



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:08 AM UTC

PDB ID : 6KPP / pdb_00006kpp
Title : BNC105 in complex with tubulin
Authors : Wang, T.; Wu, C.; Pu, D.
Deposited on : 2019-08-15
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

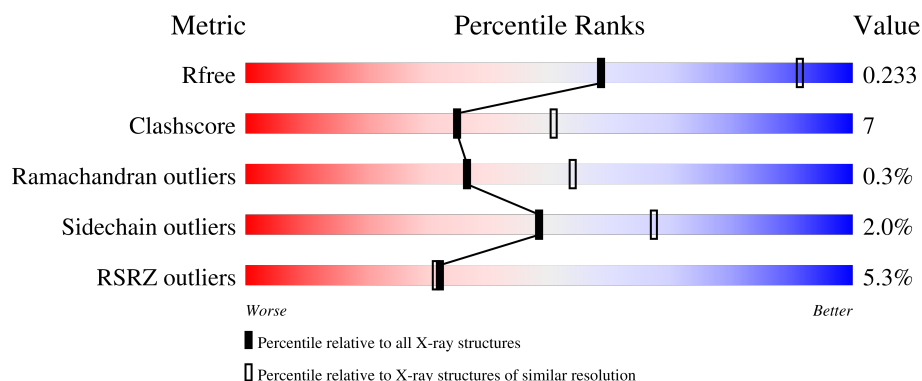
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	450	0% 82% 15% ..
1	C	450	3% 83% 14% .
2	B	445	4% 77% 20% .
2	D	445	8% 71% 22% . 6%
3	E	143	2% 77% 9% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	10% 63% 17% • 17%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17583 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	438	Total	C	N	O	S	0	2	0
			3430	2171	582	653	24			
1	C	441	Total	C	N	O	S	0	5	0
			3462	2190	586	663	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3376	2119	578	652	27			
2	D	418	Total	C	N	O	S	0	2	0
			3297	2073	559	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	633	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	expression tag	UNP P63042
E	2	ALA	-	expression tag	UNP P63042

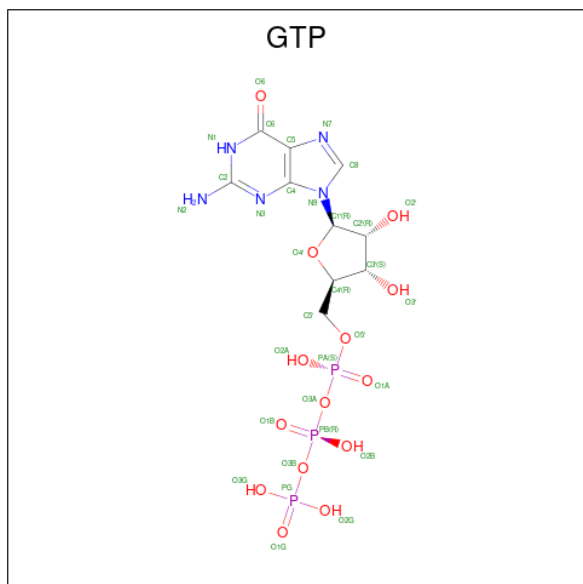
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	0	0
			2615	1681	454	466	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		

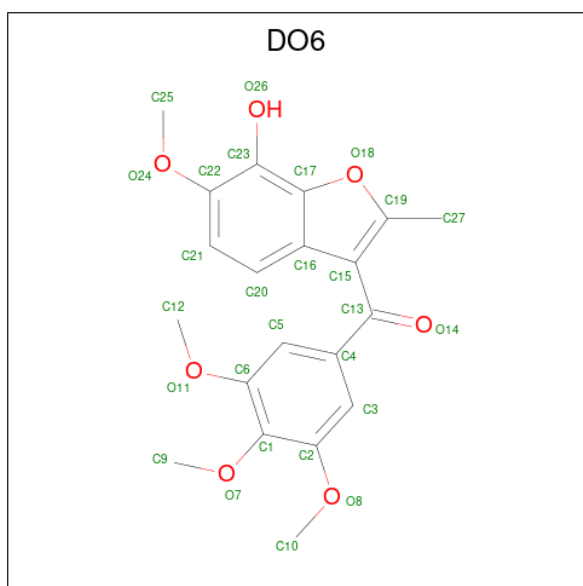
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

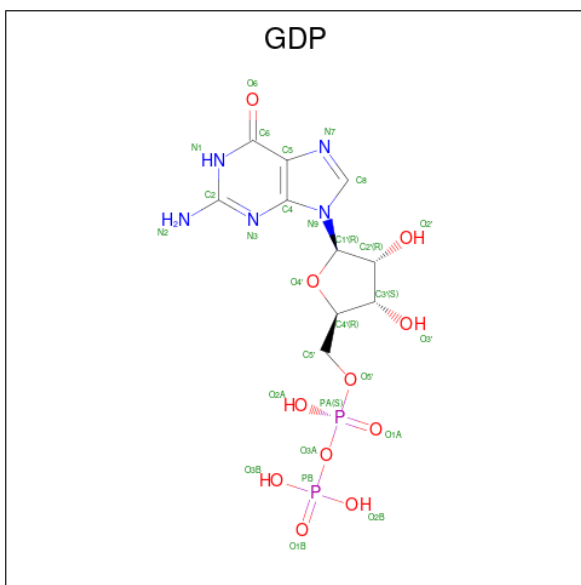
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is (6-methoxy-2-methyl-7-oxidanyl-1-benzofuran-3-yl)-(3,4,5-trimethoxyphenyl)methanone (CCD ID: DO6) (formula: C₂₀H₂₀O₇) (labeled as "Ligand of Interest" by depositor).



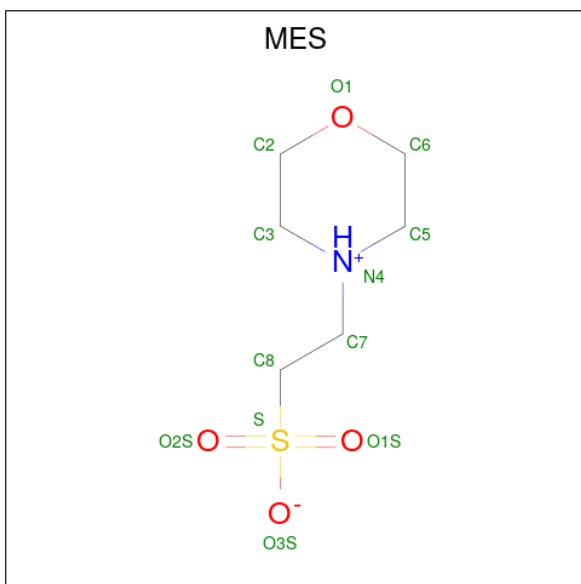
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			27	20	7		
8	D	1	Total	C	O	0	0
			27	20	7		

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



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



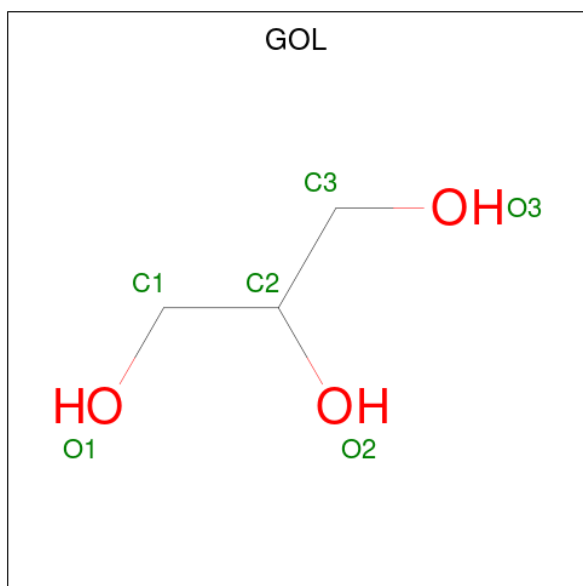
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		

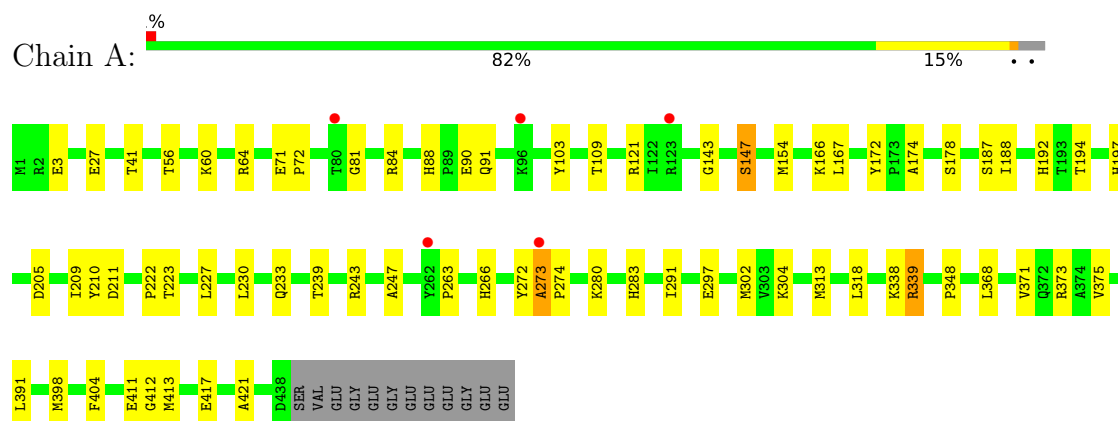
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	34	Total	O	0	0
			34	34		
12	B	27	Total	O	0	0
			27	27		
12	C	82	Total	O	0	0
			82	82		
12	D	5	Total	O	0	0
			5	5		
12	E	5	Total	O	0	0
			5	5		
12	F	8	Total	O	0	0
			8	8		

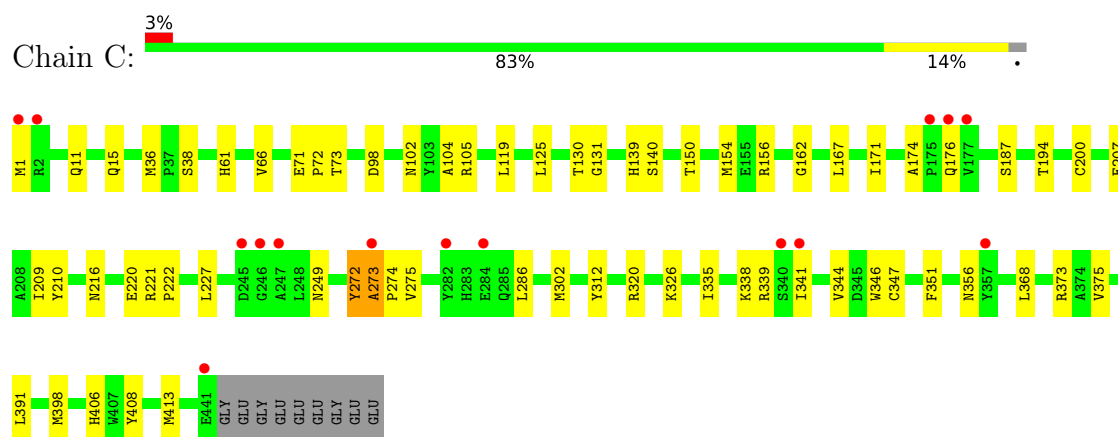
3 Residue-property plots

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

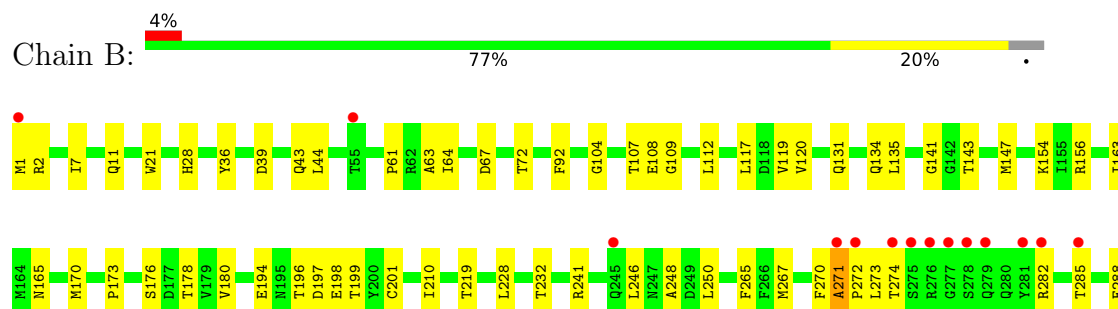
• Molecule 1: Tubulin alpha-1B chain

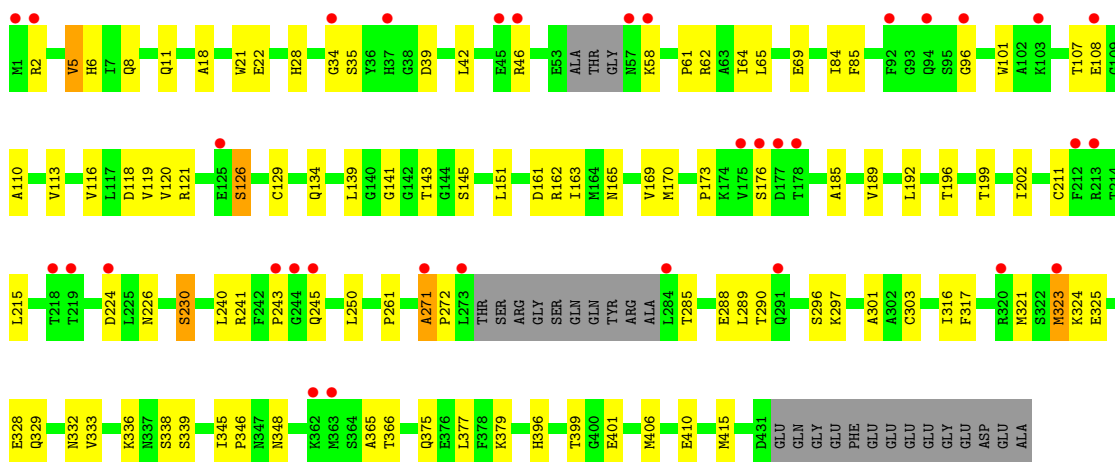


• Molecule 1: Tubulin alpha-1B chain

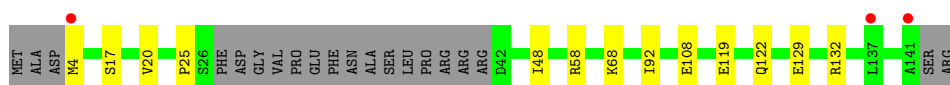


• Molecule 2: Tubulin beta chain

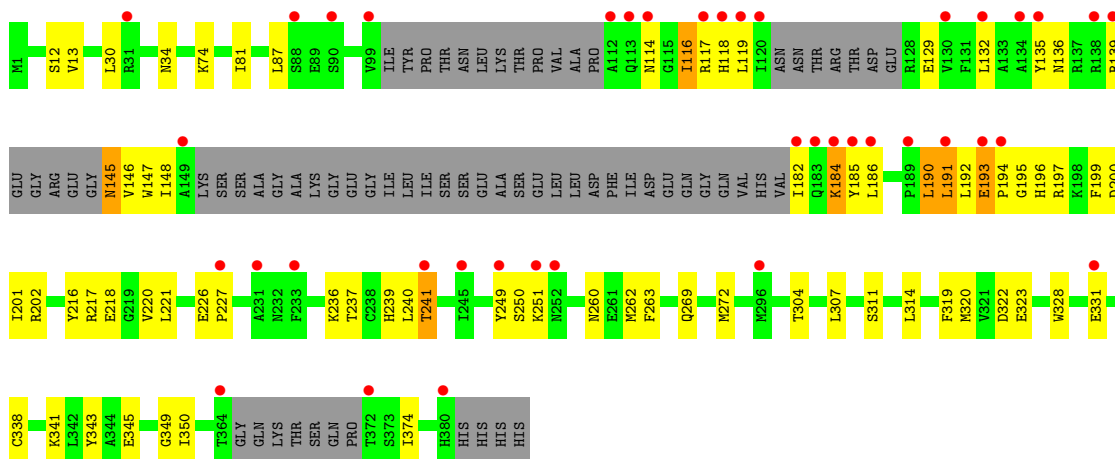




- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.45Å 157.66Å 183.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 – 2.75 48.27 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.27-2.75) 98.7 (48.27-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.194 , 0.235 0.195 , 0.233	Depositor DCC
R_{free} test set	4035 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.1	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	0.93	EDS
Total number of atoms	17583	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MES, GTP, GOL, MG, DO6, GDP

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	0.17	0/3514	0.43	2/4770 (0.0%)
1	C	0.16	0/3552	0.42	2/4822 (0.0%)
2	B	0.16	0/3451	0.41	2/4674 (0.0%)
2	D	0.15	0/3374	0.42	0/4568
3	E	0.13	0/1041	0.32	0/1382
4	F	0.16	0/2674	0.42	0/3609
All	All	0.16	0/17606	0.42	6/23825 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	270	PHE	CA-C-N	6.42	137.45	121.80
2	B	270	PHE	C-N-CA	6.42	137.45	121.80
1	A	272	TYR	CA-C-N	6.34	137.27	121.80
1	A	272	TYR	C-N-CA	6.34	137.27	121.80
1	C	272	TYR	CA-C-N	5.72	135.76	121.80
1	C	272	TYR	C-N-CA	5.72	135.76	121.80

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	3430	0	3345	41	0
1	C	3462	0	3373	47	0
2	B	3376	0	3257	54	0
2	D	3297	0	3175	66	0
3	E	1026	0	1042	7	0
4	F	2615	0	2598	53	0
5	A	32	0	12	0	0
5	C	32	0	12	2	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	B	27	0	0	1	0
8	D	27	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	B	24	0	24	2	0
11	B	6	0	8	0	0
11	C	6	0	8	1	0
12	A	34	0	0	0	0
12	B	27	0	0	0	0
12	C	82	0	0	0	0
12	D	5	0	0	0	0
12	E	5	0	0	0	0
12	F	8	0	0	0	0
All	All	17583	0	16878	256	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 7.

All (256) 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:D:271:ALA:HB2	2:D:365:ALA:H	1.29	0.97
1:A:273:ALA:HB2	1:A:375:VAL:H	1.36	0.90
2:B:271:ALA:HB2	2:B:365:ALA:H	1.44	0.83
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.67	0.75
2:B:295:ASP:HA	10:B:505:MES:H32	1.69	0.75
2:D:6:HIS:HD2	2:D:134:GLN:HE21	1.35	0.74
1:C:273:ALA:HB2	1:C:375:VAL:H	1.51	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ALA:HB2	1:C:413:MET:HE2	1.70	0.72
2:B:173:PRO:HA	2:B:176:SER:HB2	1.73	0.70
1:C:1:MET:SD	1:C:130:THR:OG1	2.49	0.70
2:D:173:PRO:HA	2:D:176:SER:HB2	1.74	0.69
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.74	0.69
3:E:119:GLU:HA	3:E:122:GLN:HG2	1.73	0.69
2:D:6:HIS:CE1	2:D:8:GLN:HG2	2.29	0.68
2:D:6:HIS:CD2	2:D:134:GLN:HE21	2.12	0.67
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.27	0.67
2:D:271:ALA:HB2	2:D:365:ALA:N	2.08	0.67
1:A:166:LYS:NZ	1:A:197:HIS:O	2.27	0.67
2:D:396:HIS:HA	2:D:399:THR:HG22	1.76	0.66
1:A:273:ALA:HB1	1:A:274:PRO:CD	2.26	0.66
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.77	0.66
2:B:338:SER:HB3	4:F:34:ASN:HD21	1.60	0.66
4:F:117:ARG:HG2	4:F:118:HIS:H	1.60	0.66
1:C:220:GLU:HB3	2:D:324:LYS:HD3	1.79	0.65
4:F:182:ILE:HG12	4:F:241:THR:HG23	1.77	0.65
4:F:114:ASN:HB2	4:F:147:TRP:O	1.97	0.65
1:C:408:TYR:HB3	1:C:413:MET:HE3	1.80	0.64
4:F:190:LEU:HD23	4:F:323:GLU:HA	1.79	0.64
2:D:6:HIS:HE1	2:D:8:GLN:HG2	1.62	0.64
1:A:412:GLY:O	3:E:58:ARG:NH1	2.30	0.64
2:D:35:SER:OG	2:D:58:LYS:NZ	2.29	0.63
4:F:217:ARG:NH2	4:F:345:GLU:OE2	2.32	0.62
4:F:184:LYS:NZ	4:F:239:HIS:O	2.32	0.62
2:D:42:LEU:HD22	2:D:243:PRO:HG3	1.82	0.62
2:D:143:THR:N	9:D:503:GDP:O3B	2.28	0.61
2:B:36:TYR:CZ	2:B:44:LEU:HD21	2.35	0.61
2:D:317:PHE:HB3	2:D:321:MET:HE1	1.81	0.61
4:F:30:LEU:HD13	4:F:34:ASN:ND2	2.16	0.60
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.82	0.60
4:F:314:LEU:HD13	4:F:350:ILE:HD11	1.84	0.60
4:F:237:THR:HG21	4:F:250:SER:HA	1.82	0.60
1:C:273:ALA:HB1	1:C:274:PRO:HD2	1.83	0.59
1:C:273:ALA:HB1	1:C:274:PRO:CD	2.31	0.59
1:C:102:ASN:HB3	1:C:105:ARG:HG3	1.84	0.59
2:D:11:GLN:N	9:D:503:GDP:O2B	2.31	0.58
2:B:271:ALA:CB	2:B:365:ALA:H	2.15	0.58
4:F:13:VAL:HG12	4:F:343:TYR:HE1	1.67	0.58
1:C:221:ARG:HG3	2:D:324:LYS:HG3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:GLU:HG3	2:D:96:GLY:HA2	1.85	0.58
2:B:134:GLN:HA	2:B:165:ASN:O	2.05	0.57
2:B:330:MET:HG2	2:B:351:THR:HG21	1.87	0.57
2:D:134:GLN:HA	2:D:165:ASN:O	2.04	0.57
4:F:193:GLU:C	4:F:195:GLY:H	2.12	0.57
2:B:219:THR:HG21	1:C:326:LYS:HA	1.86	0.57
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.87	0.57
1:C:1:MET:SD	1:C:1:MET:O	2.64	0.56
2:B:282:ARG:HH12	2:B:288:GLU:CD	2.13	0.56
4:F:184:LYS:HE3	4:F:239:HIS:HB2	1.88	0.56
2:D:161:ASP:OD1	2:D:162:ARG:NH1	2.39	0.56
1:A:273:ALA:HB2	1:A:375:VAL:O	2.07	0.55
1:A:273:ALA:CB	1:A:375:VAL:H	2.15	0.55
1:C:275:VAL:HA	1:C:368:LEU:HD21	1.89	0.55
2:D:64:ILE:HD13	2:D:120:VAL:HG22	1.88	0.55
4:F:114:ASN:HB3	4:F:148:ILE:HG13	1.89	0.55
4:F:226:GLU:OE1	4:F:250:SER:OG	2.25	0.54
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.90	0.54
2:D:271:ALA:HB1	2:D:289:LEU:HD11	1.90	0.54
4:F:190:LEU:HB2	4:F:322:ASP:C	2.32	0.54
1:C:11:GLN:HB3	5:C:501:GTP:O2A	2.08	0.54
1:A:348:PRO:HB3	3:E:25:PRO:HD3	1.90	0.53
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.91	0.53
2:B:196:THR:HG21	2:B:199:THR:OG1	2.08	0.53
4:F:30:LEU:HD13	4:F:34:ASN:HD22	1.73	0.53
1:A:81:GLY:O	1:A:84:ARG:HG3	2.07	0.53
1:A:273:ALA:HB1	1:A:274:PRO:HD2	1.90	0.53
2:D:107:THR:OG1	2:D:108:GLU:N	2.42	0.53
4:F:221:LEU:HB2	4:F:262:MET:O	2.09	0.53
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.90	0.52
2:B:64:ILE:HD13	2:B:120:VAL:HG22	1.91	0.52
4:F:116:ILE:HG23	4:F:135:TYR:OH	2.09	0.52
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.92	0.52
2:D:116:VAL:HG11	2:D:151:LEU:HD11	1.90	0.52
1:C:312:TYR:CD1	1:C:341:ILE:HG13	2.44	0.52
4:F:148:ILE:HG22	4:F:185:TYR:CE1	2.45	0.52
1:C:398:MET:HE2	2:D:346:PRO:HD2	1.92	0.51
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.91	0.51
2:B:306:ARG:HE	10:B:505:MES:H62	1.76	0.51
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.41	0.51
4:F:269:GLN:HA	4:F:272:MET:HE2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HD23	2:B:147:MET:HE1	1.94	0.50
1:C:221:ARG:NH2	2:D:323:MET:HB2	2.25	0.50
2:D:192:LEU:O	2:D:196:THR:HG22	2.10	0.50
1:A:143:GLY:O	1:A:147:SER:HB3	2.10	0.50
1:A:247:ALA:HB3	3:E:17:SER:OG	2.11	0.50
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.44	0.50
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.94	0.50
3:E:129:GLU:OE1	3:E:132:ARG:NH2	2.45	0.50
2:D:196:THR:HG21	2:D:199:THR:CG2	2.42	0.49
2:D:65:LEU:HD11	2:D:85:PHE:CD2	2.46	0.49
2:D:211:CYS:HA	2:D:215:LEU:HD12	1.94	0.49
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.47	0.49
2:B:178:THR:HG22	2:B:180:VAL:H	1.78	0.49
2:B:378:PHE:HD1	2:B:415:MET:HE2	1.78	0.49
1:A:297:GLU:CD	1:A:339:ARG:HH22	2.21	0.49
2:B:228:LEU:HB3	2:B:300:MET:HE1	1.94	0.48
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.48
3:E:4:MET:HE3	3:E:20:VAL:HG21	1.93	0.48
1:C:286:LEU:O	1:C:373:ARG:NH1	2.45	0.48
2:D:169:VAL:HA	2:D:202:ILE:O	2.13	0.48
4:F:184:LYS:HE3	4:F:239:HIS:CG	2.48	0.48
1:A:109:THR:HG21	1:A:411:GLU:OE2	2.13	0.48
1:A:263:PRO:O	1:A:266:HIS:ND1	2.26	0.48
2:B:36:TYR:CE2	2:B:44:LEU:HD21	2.48	0.48
1:C:272:TYR:CE2	1:C:273:ALA:HB3	2.48	0.48
2:B:386:THR:O	2:B:390:ARG:HG2	2.14	0.48
2:D:39:ASP:OD1	2:D:39:ASP:N	2.46	0.48
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.95	0.48
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.96	0.48
2:B:392:LYS:HB3	2:B:395:LEU:HD12	1.95	0.47
2:D:375:GLN:O	2:D:379:LYS:HG2	2.14	0.47
2:B:271:ALA:HB1	2:B:272:PRO:CD	2.45	0.47
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.95	0.47
1:A:56:THR:OG1	1:A:60:LYS:HB3	2.15	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.96	0.47
4:F:196:HIS:O	4:F:227:PRO:HA	2.14	0.47
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.96	0.47
2:B:156:ARG:NH1	2:B:194:GLU:O	2.48	0.46
1:A:280:LYS:HD3	1:A:283:HIS:HB2	1.97	0.46
2:B:332:ASN:O	2:B:336:LYS:HB2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:132:LEU:O	4:F:136:ASN:N	2.49	0.46
1:A:103:TYR:HD2	1:A:147:SER:OG	1.98	0.46
1:C:1:MET:HE1	1:C:131:GLY:HA3	1.96	0.46
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.81	0.46
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.96	0.46
1:A:174:ALA:O	1:A:178:SER:HB3	2.16	0.46
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.56	0.46
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.98	0.46
2:D:285:THR:HG23	2:D:288:GLU:H	1.79	0.46
2:D:316:ILE:HG23	2:D:366:THR:HB	1.97	0.46
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.46
2:B:1:MET:SD	2:B:1:MET:N	2.82	0.46
2:D:110:ALA:O	2:D:113:VAL:HG12	2.15	0.46
1:A:154:MET:HG3	1:A:194:THR:HG23	1.98	0.46
1:A:209:ILE:HD11	1:A:302:MET:SD	2.56	0.46
2:D:271:ALA:CB	2:D:272:PRO:CD	2.94	0.46
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.46	0.45
1:C:216:ASN:HB3	1:C:275:VAL:O	2.17	0.45
2:D:107:THR:HG21	2:D:401:GLU:OE1	2.15	0.45
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.98	0.45
1:C:140:SER:HA	1:C:171:ILE:HB	1.98	0.45
1:C:209:ILE:HD11	1:C:302:MET:SD	2.56	0.45
11:C:504:GOL:H11	2:D:245:GLN:HG2	1.98	0.45
2:D:189:VAL:HG11	2:D:415:MET:HE3	1.98	0.45
2:B:317:PHE:HB2	2:B:353:VAL:HG22	1.97	0.45
1:C:71:GLU:OE1	1:C:73:THR:HB	2.17	0.45
4:F:236:LYS:O	4:F:240:LEU:HB2	2.17	0.45
4:F:148:ILE:HG22	4:F:185:TYR:HE1	1.80	0.45
1:C:221:ARG:HH21	2:D:323:MET:HB2	1.82	0.45
2:D:65:LEU:HD11	2:D:85:PHE:HD2	1.82	0.45
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.51	0.45
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.99	0.45
1:C:154:MET:HG3	1:C:194:THR:HG23	1.99	0.45
4:F:191:LEU:HD13	4:F:193:GLU:HB3	1.99	0.44
4:F:191:LEU:CD1	4:F:193:GLU:HB3	2.47	0.44
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.53	0.44
2:B:232:THR:OG1	2:B:300:MET:HE2	2.16	0.44
4:F:201:ILE:HG12	4:F:221:LEU:HD21	1.99	0.44
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.99	0.44
4:F:199:PHE:HB2	4:F:221:LEU:HD22	2.00	0.44
1:A:90:GLU:O	1:A:121:ARG:HD2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:VAL:HG12	1:A:373:ARG:H	1.82	0.44
2:D:34:GLY:HA2	2:D:84:ILE:HD11	1.98	0.44
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.98	0.44
2:D:118:ASP:OD1	2:D:121:ARG:NH2	2.47	0.44
1:A:413:MET:HE3	1:A:417:GLU:HB3	2.00	0.44
1:C:221:ARG:HE	1:C:221:ARG:HB3	1.68	0.44
2:D:332:ASN:CG	2:D:336:LYS:HZ2	2.22	0.44
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.44
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.44
2:D:297:LYS:HB2	2:D:297:LYS:HE2	1.85	0.44
1:C:176:GLN:NE2	1:C:207:GLU:OE2	2.51	0.44
2:B:28:HIS:CE1	2:B:241:ARG:HB3	2.53	0.44
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.53	0.44
2:D:2:ARG:HA	2:D:129:CYS:O	2.17	0.44
2:D:46:ARG:NH2	2:D:240:LEU:O	2.50	0.44
2:D:301:ALA:O	2:D:303:CYS:N	2.50	0.44
2:B:246:LEU:HD23	2:B:246:LEU:HA	1.86	0.43
2:D:28:HIS:CE1	2:D:241:ARG:HB3	2.53	0.43
2:D:101:TRP:HD1	2:D:145[A]:SER:OG	2.00	0.43
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.00	0.43
4:F:237:THR:OG1	4:F:249:TYR:HB3	2.18	0.43
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.52	0.43
2:B:39:ASP:N	2:B:39:ASP:OD1	2.50	0.43
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.54	0.43
2:B:197:ASP:C	2:B:198:GLU:HG3	2.43	0.43
2:D:290:THR:HG22	2:D:333:VAL:HG21	2.01	0.43
4:F:320:MET:HB3	4:F:328:TRP:HB2	2.01	0.43
2:B:117:LEU:HD11	2:B:154:LYS:HD2	2.00	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.43
1:C:273:ALA:CB	1:C:375:VAL:H	2.26	0.43
2:D:139:LEU:HB3	2:D:185:ALA:HA	2.00	0.43
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.52	0.42
1:C:162:GLY:HA2	3:E:92:ILE:HD11	2.01	0.42
4:F:260:ASN:N	4:F:260:ASN:HD22	2.17	0.42
2:D:126:SER:O	2:D:126:SER:OG	2.30	0.42
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.53	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.01	0.42
2:D:332:ASN:O	2:D:336:LYS:HG3	2.19	0.42
4:F:193:GLU:C	4:F:195:GLY:N	2.78	0.42
2:B:210:ILE:HG23	2:B:273:LEU:HD13	2.02	0.42
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.02	0.42
2:B:104:GLY:O	2:B:109:GLY:HA3	2.20	0.42
2:D:406:MET:O	2:D:410:GLU:N	2.41	0.42
4:F:202:ARG:HB3	4:F:220:VAL:HG12	2.01	0.42
1:C:338:LYS:HE2	1:C:338:LYS:HB3	1.83	0.42
4:F:184:LYS:HE2	4:F:184:LYS:HB2	1.74	0.42
2:B:7:ILE:O	2:B:135:LEU:HA	2.20	0.42
2:B:21:TRP:CZ2	2:B:63:ALA:HB2	2.54	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.55	0.42
2:D:28:HIS:NE2	2:D:241:ARG:HD2	2.35	0.42
4:F:320:MET:O	4:F:328:TRP:N	2.45	0.42
1:A:223:THR:O	1:A:227:LEU:HG	2.20	0.41
2:D:329:GLN:O	2:D:333:VAL:HG23	2.21	0.41
4:F:200:ASP:O	4:F:221:LEU:HD23	2.20	0.41
2:B:317:PHE:HZ	2:B:330:MET:HE1	1.85	0.41
1:A:398:MET:HE3	1:A:404:PHE:CD2	2.56	0.41
2:B:107:THR:OG1	2:B:108:GLU:N	2.54	0.41
2:B:28:HIS:HA	2:B:43:GLN:HB3	2.02	0.41
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.41
2:B:141:GLY:HA3	9:B:503:GDP:O3A	2.21	0.41
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.02	0.41
2:D:141:GLY:HA3	9:D:503:GDP:O3A	2.20	0.41
2:B:64:ILE:HG12	2:B:119:VAL:HG12	2.03	0.41
2:B:248:ALA:HB1	8:B:501:DO6:C5	2.51	0.41
4:F:184:LYS:HE3	4:F:239:HIS:CD2	2.56	0.41
4:F:304:THR:HG21	4:F:311:SER:HB2	2.01	0.41
2:B:143:THR:HG23	2:B:147:MET:HE2	2.03	0.41
2:B:285:THR:HG23	2:B:288:GLU:H	1.86	0.41
2:D:18:ALA:O	2:D:22:GLU:HG3	2.20	0.41
4:F:263:PHE:HE2	4:F:341:LYS:HD2	1.85	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.02	0.41
1:A:318:LEU:O	1:A:375:VAL:HA	2.20	0.41
4:F:191:LEU:H	4:F:191:LEU:HG	1.63	0.41
2:D:325:GLU:HA	2:D:328:GLU:HG2	2.03	0.40
4:F:201:ILE:HB	4:F:319:PHE:HB2	2.03	0.40
1:C:15:GLN:NE2	5:C:501:GTP:O6	2.54	0.40
4:F:129:GLU:O	4:F:132:LEU:HG	2.21	0.40
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.56	0.40
2:B:271:ALA:HB1	2:B:272:PRO:HD2	2.03	0.40
2:D:5:VAL:HG12	2:D:62:ARG:CD	2.52	0.40
4:F:192:LEU:HB3	4:F:197:ARG:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:GLN:HA	2:B:72:THR:HG21	2.02	0.40
4:F:145:ASN:CG	4:F:146:VAL:H	2.30	0.40
2:D:226:ASN:O	2:D:230:SER:OG	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/450 (97%)	424 (97%)	13 (3%)	1 (0%)	43	62
1	C	443/450 (98%)	428 (97%)	14 (3%)	1 (0%)	43	62
2	B	427/445 (96%)	415 (97%)	11 (3%)	1 (0%)	43	62
2	D	413/445 (93%)	400 (97%)	12 (3%)	1 (0%)	43	62
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100
4	F	305/384 (79%)	285 (93%)	17 (6%)	3 (1%)	12	22
All	All	2147/2317 (93%)	2072 (96%)	68 (3%)	7 (0%)	36	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	ALA
2	B	271	ALA
1	C	273	ALA
2	D	271	ALA
4	F	190	LEU
4	F	193	GLU
4	F	194	PRO

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	371/378 (98%)	364 (98%)	7 (2%)	50	68
1	C	376/378 (100%)	373 (99%)	3 (1%)	73	83
2	B	371/383 (97%)	367 (99%)	4 (1%)	65	79
2	D	364/383 (95%)	355 (98%)	9 (2%)	42	63
3	E	112/127 (88%)	109 (97%)	3 (3%)	39	61
4	F	286/342 (84%)	275 (96%)	11 (4%)	29	51
All	All	1880/1991 (94%)	1843 (98%)	37 (2%)	48	67

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	147	SER
1	A	167	LEU
1	A	188	ILE
1	A	313	MET
1	A	338	LYS
1	A	339	ARG
2	B	274	THR
2	B	320	ARG
2	B	339	SER
2	B	350	LYS
1	C	38	SER
1	C	320	ARG
1	C	347	CYS
2	D	5	VAL
2	D	119	VAL
2	D	126	SER
2	D	224	ASP
2	D	230	SER
2	D	296	SER
2	D	323	MET
2	D	338	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	339	SER
3	E	48	ILE
3	E	68	LYS
3	E	108	GLU
4	F	12	SER
4	F	116	ILE
4	F	119	LEU
4	F	139	ARG
4	F	145	ASN
4	F	184	LYS
4	F	186	LEU
4	F	191	LEU
4	F	241	THR
4	F	251	LYS
4	F	307	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	301	GLN
1	A	393	HIS
2	B	134	GLN
2	B	245	GLN
2	B	375	GLN
1	C	11	GLN
1	C	15	GLN
1	C	128	GLN
1	C	309	HIS
2	D	6	HIS
2	D	165	ASN
2	D	191	GLN
2	D	195	ASN
2	D	396	HIS
3	E	10	ASN
3	E	134	ASN
4	F	26	GLN
4	F	260	ASN
4	F	340	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GTP	C	501	6	33,34,34	1.03	2 (6%)	50,54,54	1.51	9 (18%)
11	GOL	B	506	-	5,5,5	0.37	0	5,5,5	0.32	0
8	DO6	B	501	-	29,29,29	0.20	0	40,42,42	0.45	0
9	GDP	D	503	6	29,30,30	1.19	3 (10%)	45,47,47	1.74	6 (13%)
5	GTP	A	501	6	33,34,34	1.02	3 (9%)	50,54,54	1.50	8 (16%)
9	GDP	B	503	6	29,30,30	1.21	4 (13%)	45,47,47	1.69	6 (13%)
11	GOL	C	504	-	5,5,5	0.37	0	5,5,5	0.31	0
10	MES	B	505	-	12,12,12	2.40	1 (8%)	15,16,16	1.97	3 (20%)
8	DO6	D	501	-	29,29,29	0.19	0	40,42,42	0.40	0
10	MES	B	504	-	12,12,12	2.31	1 (8%)	15,16,16	1.97	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	2/22/38/38	0/3/3/3
11	GOL	B	506	-	-	2/4/4/4	-
8	DO6	B	501	-	-	0/16/16/16	0/3/3/3
9	GDP	D	503	6	-	6/16/32/32	0/3/3/3
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
9	GDP	B	503	6	-	3/16/32/32	0/3/3/3
11	GOL	C	504	-	-	4/4/4/4	-
10	MES	B	505	-	-	3/6/14/14	0/1/1/1
8	DO6	D	501	-	-	0/16/16/16	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-8.05	1.66	1.77
10	B	504	MES	C8-S	-7.72	1.66	1.77
9	D	503	GDP	C5-C4	3.15	1.47	1.38
9	B	503	GDP	C5-C4	3.11	1.47	1.38
5	C	501	GTP	PB-O3A	2.60	1.62	1.59
9	B	503	GDP	C6-N1	-2.44	1.34	1.38
5	A	501	GTP	PA-O3A	2.31	1.62	1.59
9	D	503	GDP	PA-O3A	2.29	1.62	1.59
9	B	503	GDP	PA-O3A	2.29	1.62	1.59
9	D	503	GDP	C6-N1	-2.24	1.34	1.38
5	C	501	GTP	PA-O3A	2.22	1.61	1.59
5	A	501	GTP	PB-O3B	2.18	1.61	1.59
5	A	501	GTP	C2-N3	2.09	1.38	1.33
9	B	503	GDP	C5-N7	-2.07	1.34	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	GDP	C5-C4-N3	-5.98	118.88	128.39
9	D	503	GDP	C5-C4-N3	-5.91	118.99	128.39
10	B	505	MES	C5-N4-C3	5.81	121.37	108.84
9	D	503	GDP	C2-N3-C4	4.92	120.77	112.30
9	B	503	GDP	C2-N3-C4	4.86	120.67	112.30
5	A	501	GTP	C5-C4-N3	-4.69	120.92	128.39
5	C	501	GTP	C5-C4-N3	-4.69	120.93	128.39
5	A	501	GTP	C2-N3-C4	4.54	120.12	112.30
5	C	501	GTP	C2-N3-C4	4.54	120.11	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	C5-N4-C3	4.47	118.47	108.84
9	D	503	GDP	N9-C4-N3	4.41	134.76	125.95
9	B	503	GDP	N9-C4-N3	4.37	134.69	125.95
9	B	503	GDP	C6-C5-N7	3.30	136.30	130.29
9	D	503	GDP	C6-C5-N7	3.27	136.23	130.29
10	B	504	MES	C7-N4-C3	2.94	119.07	111.24
10	B	504	MES	C2-C3-N4	-2.92	105.68	110.12
5	A	501	GTP	N9-C4-N3	2.89	131.73	125.95
5	C	501	GTP	N9-C8-N7	-2.88	108.07	113.40
5	C	501	GTP	C2-N1-C6	-2.84	119.95	125.11
5	A	501	GTP	N9-C8-N7	-2.76	108.28	113.40
5	C	501	GTP	C8-N7-C5	2.73	109.13	104.26
5	A	501	GTP	C2-N1-C6	-2.70	120.21	125.11
5	C	501	GTP	N9-C4-N3	2.67	131.29	125.95
9	B	503	GDP	C4-C5-N7	-2.65	106.47	110.67
9	D	503	GDP	C4-C5-N7	-2.60	106.55	110.67
5	A	501	GTP	C8-N7-C5	2.57	108.83	104.26
10	B	505	MES	O1S-S-C8	2.43	110.40	106.73
5	A	501	GTP	C5-C6-N1	2.39	119.34	113.25
5	C	501	GTP	C5-C6-N1	2.32	119.16	113.25
5	A	501	GTP	O6-C6-C5	-2.31	120.44	126.53
5	C	501	GTP	O6-C6-C5	-2.24	120.62	126.53
10	B	505	MES	O2S-S-C8	2.21	110.06	106.73
5	C	501	GTP	C4-C5-N7	-2.14	107.28	110.67
10	B	504	MES	O1S-S-C8	2.11	109.91	106.73
9	D	503	GDP	O6-C6-C5	-2.10	121.00	126.53
9	B	503	GDP	O6-C6-C5	-2.03	121.19	126.53

There are no chirality outliers.

All (28) 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	A	501	GTP	C5'-O5'-PA-O2A
9	B	503	GDP	C5'-O5'-PA-O3A
9	B	503	GDP	C5'-O5'-PA-O1A
9	B	503	GDP	C5'-O5'-PA-O2A
9	D	503	GDP	PA-O3A-PB-O2B
9	D	503	GDP	C5'-O5'-PA-O3A
9	D	503	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

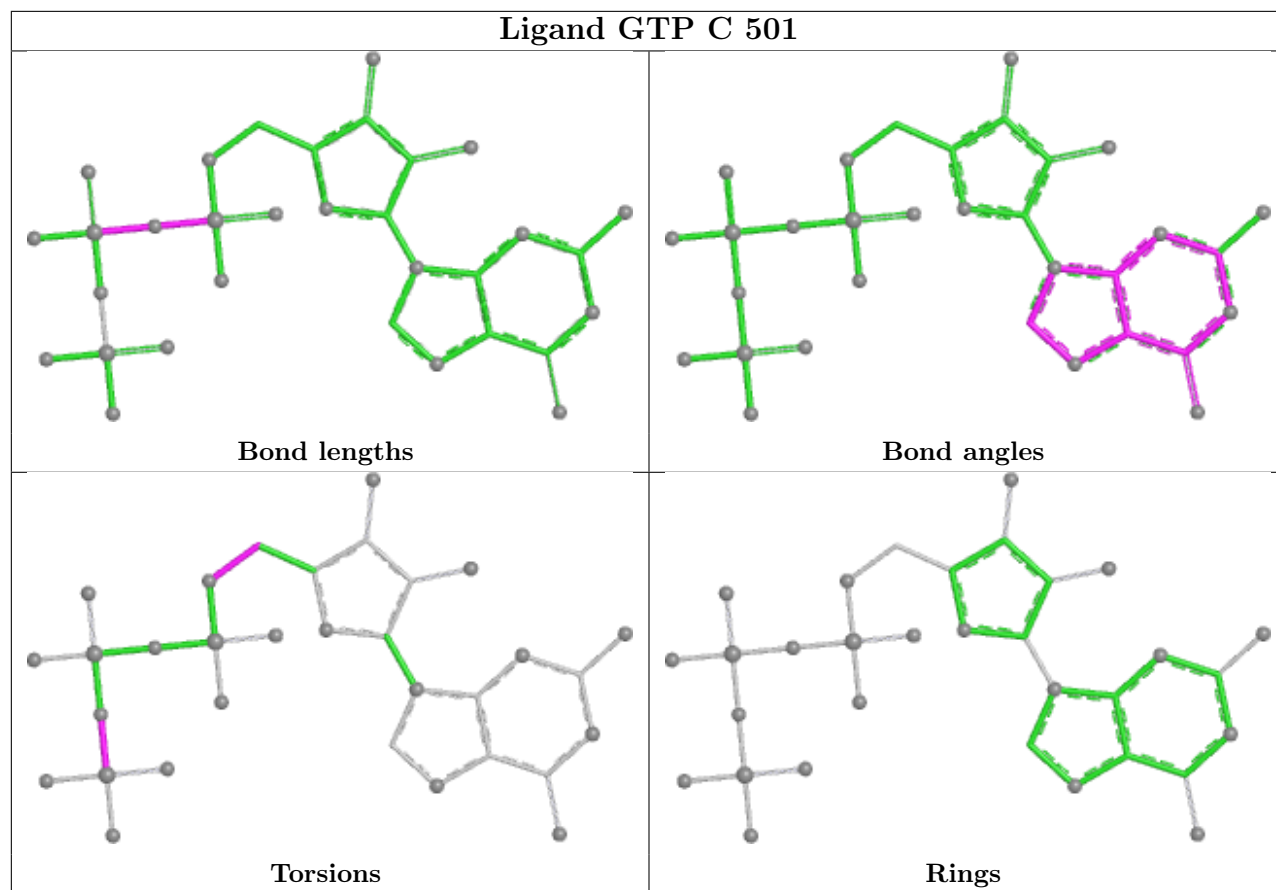
Mol	Chain	Res	Type	Atoms
10	B	504	MES	C8-C7-N4-C3
10	B	504	MES	C7-C8-S-O2S
10	B	504	MES	C7-C8-S-O3S
10	B	505	MES	C8-C7-N4-C3
11	C	504	GOL	O1-C1-C2-C3
11	C	504	GOL	C1-C2-C3-O3
11	C	504	GOL	O2-C2-C3-O3
11	B	506	GOL	O1-C1-C2-C3
11	B	506	GOL	O1-C1-C2-O2
11	C	504	GOL	O1-C1-C2-O2
10	B	505	MES	N4-C7-C8-S
10	B	505	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O1S
5	C	501	GTP	PB-O3B-PG-O2G
9	D	503	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
9	D	503	GDP	PA-O3A-PB-O1B
9	D	503	GDP	PA-O3A-PB-O3B

There are no ring outliers.

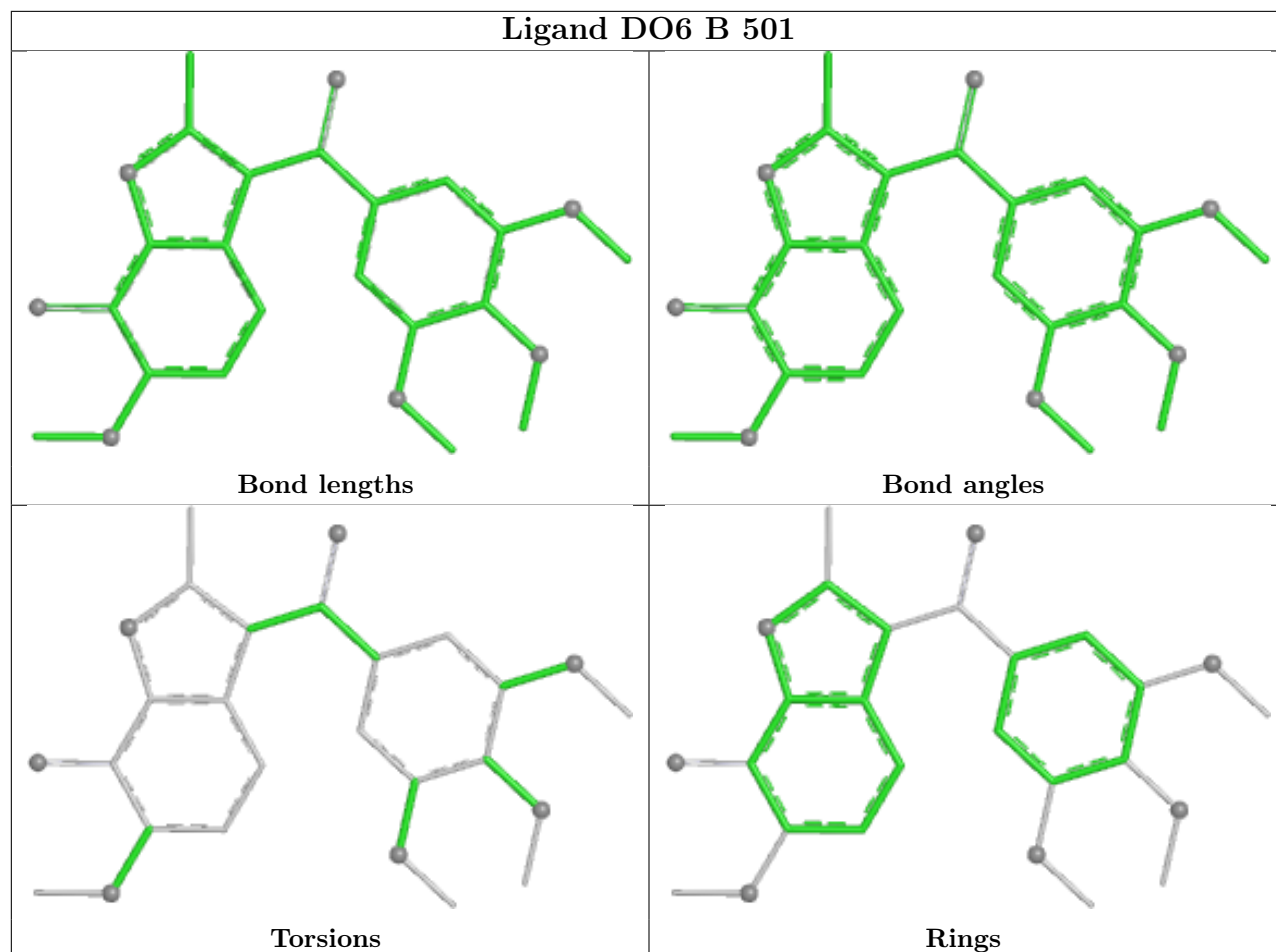
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	2	0
8	B	501	DO6	1	0
9	D	503	GDP	3	0
9	B	503	GDP	1	0
11	C	504	GOL	1	0
10	B	505	MES	2	0

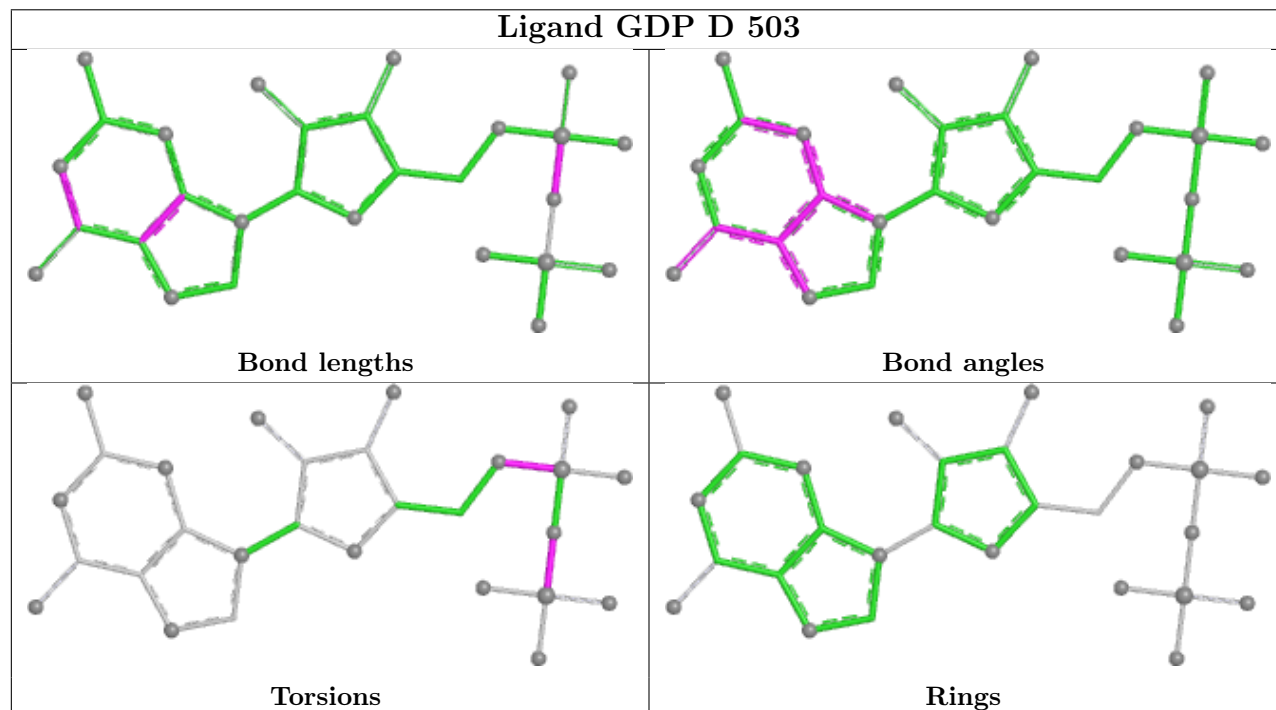
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

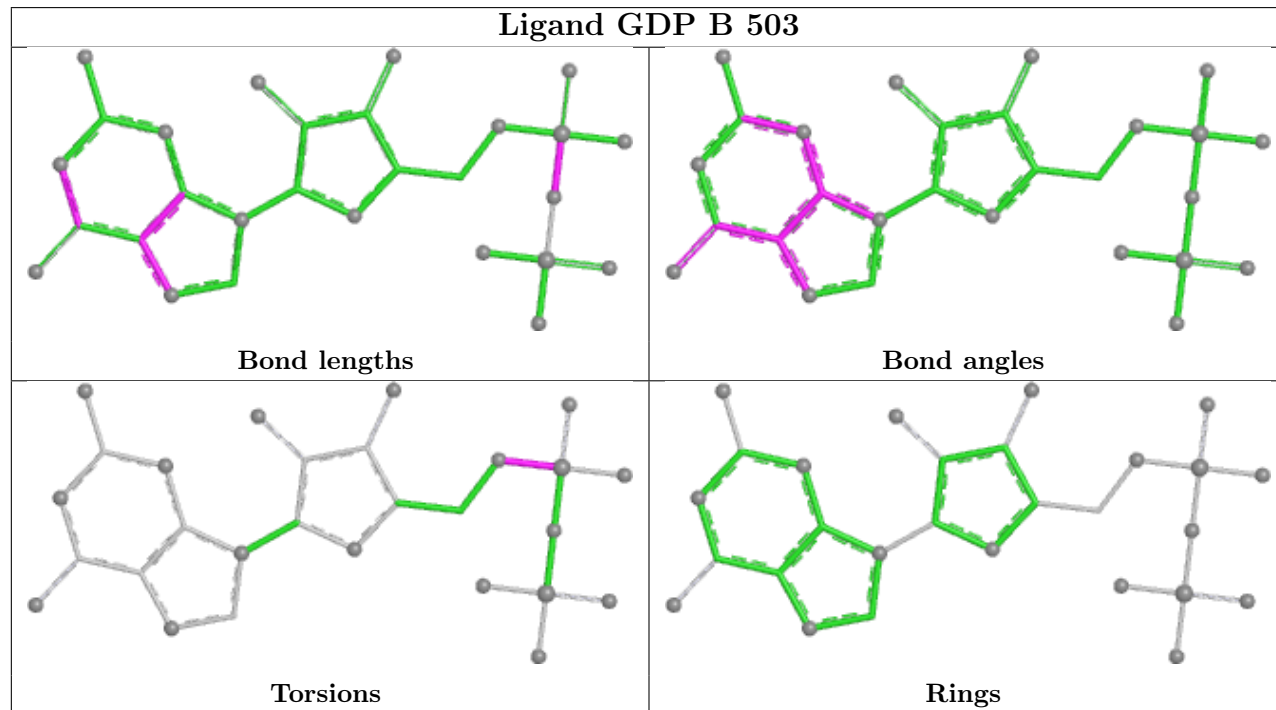
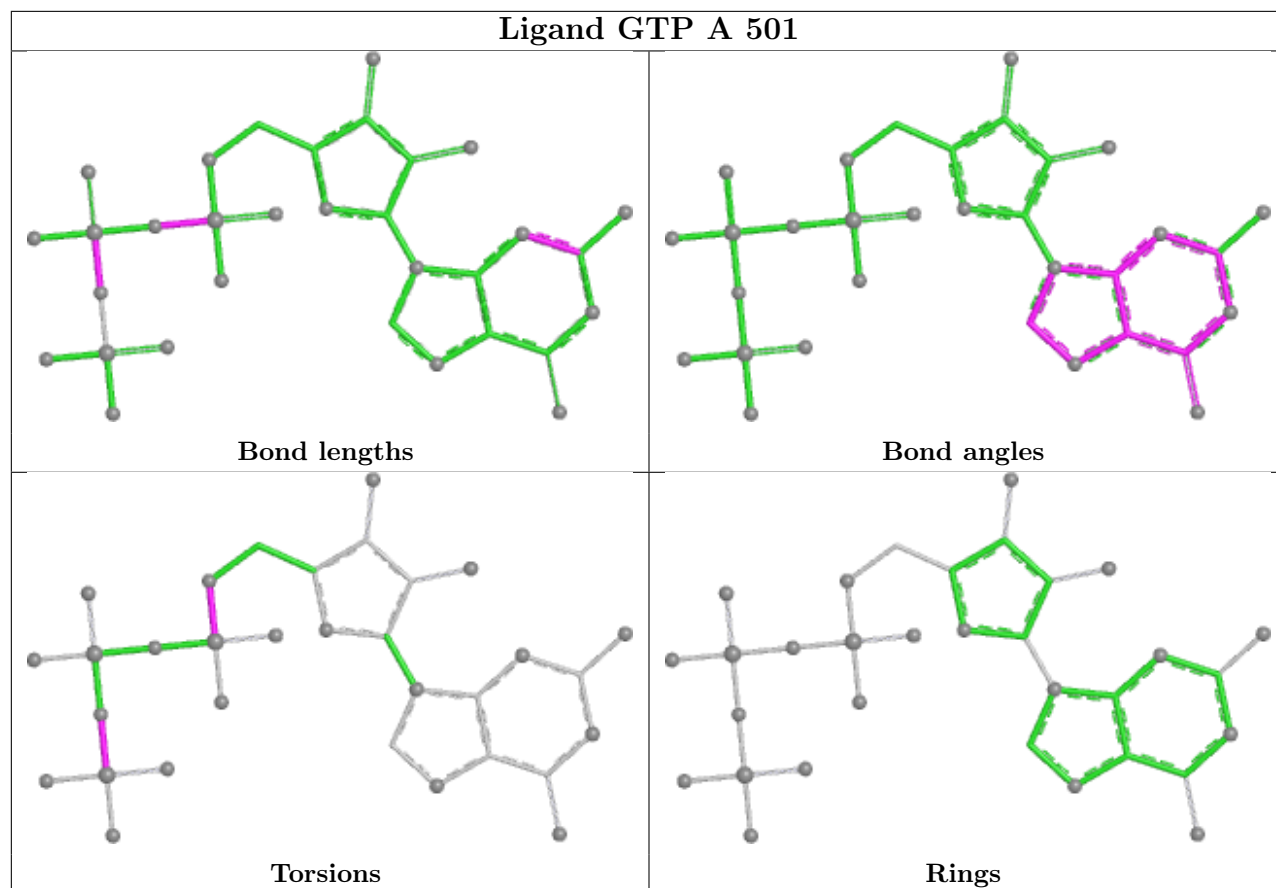


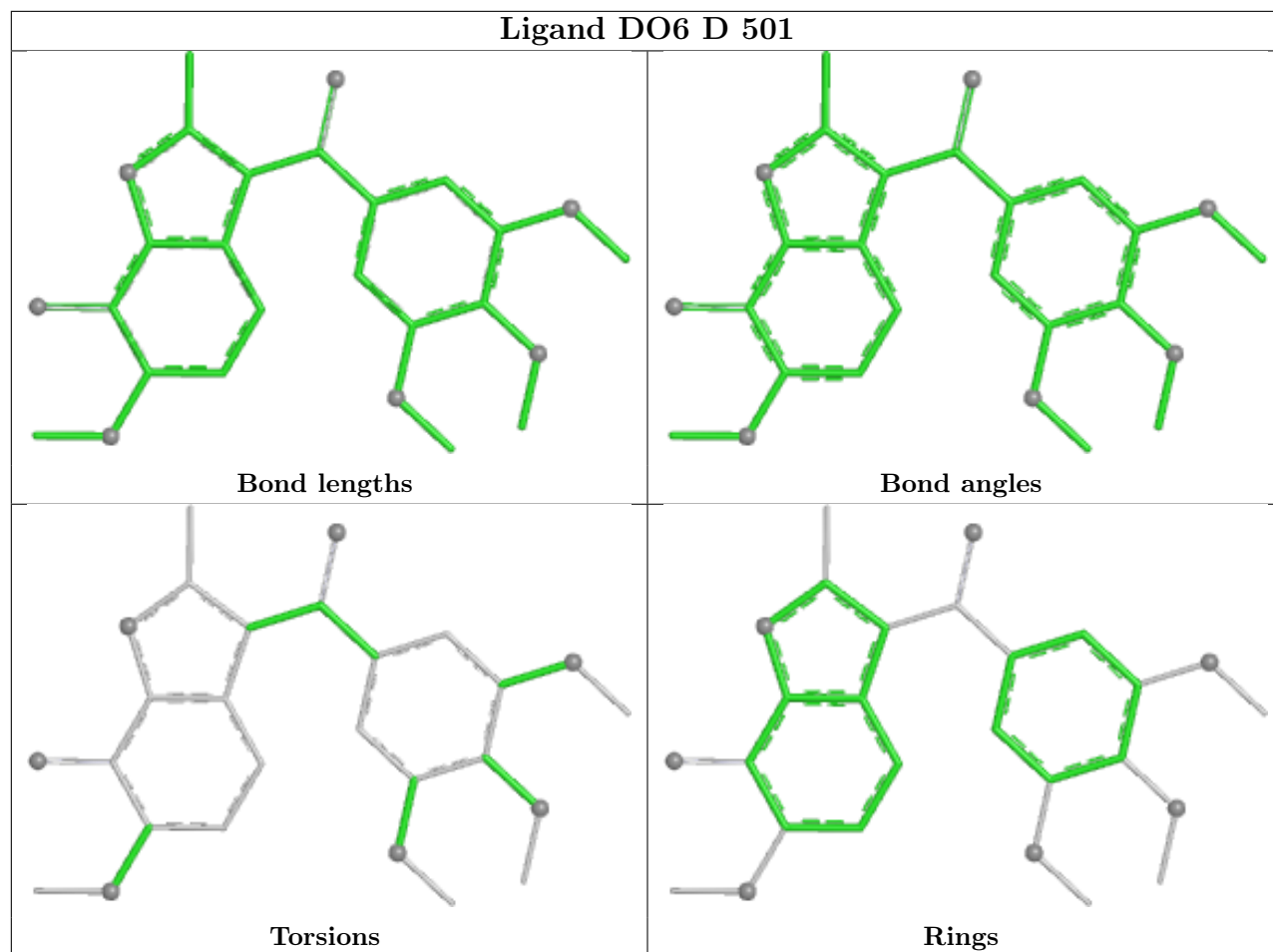
Ligand DO6 B 501



Ligand GDP D 503







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	438/450 (97%)	-0.06	5 (1%) 78 77	27, 47, 77, 110	2 (0%)
1	C	441/450 (98%)	-0.19	15 (3%) 48 46	15, 34, 65, 146	5 (1%)
2	B	429/445 (96%)	0.05	17 (3%) 42 40	20, 44, 90, 137	3 (0%)
2	D	418/445 (93%)	0.76	34 (8%) 18 18	30, 78, 117, 175	2 (0%)
3	E	123/143 (86%)	0.45	3 (2%) 59 56	23, 67, 115, 141	2 (1%)
4	F	317/384 (82%)	0.74	40 (12%) 8 8	38, 78, 137, 175	0
All	All	2166/2317 (93%)	0.24	114 (5%) 32 31	15, 54, 113, 175	14 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	7.8
2	B	277	GLY	6.1
2	D	273	LEU	5.3
4	F	99	VAL	4.7
2	D	46	ARG	4.4
4	F	191	LEU	4.3
2	B	271	ALA	4.3
2	B	1	MET	4.3
2	D	284	LEU	4.2
2	D	219	THR	4.2
4	F	149	ALA	3.9
1	C	273	ALA	3.8
2	B	275	SER	3.8
2	D	175	VAL	3.7
2	D	323	MET	3.7
2	B	274	THR	3.6
4	F	132	LEU	3.6
2	D	243	PRO	3.6
4	F	364	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	3.5
4	F	231	ALA	3.4
4	F	120	ILE	3.4
4	F	245	ILE	3.4
1	A	262	TYR	3.3
2	B	278	SER	3.3
2	D	92	PHE	3.2
4	F	296	MET	3.2
4	F	119	LEU	3.2
4	F	380	HIS	3.1
4	F	134	ALA	3.1
4	F	233	PHE	3.1
4	F	194	PRO	3.1
1	A	273	ALA	3.1
2	D	57	ASN	3.1
2	B	245	GLN	3.1
2	B	429	THR	3.1
4	F	112	ALA	3.1
1	C	176	GLN	3.0
2	B	279	GLN	3.0
4	F	130	VAL	3.0
2	D	291	GLN	3.0
4	F	251	LYS	3.0
2	D	218	THR	3.0
2	D	244	GLY	3.0
1	C	177	VAL	2.9
2	D	125	GLU	2.9
1	C	245	ASP	2.9
2	D	271	ALA	2.9
4	F	185	TYR	2.9
4	F	114	ASN	2.8
4	F	183	GLN	2.8
2	D	245	GLN	2.7
1	A	123	ARG	2.7
2	D	94	GLN	2.6
4	F	182	ILE	2.6
2	D	177	ASP	2.6
2	D	45	GLU	2.6
4	F	227	PRO	2.6
4	F	139	ARG	2.6
1	C	247	ALA	2.6
2	D	213	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	2.6
1	A	96	LYS	2.6
2	D	2	ARG	2.5
2	B	281	TYR	2.5
1	C	175	PRO	2.5
4	F	184	LYS	2.5
1	C	246	GLY	2.5
4	F	135	TYR	2.5
3	E	141	ALA	2.5
2	B	272	PRO	2.4
4	F	252	ASN	2.4
2	D	58	LYS	2.4
1	C	341	ILE	2.3
2	B	55	THR	2.3
2	D	37	HIS	2.3
4	F	138	ARG	2.3
2	D	96	GLY	2.3
4	F	186	LEU	2.3
4	F	331	GLU	2.3
2	D	34	GLY	2.3
1	C	357	TYR	2.3
1	C	2	ARG	2.3
2	D	212	PHE	2.3
2	B	285	THR	2.2
2	D	178	THR	2.2
4	F	372	THR	2.2
2	B	276	ARG	2.2
2	B	364	SER	2.2
1	C	282	TYR	2.2
3	E	4	MET	2.2
2	B	428	ALA	2.2
4	F	193	GLU	2.2
1	C	340	SER	2.2
2	D	103	LYS	2.2
4	F	90	SER	2.1
2	D	108	GLU	2.1
4	F	31	ARG	2.1
2	D	362	LYS	2.1
4	F	117	ARG	2.1
4	F	189	PRO	2.1
3	E	137	LEU	2.1
2	D	224	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	118	HIS	2.1
1	A	80	THR	2.0
4	F	113	GLN	2.0
2	B	282	ARG	2.0
2	D	320	ARG	2.0
1	C	284	GLU	2.0
1	C	441	GLU	2.0
2	D	176	SER	2.0
4	F	88	SER	2.0
2	D	363	MET	2.0
4	F	241	THR	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	GOL	B	506	6/6	0.77	0.23	77,78,78,78	0
11	GOL	C	504	6/6	0.83	0.20	70,72,75,77	0
10	MES	B	505	12/12	0.85	0.20	83,90,115,115	0
9	GDP	D	503	28/28	0.88	0.12	51,62,77,79	0
6	MG	D	502	1/1	0.88	0.10	68,68,68,68	0
6	MG	A	502	1/1	0.89	0.19	31,31,31,31	0
10	MES	B	504	12/12	0.90	0.13	45,59,82,83	0
6	MG	C	502	1/1	0.90	0.27	32,32,32,32	0
8	DO6	B	501	27/27	0.94	0.11	31,40,56,58	0
7	CA	A	503	1/1	0.95	0.10	82,82,82,82	0
8	DO6	D	501	27/27	0.96	0.09	32,47,62,65	0
6	MG	B	502	1/1	0.96	0.13	27,27,27,27	0

Continued on next page...

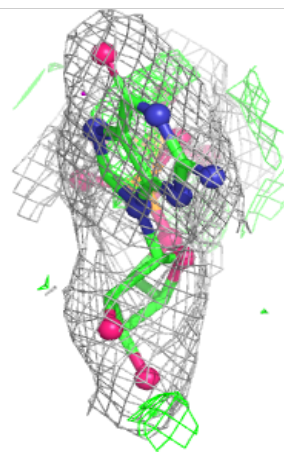
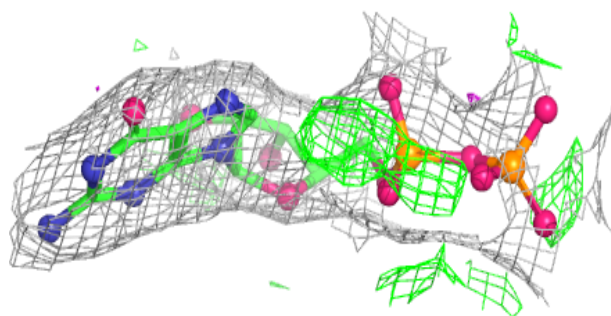
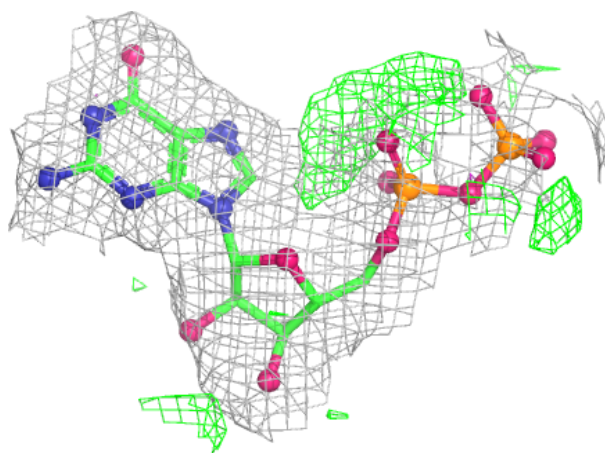
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GDP	B	503	28/28	0.97	0.07	12,30,35,38	0
5	GTP	C	501	32/32	0.97	0.07	17,26,32,38	0
5	GTP	A	501	32/32	0.97	0.06	24,30,37,41	0
7	CA	C	503	1/1	0.98	0.03	55,55,55,55	0

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

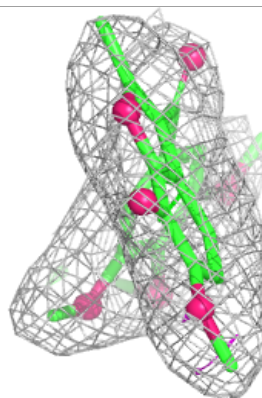
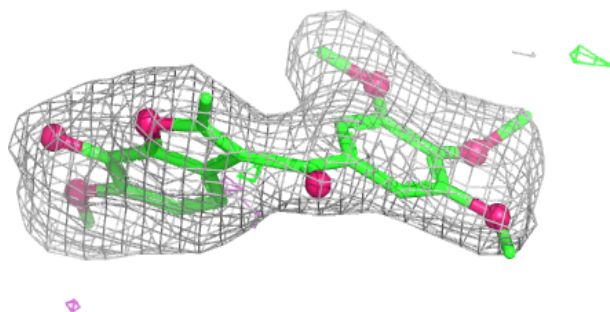
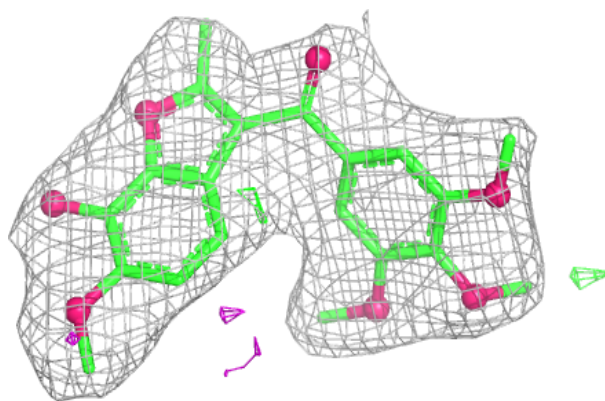
Electron density around GDP D 503:

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

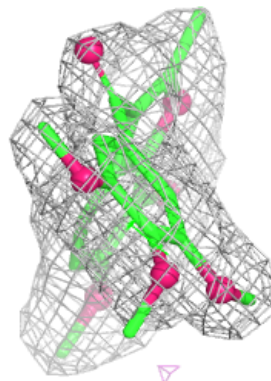
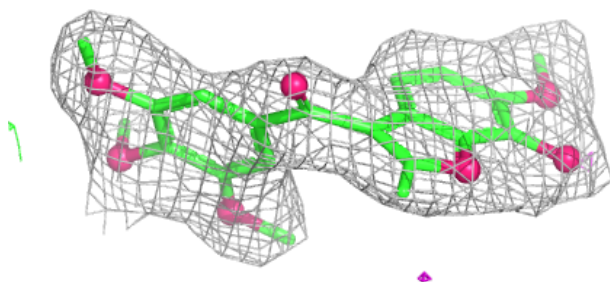
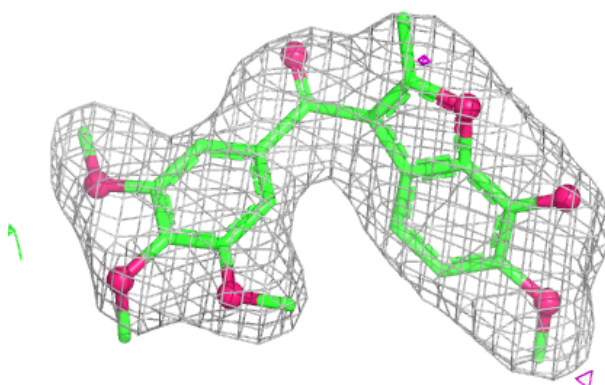


Electron density around DO6 B 501:

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

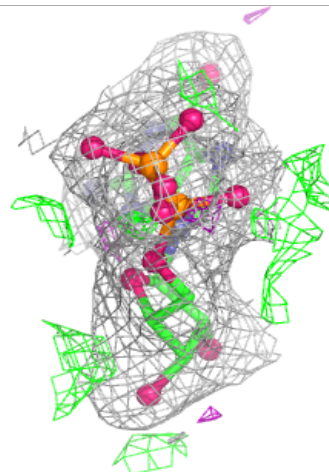
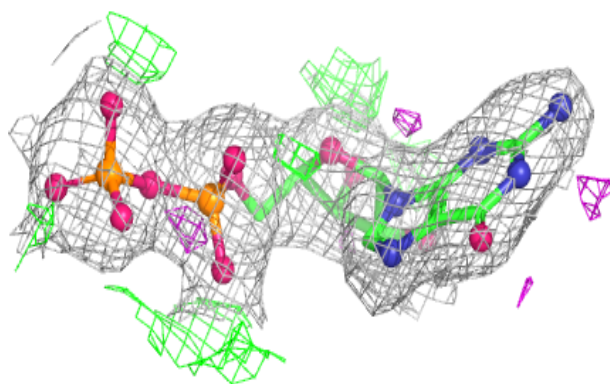
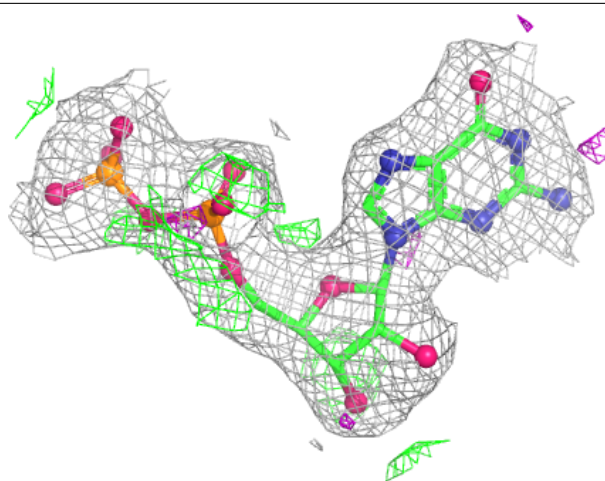
**Electron density around DO6 D 501:**

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



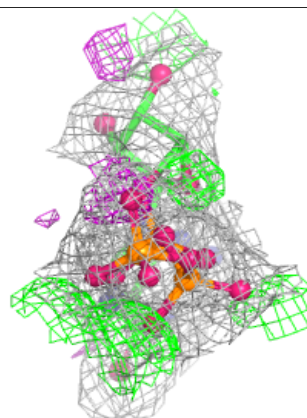
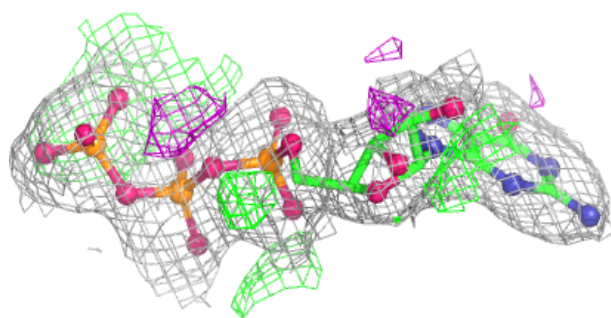
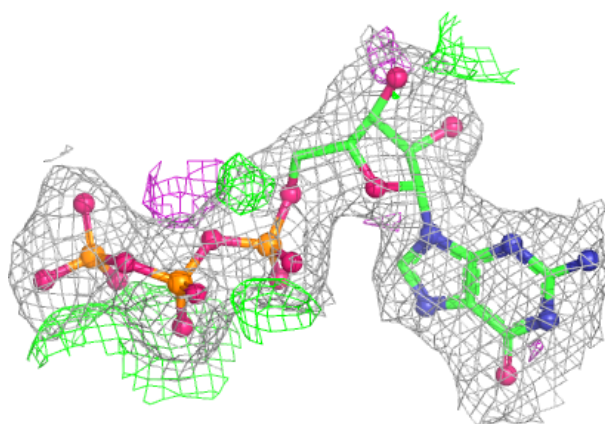
Electron density around GDP B 503:

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

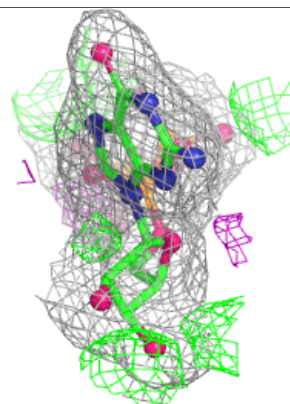
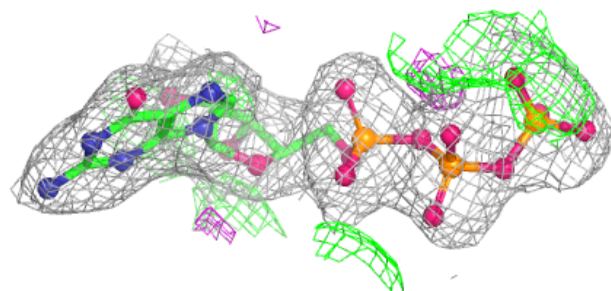
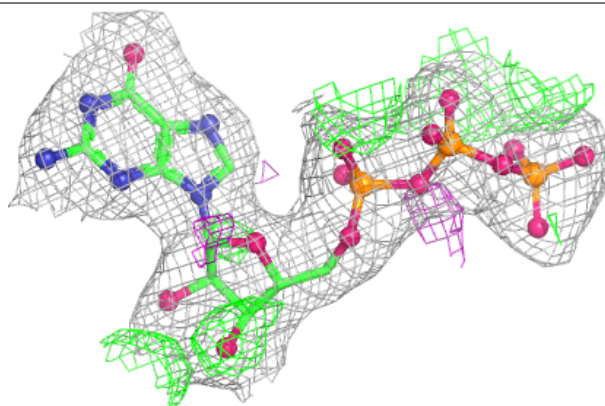


Electron density around GTP C 501:

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

**Electron density around GTP A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.