



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:43 PM UTC

PDB ID : 5OSK / pdb_00005osk
Title : Tubulin-7j complex
Authors : Menchon, G.; Protá, A.E.; Steinmetz, M.O.; Potter, B.V.L.
Deposited on : 2017-08-17
Resolution : 2.11 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

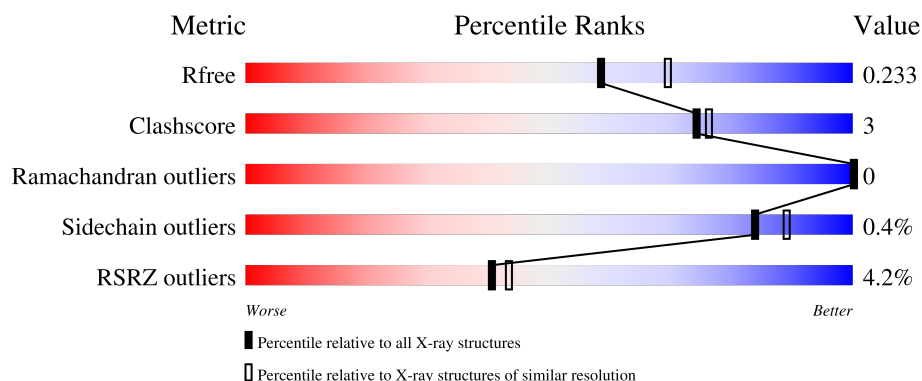
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

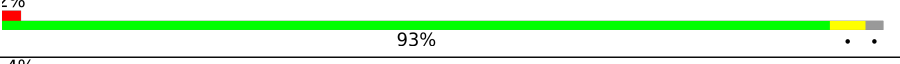
The reported resolution of this entry is 2.11 Å.

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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	7%71%11%18%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18295 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	5	0
			3445	2181	585	654	25			
1	C	440	Total	C	N	O	S	0	8	0
			3476	2199	587	665	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	6	0
			3362	2114	576	644	28			
2	D	420	Total	C	N	O	S	0	1	0
			3306	2079	561	639	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	1	0
			1020	629	184	202	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	316	Total	C	N	O	S	0	0	0
			2592	1665	445	468	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		

Continued on next page...

Continued from previous page...

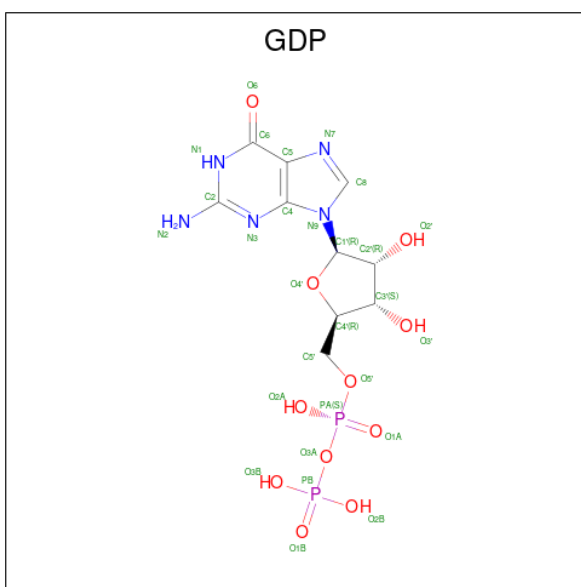
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



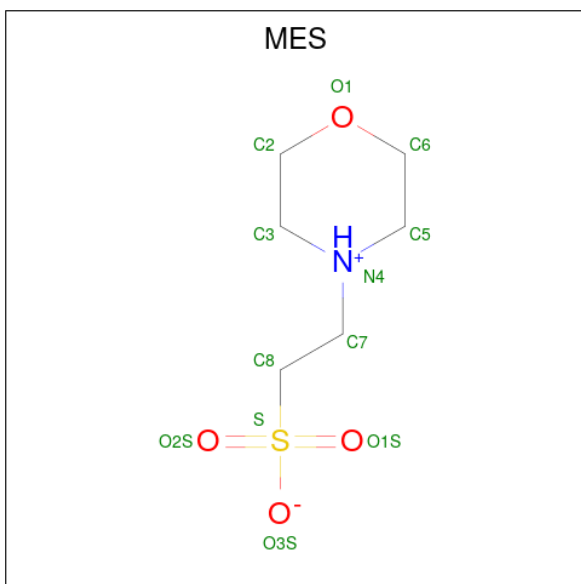
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



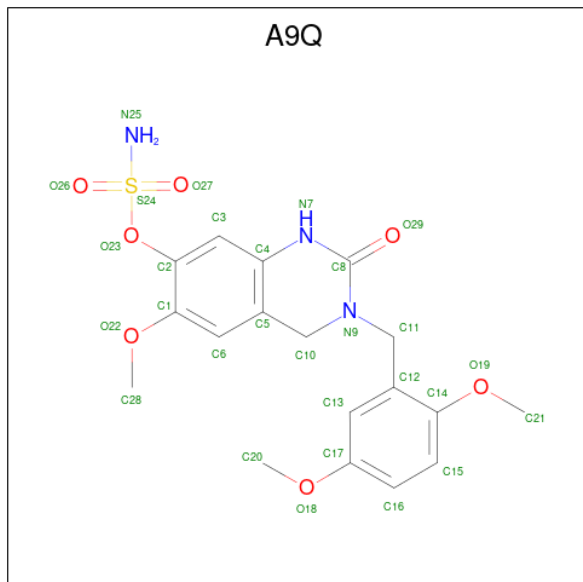
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is 3-(2,5-Dimethoxybenzyl)-7-sulfamoyloxy-6-methoxy-3,4-dihydroquinazolin-2(1H)-one (CCD ID: A9Q) (formula: $C_{18}H_{21}N_3O_7S$).

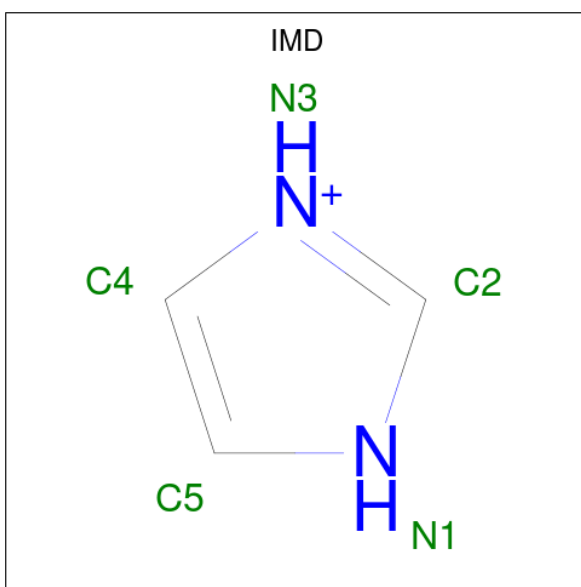


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			29	18	3	7	1		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

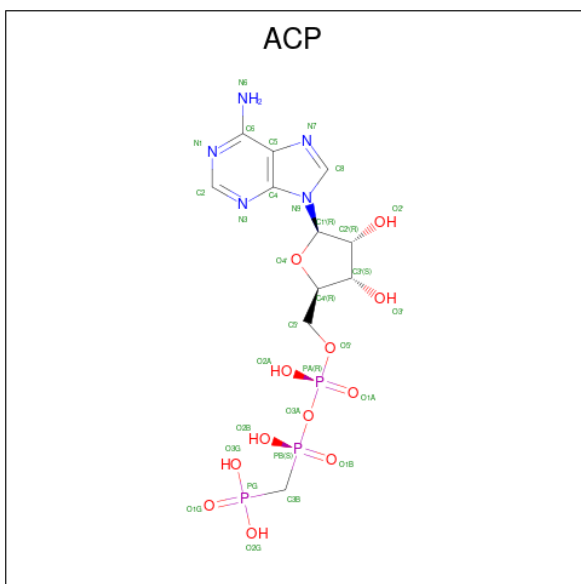
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	Ca	0	0
			1	1		

- Molecule 12 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C N 5 3 2	0	0
12	C	1	Total C N 5 3 2	0	0

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

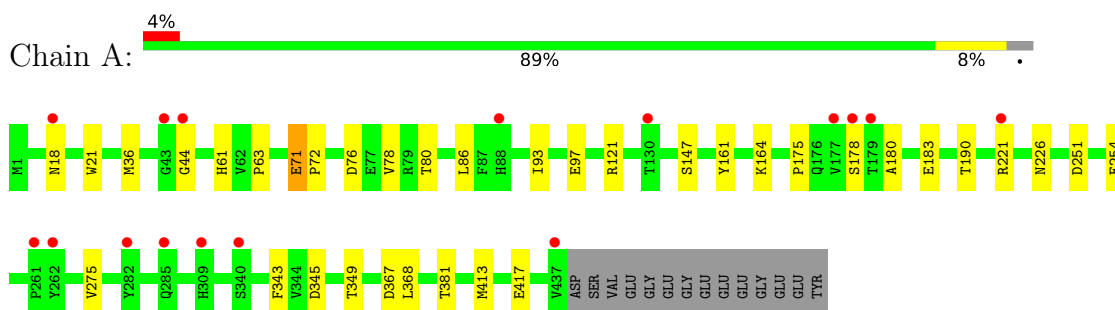
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	150	Total 150	O 150	0	0
14	B	186	Total 186	O 186	0	0
14	C	284	Total 284	O 284	0	0
14	D	96	Total 96	O 96	0	0
14	E	53	Total 53	O 53	0	0
14	F	75	Total 75	O 75	0	0

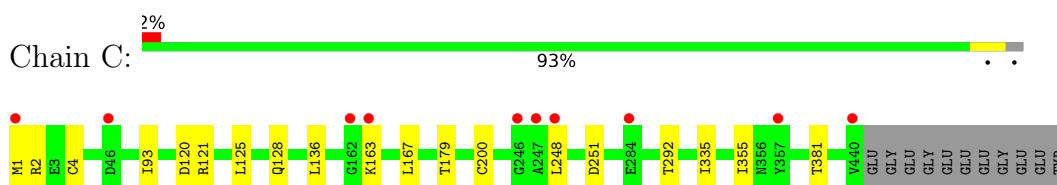
3 Residue-property plots [i](#)

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.

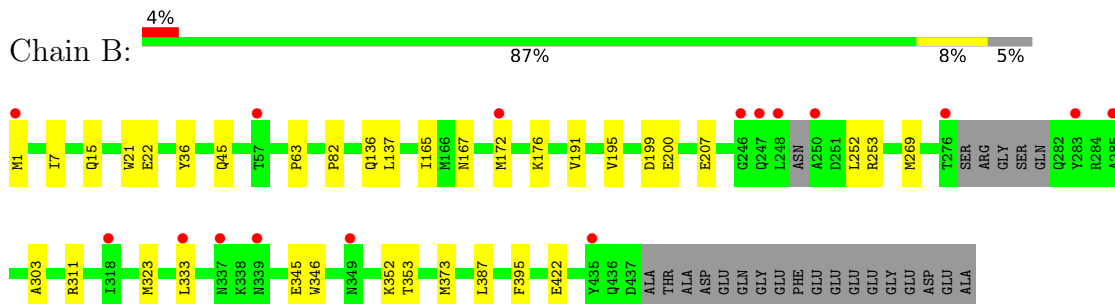
- Molecule 1: Tubulin alpha-1B chain



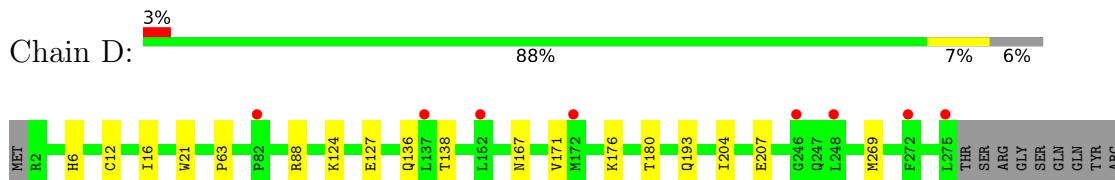
- Molecule 1: Tubulin alpha-1B chain

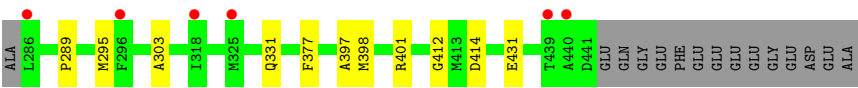


- Molecule 2: Tubulin beta-2B chain

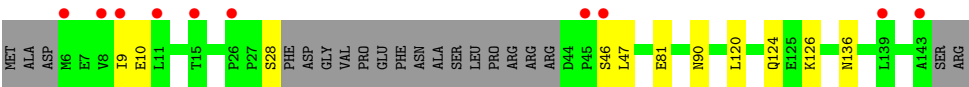
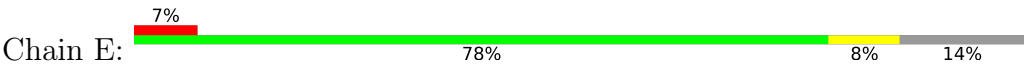


- Molecule 2: Tubulin beta-2B chain

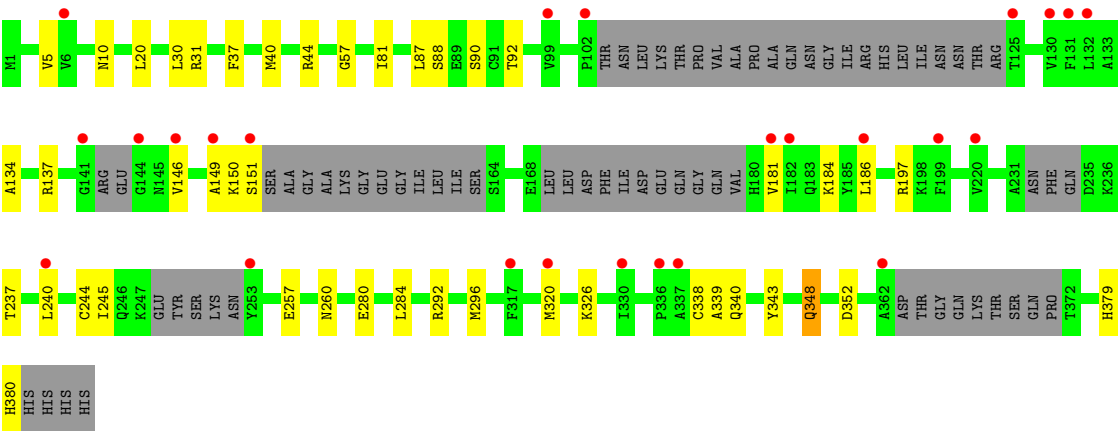




• Molecule 3: Stathmin-4



• 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	105.67Å 159.92Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 2.11 49.79 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.79-2.11) 98.0 (49.79-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.195 , 0.232 0.197 , 0.233	Depositor DCC
R_{free} test set	8558 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18295	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: ACP, CA, GTP, GOL, MES, IMD, MG, GDP, A9Q

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	0.30	0/3529	0.49	0/4790
1	C	0.41	0/3572	0.57	0/4851
2	B	0.34	0/3444	0.51	0/4659
2	D	0.28	0/3382	0.46	0/4582
3	E	0.34	0/1031	0.45	0/1368
4	F	0.20	0/2649	0.37	0/3573
All	All	0.32	0/17607	0.49	0/23823

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	3445	0	3363	21	0
1	C	3476	0	3391	14	0
2	B	3362	0	3255	26	0
2	D	3306	0	3186	17	0
3	E	1020	0	1037	9	0
4	F	2592	0	2565	26	0
5	A	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	12	0	16	0	0
7	B	18	0	24	0	0
7	C	12	0	16	1	0
8	B	28	0	12	1	0
8	D	28	0	12	1	0
9	B	12	0	12	1	0
10	B	29	0	0	0	0
11	C	1	0	0	0	0
12	C	10	0	10	0	0
13	F	31	0	14	0	0
14	A	150	0	0	1	0
14	B	186	0	0	3	0
14	C	284	0	0	3	0
14	D	96	0	0	2	0
14	E	53	0	0	1	0
14	F	75	0	0	0	0
All	All	18295	0	16937	106	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 (106) 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:348:GLN:NE2	4:F:352:ASP:OD1	2.17	0.73
2:B:422:GLU:HG3	14:B:615:HOH:O	1.96	0.66
1:A:345:ASP:HB2	3:E:28:SER:HB2	1.78	0.65
1:C:120[A]:ASP:OD1	14:C:601:HOH:O	2.15	0.65
2:B:253[A]:ARG:NH1	9:B:506:MES:O3S	2.27	0.65
4:F:20:LEU:HD21	4:F:348:GLN:HG2	1.80	0.63
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.22	0.62
4:F:134:ALA:HA	4:F:137:ARG:HE	1.65	0.62
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.83	0.61
2:D:412:GLY:HA2	3:E:136:ASN:HD22	1.67	0.59
1:A:44:GLY:O	14:A:601:HOH:O	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:150:LYS:HG2	4:F:151:SER:H	1.68	0.59
1:C:163:LYS:HG2	3:E:90:ASN:OD1	2.03	0.58
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.86	0.58
1:C:2:ARG:NH2	1:C:251:ASP:OD1	2.38	0.57
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.39	0.57
3:E:120:LEU:O	3:E:124:GLN:HG2	2.05	0.56
2:B:323:MET:HB3	2:B:373:MET:HE1	1.87	0.56
1:C:179:THR:HG21	14:C:625:HOH:O	2.05	0.56
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.87	0.56
1:A:221:ARG:HD3	1:A:221:ARG:O	2.05	0.55
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.72	0.55
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.88	0.55
2:B:323:MET:HE2	2:B:373:MET:HE2	1.88	0.55
4:F:296:MET:SD	4:F:380:HIS:HB2	2.46	0.55
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.87	0.55
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.89	0.55
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.88	0.54
2:D:431:GLU:OE1	14:D:601:HOH:O	2.18	0.54
3:E:81:GLU:OE1	14:E:201:HOH:O	2.18	0.54
4:F:88:SER:O	4:F:90:SER:N	2.37	0.54
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.42	0.53
2:D:176:LYS:HD2	2:D:207:GLU:HG3	1.89	0.53
2:D:397:ALA:O	2:D:401:ARG:NH1	2.41	0.53
2:D:414:ASP:N	2:D:414:ASP:OD1	2.41	0.53
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.49	0.53
1:A:175:PRO:HA	1:A:178:SER:HB2	1.91	0.52
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.91	0.52
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.45	0.51
4:F:92:THR:O	4:F:326:LYS:NZ	2.34	0.51
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.47	0.50
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.93	0.50
14:D:602:HOH:O	3:E:126:LYS:NZ	2.43	0.50
4:F:10:ASN:HB2	4:F:44:ARG:HH12	1.76	0.50
4:F:292:ARG:HD3	4:F:379:HIS:O	2.12	0.50
2:B:345:GLU:N	2:B:345:GLU:OE1	2.45	0.50
4:F:88:SER:C	4:F:90:SER:H	2.19	0.50
2:B:22:GLU:OE1	14:B:601:HOH:O	2.20	0.50
4:F:146:VAL:H	4:F:184:LYS:NZ	2.10	0.49
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.77	0.49
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.41	0.49
2:B:345:GLU:OE2	4:F:31:ARG:NH1	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:NH1	14:C:610:HOH:O	2.45	0.49
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.94	0.48
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.95	0.48
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.95	0.48
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.96	0.48
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.23	0.46
3:E:9:ILE:HG12	3:E:10:GLU:HG3	1.96	0.46
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.50	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.51	0.45
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.98	0.45
2:B:82:PRO:O	14:B:602:HOH:O	2.20	0.45
4:F:149:ALA:HA	4:F:181:VAL:O	2.16	0.45
1:C:163:LYS:HD3	7:C:505:GOL:H12	1.99	0.45
2:D:289:PRO:HA	2:D:331:GLN:HG2	1.99	0.45
2:B:199:ASP:C	2:B:200:GLU:HG3	2.42	0.44
1:C:1:MET:HE3	1:C:1:MET:HB3	1.83	0.44
2:D:136:GLN:HA	2:D:167:ASN:O	2.18	0.44
4:F:338:CYS:SG	4:F:339:ALA:N	2.91	0.44
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.48	0.44
2:B:15:GLN:NE2	8:B:502:GDP:O6	2.51	0.43
1:A:76:ASP:O	1:A:80:THR:HG22	2.18	0.43
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.43
2:B:311:ARG:NH2	2:B:345:GLU:OE1	2.47	0.43
2:B:36:TYR:HE1	2:B:45:GLN:HG3	1.82	0.43
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.54	0.43
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.43
2:B:136:GLN:HA	2:B:167:ASN:O	2.19	0.43
2:D:16:ILE:HD11	2:D:138:THR:HB	2.02	0.42
2:D:398:MET:HE3	2:D:398:MET:HB2	1.83	0.42
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.00	0.42
2:B:373:MET:HE2	2:B:373:MET:HB3	1.66	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.42
2:B:191:VAL:O	2:B:195:VAL:HG23	2.19	0.42
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.42
4:F:260:ASN:HD22	4:F:260:ASN:HA	1.68	0.42
2:B:333:LEU:HD13	4:F:57:GLY:HA3	2.01	0.42
2:B:346:TRP:CD1	2:B:346:TRP:H	2.38	0.42
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.35	0.42
1:A:93:ILE:HD11	1:A:121:ARG:HG3	2.02	0.42
2:D:88:ARG:HH22	2:D:124:LYS:NZ	2.18	0.42
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.01	0.42
2:B:352:LYS:HD2	2:B:353:THR:H	1.85	0.41
1:A:97:GLU:HG3	2:B:1:MET:HG2	2.02	0.41
1:A:180:ALA:O	1:A:183:GLU:HG3	2.20	0.41
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
1:A:251:ASP:OD1	1:A:254:GLU:HG3	2.21	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.56	0.41
3:E:46:SER:OG	3:E:47:LEU:N	2.53	0.41
4:F:150:LYS:HG2	4:F:151:SER:N	2.36	0.41
4:F:244:CYS:SG	4:F:245:ILE:N	2.93	0.41
1:C:125:LEU:O	1:C:128:GLN:HG2	2.21	0.40
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.57	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	440/451 (98%)	432 (98%)	8 (2%)	0	100	100
1	C	446/451 (99%)	436 (98%)	10 (2%)	0	100	100
2	B	421/445 (95%)	413 (98%)	8 (2%)	0	100	100
2	D	417/445 (94%)	410 (98%)	7 (2%)	0	100	100
3	E	120/143 (84%)	120 (100%)	0	0	100	100
4	F	300/384 (78%)	291 (97%)	9 (3%)	0	100	100
All	All	2144/2319 (92%)	2102 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	373/379 (98%)	371 (100%)	2 (0%)	81	87
1	C	379/379 (100%)	378 (100%)	1 (0%)	86	91
2	B	371/383 (97%)	371 (100%)	0	100	100
2	D	364/383 (95%)	362 (100%)	2 (0%)	81	87
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	284/342 (83%)	281 (99%)	3 (1%)	65	74
All	All	1882/1993 (94%)	1874 (100%)	8 (0%)	84	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	381	THR
1	C	381	THR
2	D	127	GLU
2	D	180	THR
4	F	237	THR
4	F	240	LEU
4	F	348	GLN

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	309	HIS
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	45	GLN
2	B	136	GLN
2	B	192	HIS
2	B	193	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	300	ASN
1	C	88	HIS
1	C	393	HIS
2	D	8	GLN
2	D	14	ASN
2	D	136	GLN
2	D	192	HIS
2	D	349	ASN
2	D	406	HIS
2	D	424	ASN
2	D	426	ASN
3	E	12	ASN
3	E	136	ASN
4	F	26	GLN
4	F	45	ASN
4	F	246	GLN
4	F	333	ASN
4	F	380	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 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\# Z > 2$
7	GOL	A	504	-	5,5,5	0.41	0	5,5,5	0.32	0
7	GOL	C	503	-	5,5,5	0.37	0	5,5,5	0.29	0
7	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.26	0
5	GTP	A	501	6	33,34,34	1.05	2 (6%)	50,54,54	1.61	9 (18%)
5	GTP	C	501	6	33,34,34	1.07	3 (9%)	50,54,54	1.55	11 (22%)
7	GOL	B	504	-	5,5,5	0.33	0	5,5,5	0.51	0
8	GDP	B	502	6	29,30,30	1.12	2 (6%)	45,47,47	1.74	8 (17%)
7	GOL	B	501	-	5,5,5	0.38	0	5,5,5	0.44	0
9	MES	B	506	-	12,12,12	2.07	1 (8%)	15,16,16	2.03	4 (26%)
10	A9Q	B	507	-	30,31,31	2.51	6 (20%)	43,45,45	1.93	8 (18%)
7	GOL	B	505	-	5,5,5	0.44	0	5,5,5	0.22	0
7	GOL	C	505	-	5,5,5	0.39	0	5,5,5	0.56	0
12	IMD	C	506	-	5,5,5	0.73	0	5,5,5	0.43	0
12	IMD	C	507	-	5,5,5	0.71	0	5,5,5	0.35	0
13	ACP	F	402	6	31,33,33	1.78	7 (22%)	47,52,52	1.95	9 (19%)
8	GDP	D	501	6	29,30,30	1.18	4 (13%)	45,47,47	1.74	5 (11%)

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
7	GOL	A	504	-	-	2/4/4/4	-
7	GOL	C	503	-	-	2/4/4/4	-
7	GOL	A	503	-	-	3/4/4/4	-
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
7	GOL	B	504	-	-	2/4/4/4	-
8	GDP	B	502	6	-	5/16/32/32	0/3/3/3
7	GOL	B	501	-	-	2/4/4/4	-
9	MES	B	506	-	-	4/6/14/14	0/1/1/1
10	A9Q	B	507	-	-	2/15/27/27	0/3/3/3
7	GOL	B	505	-	-	2/4/4/4	-
7	GOL	C	505	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ACP	F	402	6	-	9/19/38/38	0/3/3/3
12	IMD	C	506	-	-	-	0/1/1/1
12	IMD	C	507	-	-	-	0/1/1/1
8	GDP	D	501	6	-	5/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	507	A9Q	S24-N25	9.24	1.69	1.58
9	B	506	MES	C8-S	-6.92	1.67	1.77
13	F	402	ACP	PG-O1G	5.64	1.61	1.50
10	B	507	A9Q	C8-N7	5.43	1.42	1.36
10	B	507	A9Q	O26-S24	4.53	1.47	1.42
10	B	507	A9Q	O27-S24	4.38	1.47	1.42
13	F	402	ACP	PB-O3A	3.33	1.62	1.58
10	B	507	A9Q	O23-S24	3.21	1.65	1.61
8	D	501	GDP	C5-C4	3.18	1.47	1.38
10	B	507	A9Q	C4-N7	3.11	1.45	1.39
5	C	501	GTP	PB-O3A	3.11	1.62	1.59
13	F	402	ACP	PA-O1A	3.09	1.61	1.50
5	A	501	GTP	PB-O3B	3.03	1.62	1.59
8	B	502	GDP	C5-C4	3.03	1.47	1.38
13	F	402	ACP	PG-O2G	-3.00	1.48	1.55
13	F	402	ACP	PG-O3G	2.90	1.61	1.55
5	C	501	GTP	PB-O3B	2.61	1.62	1.59
8	B	502	GDP	C6-N1	-2.50	1.34	1.38
13	F	402	ACP	PA-O3A	2.44	1.62	1.59
8	D	501	GDP	C6-N1	-2.38	1.34	1.38
8	D	501	GDP	C5-N7	-2.11	1.34	1.39
5	A	501	GTP	PA-O3A	2.10	1.61	1.59
8	D	501	GDP	PA-O3A	2.10	1.61	1.59
5	C	501	GTP	C2-N3	2.09	1.38	1.33
13	F	402	ACP	PB-O2B	2.05	1.61	1.56

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	507	A9Q	O27-S24-O26	-6.88	112.94	119.94
8	D	501	GDP	C5-C4-N3	-6.18	118.56	128.39
13	F	402	ACP	PB-O3A-PA	-6.13	112.35	132.37
8	B	502	GDP	C5-C4-N3	-6.05	118.77	128.39
13	F	402	ACP	C5-C4-N3	-5.37	119.32	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	506	MES	O2S-S-C8	5.29	114.72	106.73
10	B	507	A9Q	O23-C2-C1	5.10	124.31	118.03
8	B	502	GDP	C2-N3-C4	5.06	121.01	112.30
8	D	501	GDP	C2-N3-C4	4.85	120.65	112.30
8	D	501	GDP	N9-C4-N3	4.71	135.37	125.95
5	C	501	GTP	C5-C4-N3	-4.69	120.92	128.39
5	A	501	GTP	C5-C4-N3	-4.67	120.95	128.39
5	C	501	GTP	C2-N3-C4	4.58	120.18	112.30
5	A	501	GTP	C2-N3-C4	4.51	120.06	112.30
13	F	402	ACP	N3-C4-N9	4.47	134.78	127.17
8	B	502	GDP	N9-C4-N3	4.46	134.87	125.95
10	B	507	A9Q	O22-C1-C2	4.37	121.33	115.40
13	F	402	ACP	N3-C2-N1	-4.09	122.39	128.58
9	B	506	MES	C5-N4-C3	3.88	117.20	108.84
13	F	402	ACP	C5-N7-C8	3.80	109.43	103.45
13	F	402	ACP	C2-N3-C4	3.53	120.46	111.83
8	B	502	GDP	C6-C5-N7	3.38	136.45	130.29
10	B	507	A9Q	O22-C1-C6	-3.12	118.70	124.08
13	F	402	ACP	C4-C5-N7	-3.03	107.12	110.58
8	D	501	GDP	C6-C5-N7	2.91	135.59	130.29
10	B	507	A9Q	C11-N9-C8	-2.91	115.27	118.87
13	F	402	ACP	N9-C8-N7	-2.86	109.88	113.94
5	A	501	GTP	N9-C8-N7	-2.85	108.11	113.40
5	A	501	GTP	C8-N7-C5	2.80	109.25	104.26
5	C	501	GTP	N9-C4-N3	2.71	131.38	125.95
5	C	501	GTP	N9-C8-N7	-2.71	108.38	113.40
10	B	507	A9Q	O19-C14-C15	-2.70	119.75	124.30
10	B	507	A9Q	C4-N7-C8	-2.62	120.96	124.53
8	B	502	GDP	O2B-PB-O3A	2.61	113.39	104.64
8	B	502	GDP	C4-C5-N7	-2.53	106.66	110.67
13	F	402	ACP	PA-O5'-C5'	-2.42	107.46	121.35
5	A	501	GTP	O2A-PA-O3A	2.40	113.77	107.27
5	A	501	GTP	C4-C5-N7	-2.37	106.92	110.67
5	C	501	GTP	O6-C6-C5	-2.36	120.31	126.53
5	C	501	GTP	C2-N1-C6	-2.35	120.85	125.11
5	C	501	GTP	C8-N7-C5	2.34	108.43	104.26
5	A	501	GTP	N9-C4-N3	2.34	130.63	125.95
5	A	501	GTP	C2-N1-C6	-2.33	120.88	125.11
8	D	501	GDP	C4-C5-N7	-2.33	106.98	110.67
10	B	507	A9Q	C11-N9-C10	2.32	119.37	116.11
9	B	506	MES	C7-N4-C5	2.27	117.28	111.24
5	A	501	GTP	C5-C6-N1	2.26	118.99	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C5-C6-N1	2.24	118.94	113.25
9	B	506	MES	O3S-S-O2S	-2.15	106.01	111.40
8	B	502	GDP	O6-C6-C5	-2.11	120.96	126.53
5	C	501	GTP	O3'-C3'-C4'	-2.10	105.06	111.08
8	B	502	GDP	C5-C6-N1	2.08	118.55	113.25
5	C	501	GTP	N1-C2-N3	-2.07	119.53	123.32
5	C	501	GTP	N2-C2-N1	2.02	121.02	116.76

There are no chirality outliers.

All (57) 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
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
7	B	504	GOL	O1-C1-C2-C3
7	B	505	GOL	O1-C1-C2-C3
7	C	503	GOL	O1-C1-C2-C3
7	C	505	GOL	O1-C1-C2-C3
8	B	502	GDP	C5'-O5'-PA-O3A
8	B	502	GDP	C5'-O5'-PA-O1A
8	B	502	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	506	MES	C8-C7-N4-C5
9	B	506	MES	C7-C8-S-O1S
9	B	506	MES	C7-C8-S-O3S
13	F	402	ACP	PB-C3B-PG-O1G
13	F	402	ACP	PB-C3B-PG-O3G
13	F	402	ACP	C5'-O5'-PA-O1A
13	F	402	ACP	C5'-O5'-PA-O2A
13	F	402	ACP	C5'-O5'-PA-O3A
7	A	503	GOL	O1-C1-C2-C3
7	A	504	GOL	O1-C1-C2-C3
7	B	501	GOL	O1-C1-C2-C3
7	C	505	GOL	C1-C2-C3-O3
7	A	503	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	501	GOL	O1-C1-C2-O2
7	B	504	GOL	O1-C1-C2-O2
7	B	505	GOL	O1-C1-C2-O2
7	C	505	GOL	O1-C1-C2-O2
10	B	507	A9Q	C15-C14-O19-C21
10	B	507	A9Q	C12-C14-O19-C21
7	A	504	GOL	O1-C1-C2-O2
7	C	503	GOL	O1-C1-C2-O2
13	F	402	ACP	O4'-C4'-C5'-O5'
7	C	505	GOL	O2-C2-C3-O3
13	F	402	ACP	PB-O3A-PA-O1A
7	A	503	GOL	O2-C2-C3-O3
9	B	506	MES	C7-C8-S-O2S
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O3G
13	F	402	ACP	PB-C3B-PG-O2G
5	C	501	GTP	PB-O3A-PA-O2A
8	D	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
8	B	502	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
13	F	402	ACP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
8	B	502	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O1A

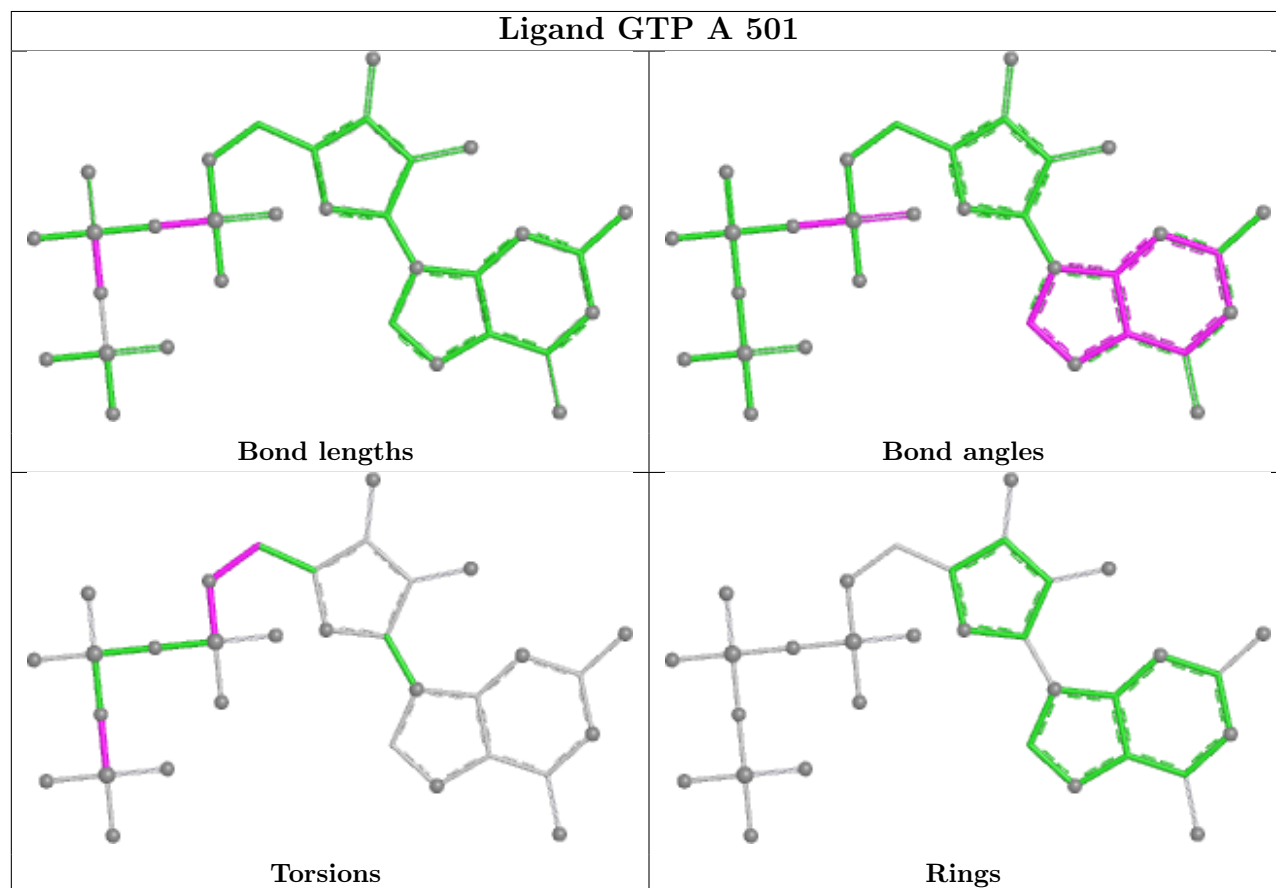
There are no ring outliers.

4 monomers are involved in 4 short contacts:

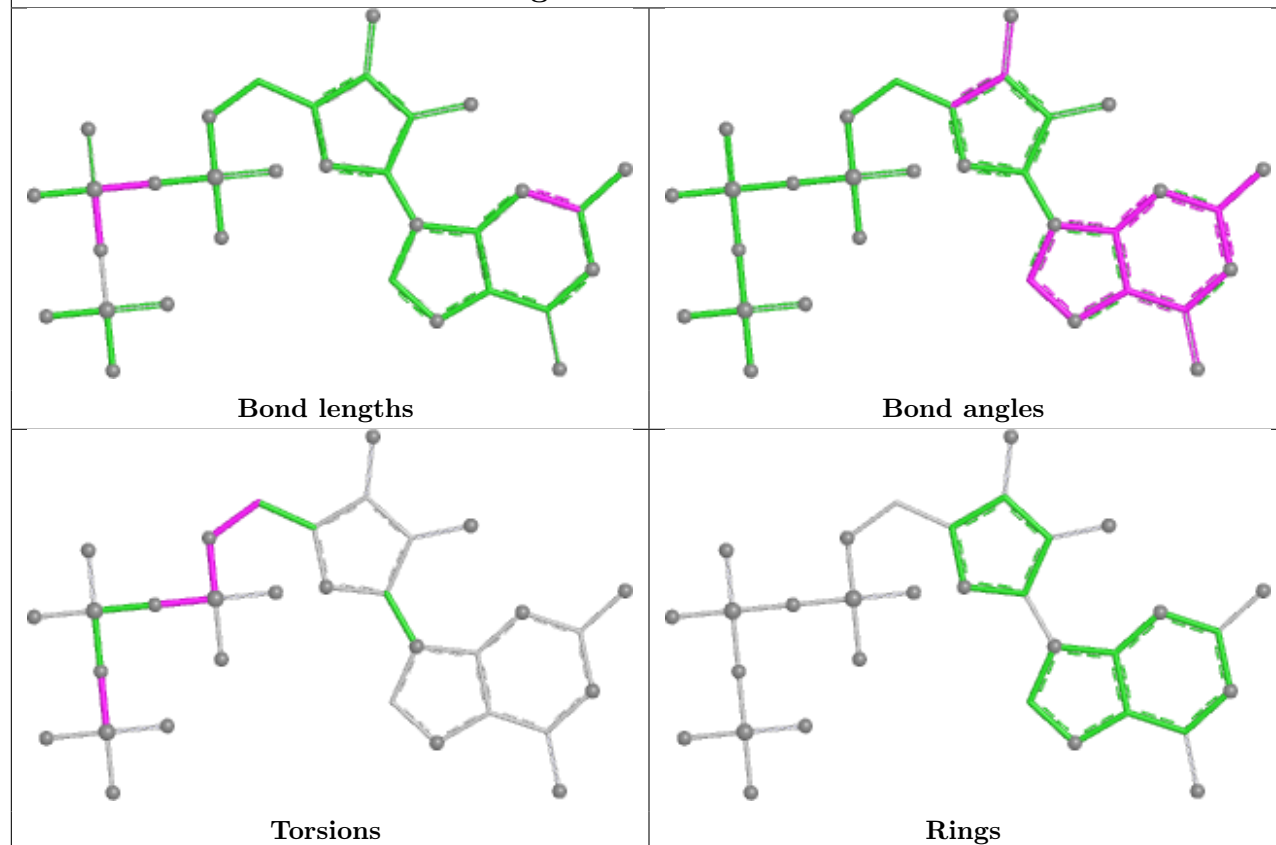
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	502	GDP	1	0
9	B	506	MES	1	0
7	C	505	GOL	1	0
8	D	501	GDP	1	0

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.

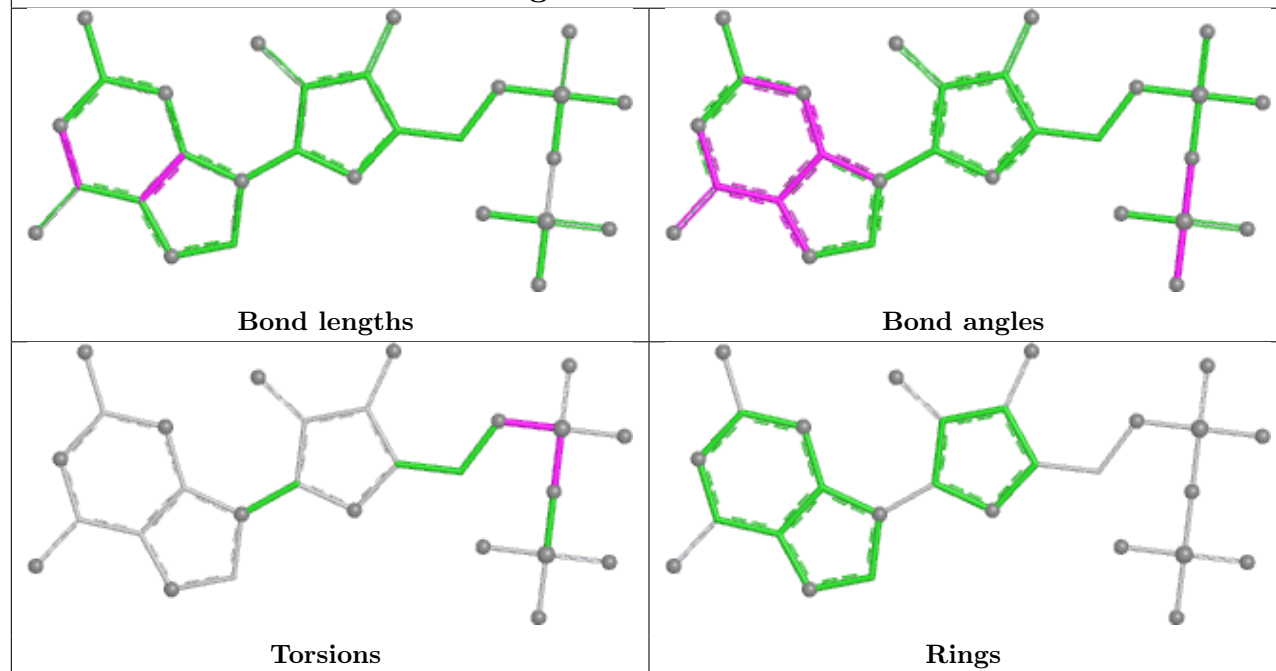
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



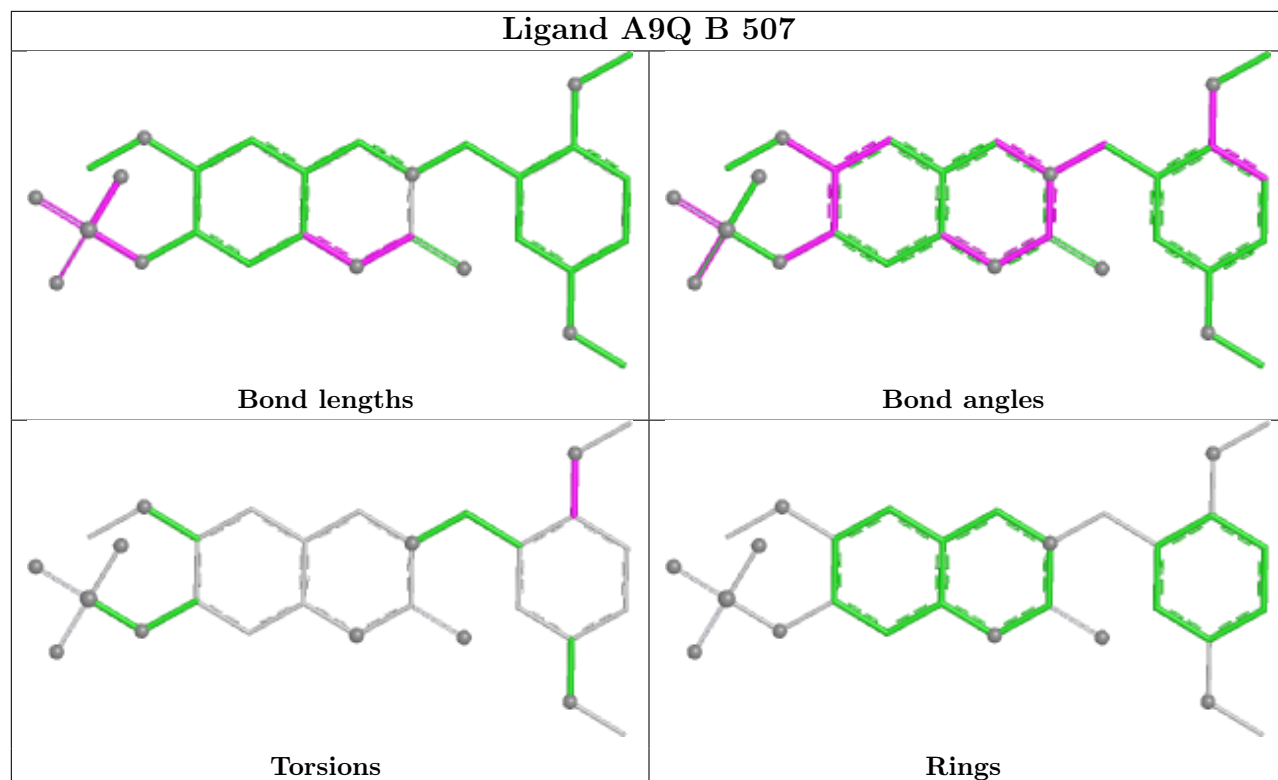
Ligand GTP C 501



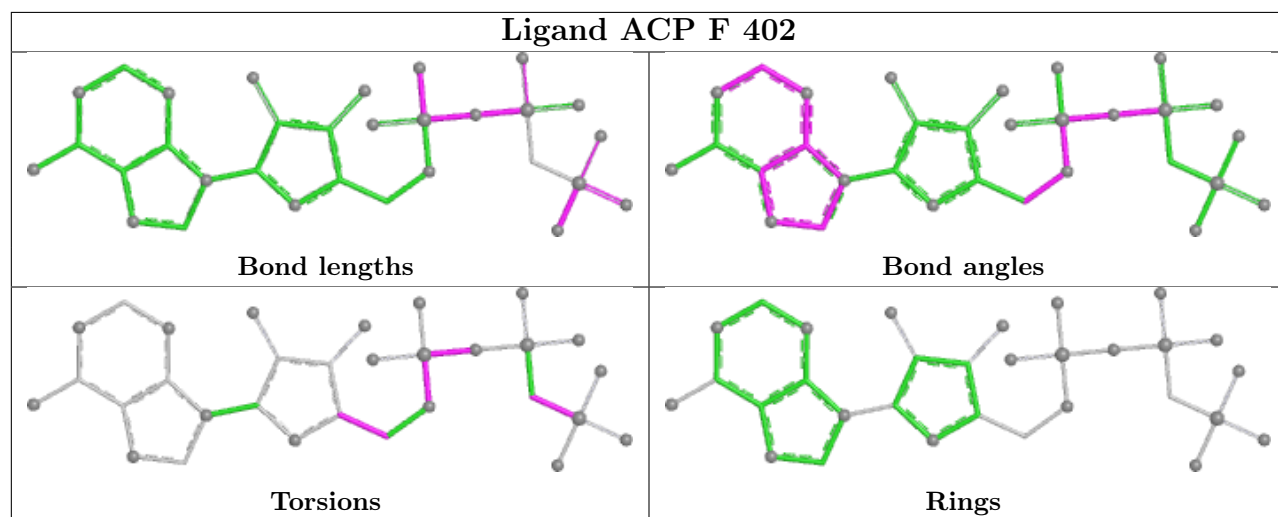
Ligand GDP B 502

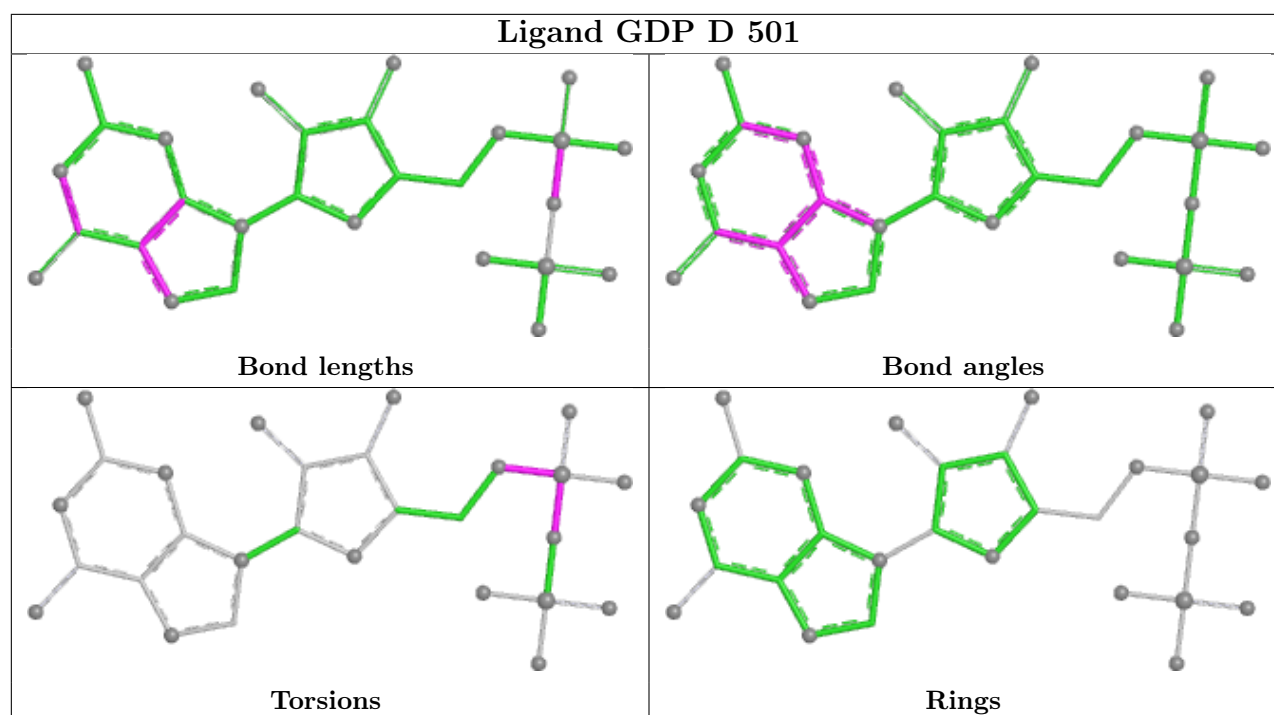


Ligand A9Q B 507



Ligand ACP F 402





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%)	0.32	16 (3%)	45 48	26, 65, 108, 156	5 (1%)
1	C	440/451 (97%)	-0.03	10 (2%)	61 64	22, 49, 80, 115	8 (1%)
2	B	421/445 (94%)	0.27	16 (3%)	44 47	25, 59, 105, 161	6 (1%)
2	D	420/445 (94%)	0.52	14 (3%)	49 52	38, 75, 113, 141	1 (0%)
3	E	123/143 (86%)	0.58	10 (8%)	18 19	32, 78, 135, 156	1 (0%)
4	F	316/384 (82%)	0.82	25 (7%)	18 20	56, 97, 164, 206	0
All	All	2157/2319 (93%)	0.37	91 (4%)	40 43	22, 67, 126, 206	21 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	248	LEU	5.5
2	B	248	LEU	5.4
3	E	143	ALA	4.3
4	F	144	GLY	4.3
2	B	276	THR	4.3
4	F	181	VAL	4.0
1	A	437	VAL	3.9
4	F	141	GLY	3.9
1	A	340	SER	3.7
4	F	132	LEU	3.6
4	F	102	PRO	3.5
4	F	131	PHE	3.5
4	F	186	LEU	3.5
3	E	8	VAL	3.4
2	D	172	MET	3.3
2	B	1	MET	3.2
4	F	240	LEU	3.1
2	B	247	GLN	3.1
1	C	1	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	435	TYR	2.9
2	D	246	GLY	2.9
2	B	333	LEU	2.8
1	C	440	VAL	2.8
1	A	130	THR	2.8
1	A	262	TYR	2.8
4	F	151	SER	2.8
2	B	246	GLY	2.8
4	F	99	VAL	2.8
1	C	163	LYS	2.7
1	A	88	HIS	2.7
4	F	320	MET	2.7
2	D	325	MET	2.6
2	B	337	ASN	2.6
4	F	125	THR	2.6
4	F	182	ILE	2.5
1	C	247	ALA	2.5
3	E	26	PRO	2.5
2	D	137	LEU	2.5
2	D	296	PHE	2.5
4	F	220	VAL	2.5
1	A	261	PRO	2.5
2	B	285	ALA	2.4
4	F	337	ALA	2.4
1	A	43	GLY	2.4
1	A	178	SER	2.4
3	E	45	PRO	2.4
1	A	177	VAL	2.4
4	F	362	ALA	2.3
2	D	318	ILE	2.3
2	D	272	PHE	2.3
2	B	339	ASN	2.3
2	B	349[A]	ASN	2.3
1	A	285	GLN	2.3
4	F	6	VAL	2.3
4	F	336	PRO	2.3
1	A	44	GLY	2.2
3	E	15	THR	2.2
4	F	130	VAL	2.2
1	C	162	GLY	2.2
4	F	149	ALA	2.2
3	E	11	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	139	LEU	2.2
1	C	357	TYR	2.2
3	E	9	ILE	2.2
4	F	330	ILE	2.2
2	D	440	ALA	2.2
1	A	179	THR	2.2
2	B	57	THR	2.2
2	D	439	THR	2.2
1	C	284	GLU	2.1
2	D	275	LEU	2.1
2	B	172	MET	2.1
3	E	6	MET	2.1
1	C	246	GLY	2.1
2	D	286	LEU	2.1
1	A	282	TYR	2.1
4	F	199	PHE	2.1
4	F	146	VAL	2.1
1	C	248	LEU	2.1
2	D	152	LEU	2.1
3	E	46	SER	2.1
1	A	18	ASN	2.1
1	A	221	ARG	2.1
1	A	309	HIS	2.1
2	B	283	TYR	2.1
4	F	317	PHE	2.1
2	B	250	ALA	2.1
2	B	318	ILE	2.0
1	C	46	ASP	2.0
2	D	82	PRO	2.0
4	F	253	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

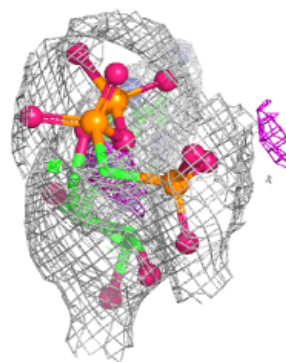
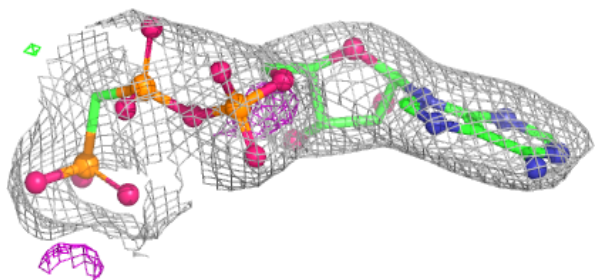
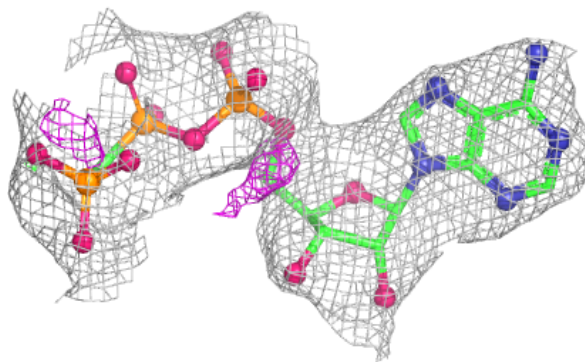
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	504	6/6	0.79	0.15	82,96,103,106	0
7	GOL	B	504	6/6	0.80	0.21	95,99,99,103	0
6	MG	F	401	1/1	0.82	0.09	101,101,101,101	0
7	GOL	A	503	6/6	0.84	0.15	80,90,92,92	0
13	ACP	F	402	31/31	0.84	0.11	98,109,164,165	0
7	GOL	C	505	6/6	0.85	0.17	78,91,100,104	0
7	GOL	B	501	6/6	0.85	0.18	89,90,91,95	0
12	IMD	C	507	5/5	0.86	0.30	88,89,90,90	0
7	GOL	C	503	6/6	0.87	0.14	66,80,82,85	0
10	A9Q	B	507	29/29	0.87	0.17	73,81,128,134	0
7	GOL	B	505	6/6	0.88	0.17	88,95,96,96	0
8	GDP	D	501	28/28	0.92	0.11	58,65,75,77	0
12	IMD	C	506	5/5	0.93	0.11	67,69,69,70	0
9	MES	B	506	12/12	0.94	0.10	54,61,82,84	0
6	MG	D	502	1/1	0.96	0.10	54,54,54,54	0
5	GTP	C	501	32/32	0.98	0.05	34,39,43,43	0
5	GTP	A	501	32/32	0.98	0.05	37,45,49,53	0
6	MG	C	502	1/1	0.99	0.02	38,38,38,38	0
11	CA	C	504	1/1	0.99	0.03	64,64,64,64	0
8	GDP	B	502	28/28	0.99	0.04	37,43,51,55	0
6	MG	A	502	1/1	0.99	0.02	44,44,44,44	0
6	MG	B	503	1/1	0.99	0.08	37,37,37,37	0

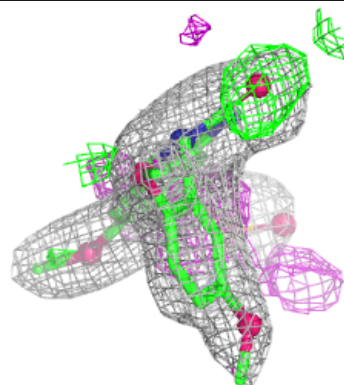
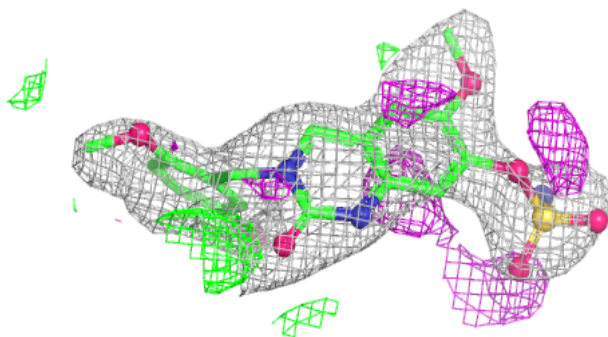
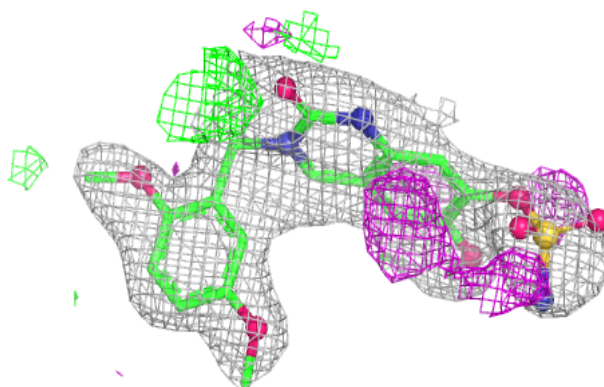
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

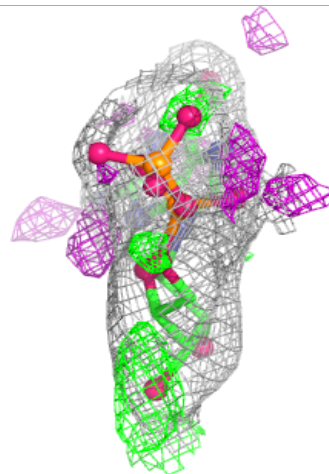
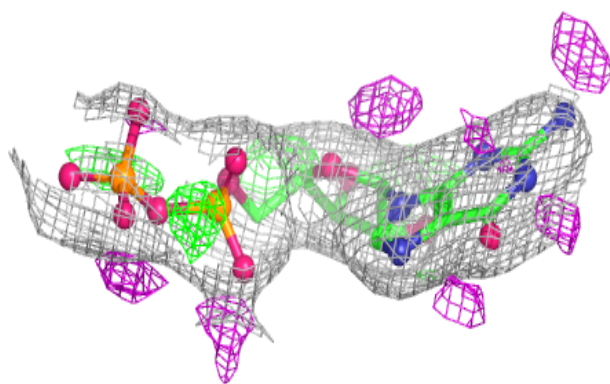
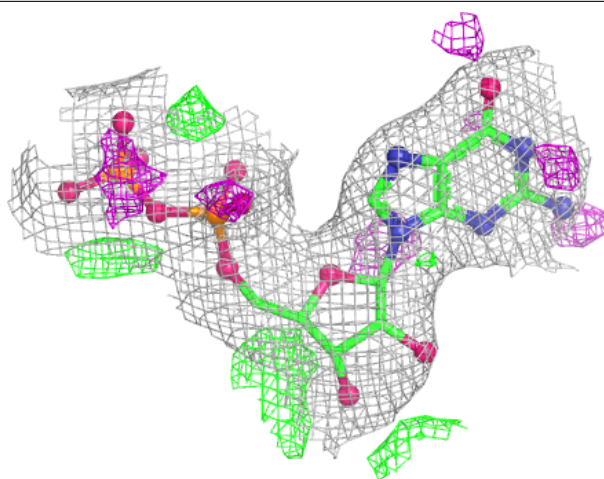
**Electron density around A9Q B 507:**

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



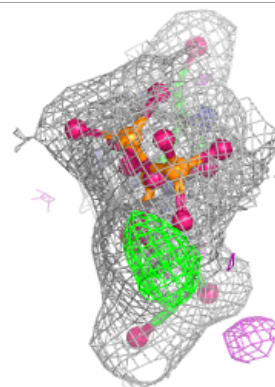
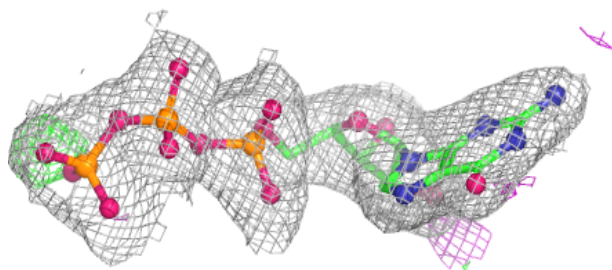
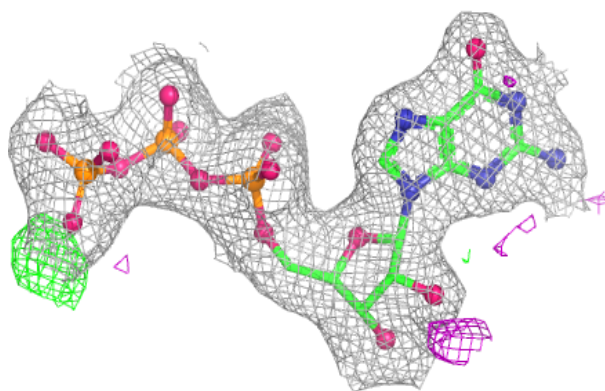
Electron density around GDP D 501:

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

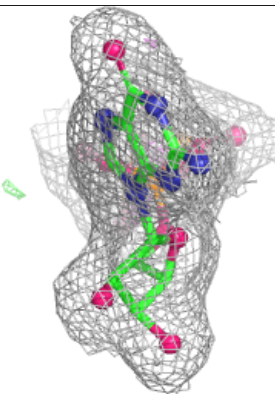
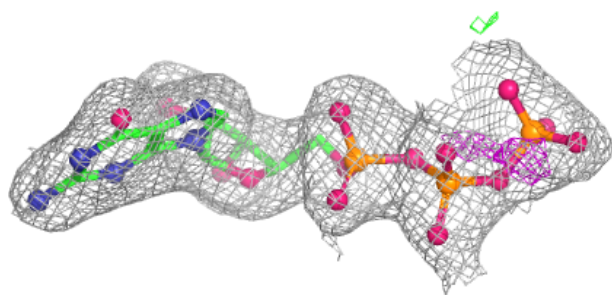
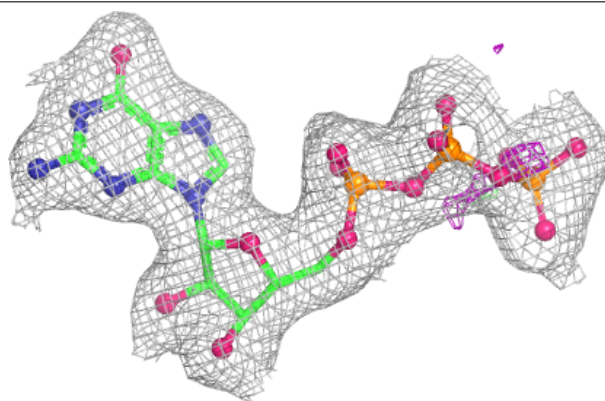


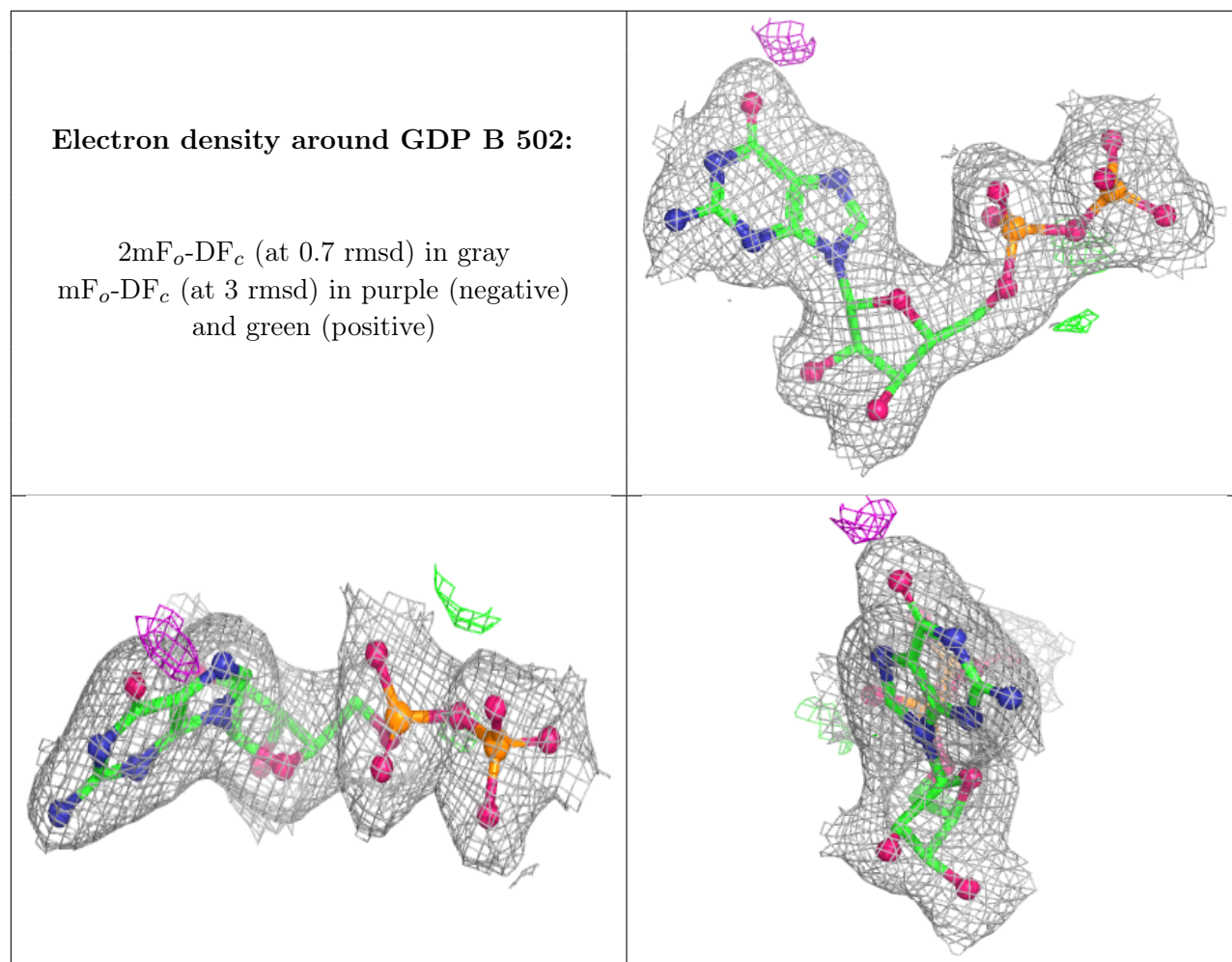
Electron density around GTP C 501:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.