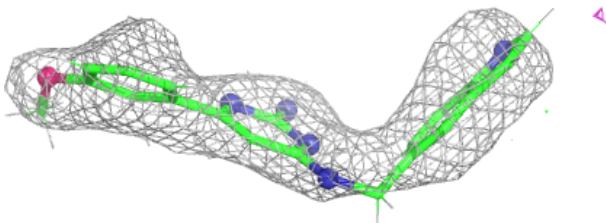
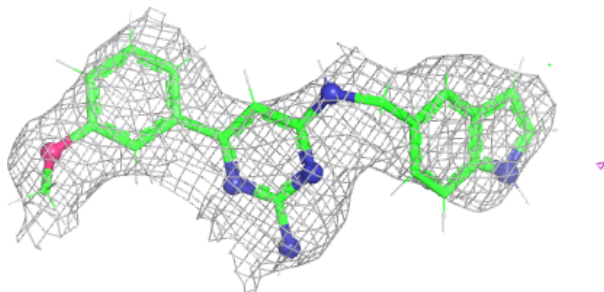


Electron density around GTP D 503:

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

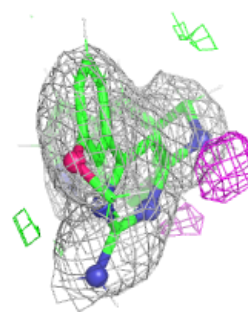
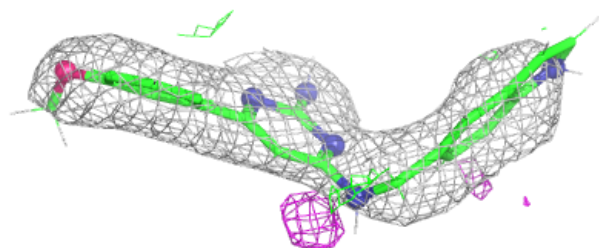
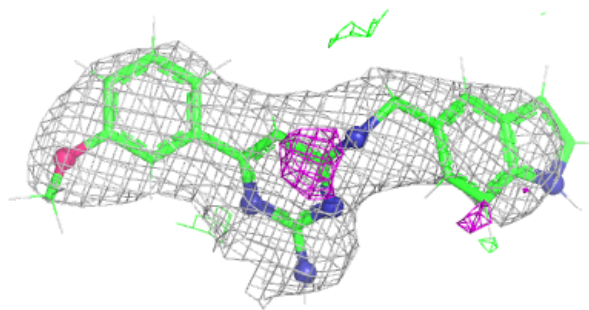
**Electron density around USI D 504:**

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



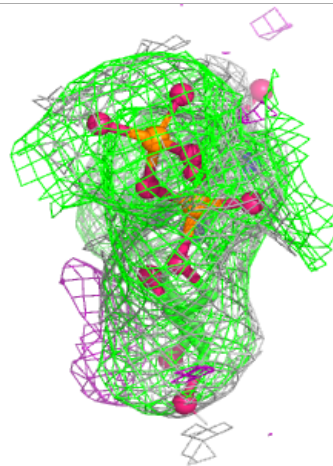
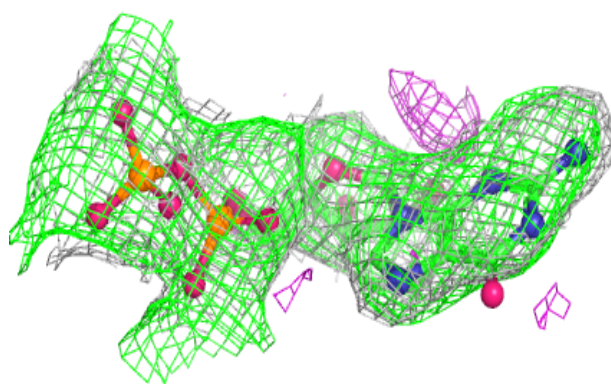
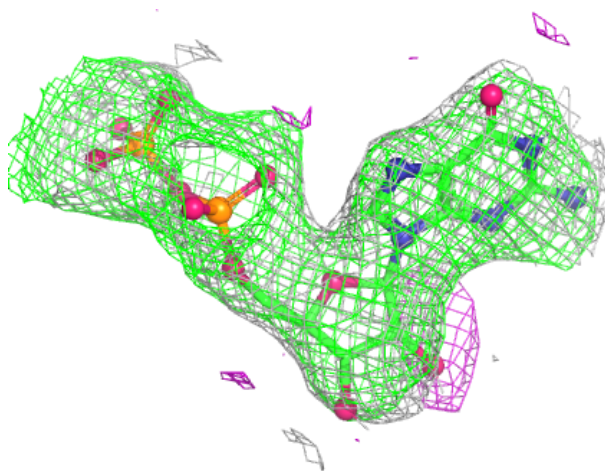
Electron density around USI B 505:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



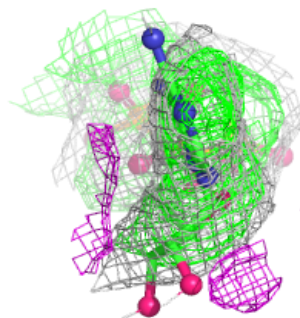
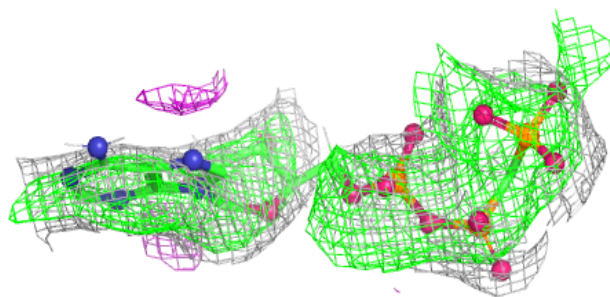
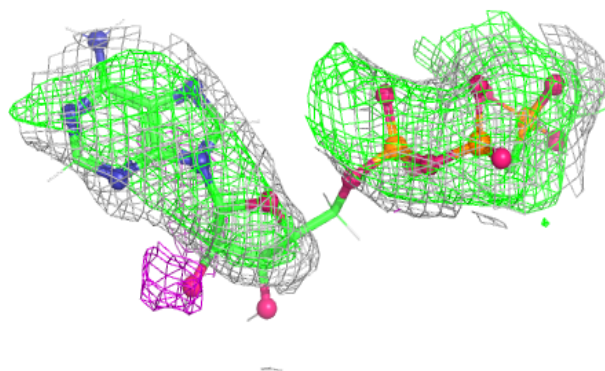
Electron density around GDP B 506:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.