



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 07:19 PM EST

PDB ID : 5S5M
Title : Tubulin-Z45527714-complex
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Deposited on : 2020-11-08
Resolution : 2.70 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

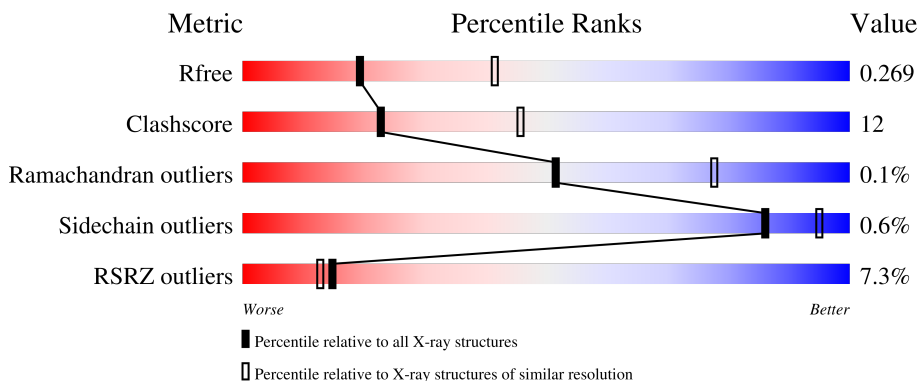
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	 8% 71% 27%
1	C	451	 3% 74% 23%
2	B	445	 5% 70% 25%
2	D	445	 8% 71% 26%
3	E	143	 12% 73% 13% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '9%', a large green segment labeled '66%', a yellow segment labeled '24%', and a grey segment on the right labeled '10%'.</p>

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 17744 atoms, of which 16 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
			Total	C	N	O	S			
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	Total	C	N	O	S	14	1	0
			3359	2109	577	646	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	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
			Total	C	N	O	S			
4	F	344	Total	C	N	O	S	0	0	0
			2826	1815	485	512	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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
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		

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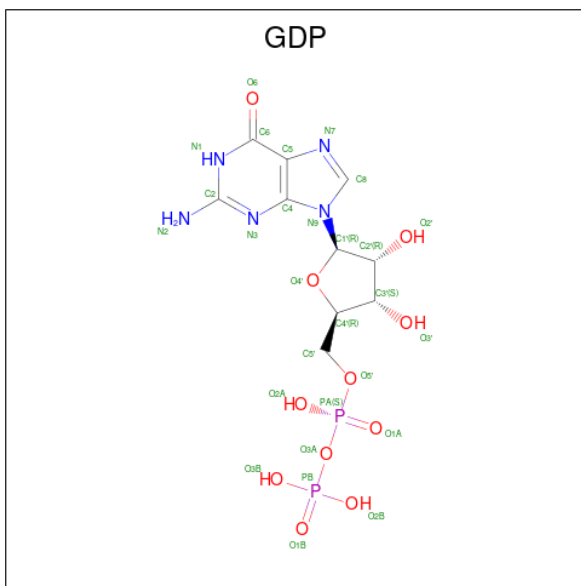
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



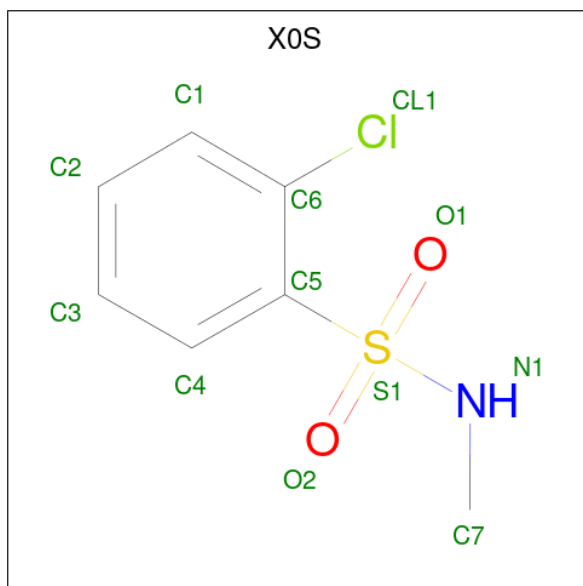
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



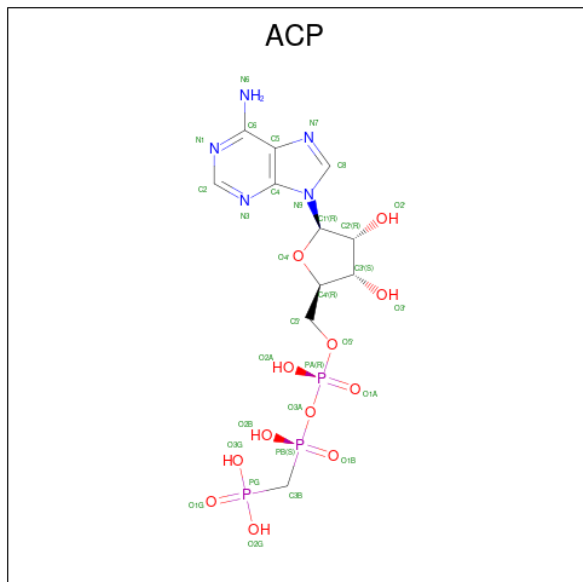
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is 2-chloro-N-methylbenzene-1-sulfonamide (three-letter code: X0S) (formula: $C_7H_8ClNO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	Cl	H	N	O			S
10	B	1	20	7	1	8	1	2	1	0	0
10	C	1	20	7	1	8	1	2	1	0	0

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



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

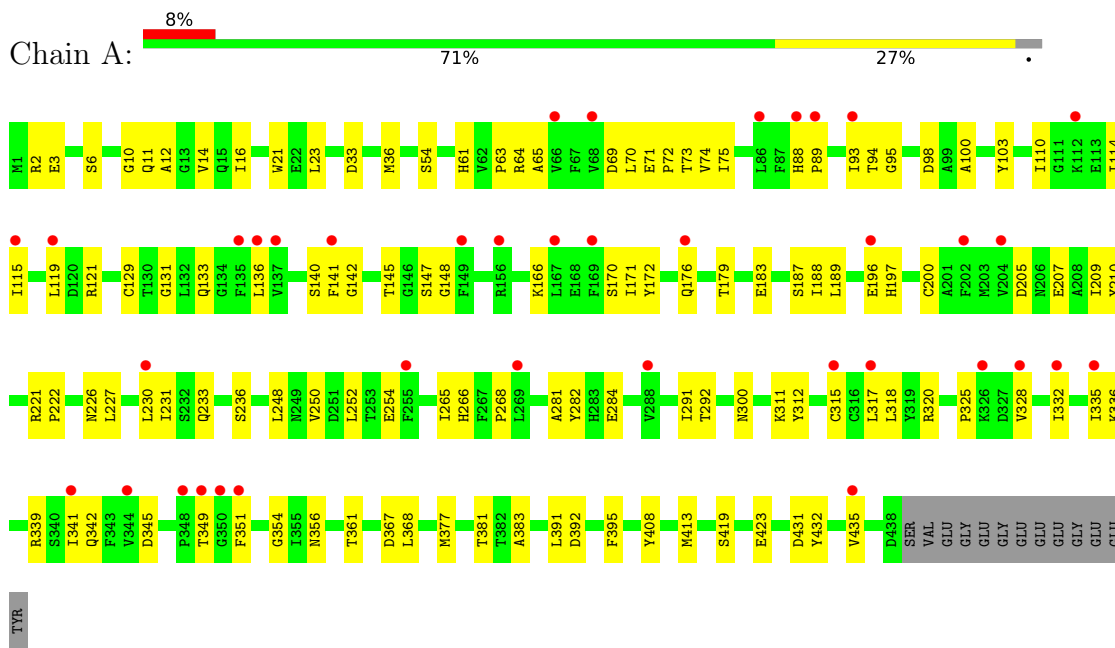
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	13	Total	O	0	0
			13	13		
12	B	25	Total	O	0	0
			25	25		
12	C	48	Total	O	0	0
			48	48		
12	D	9	Total	O	0	0
			9	9		
12	E	3	Total	O	0	0
			3	3		

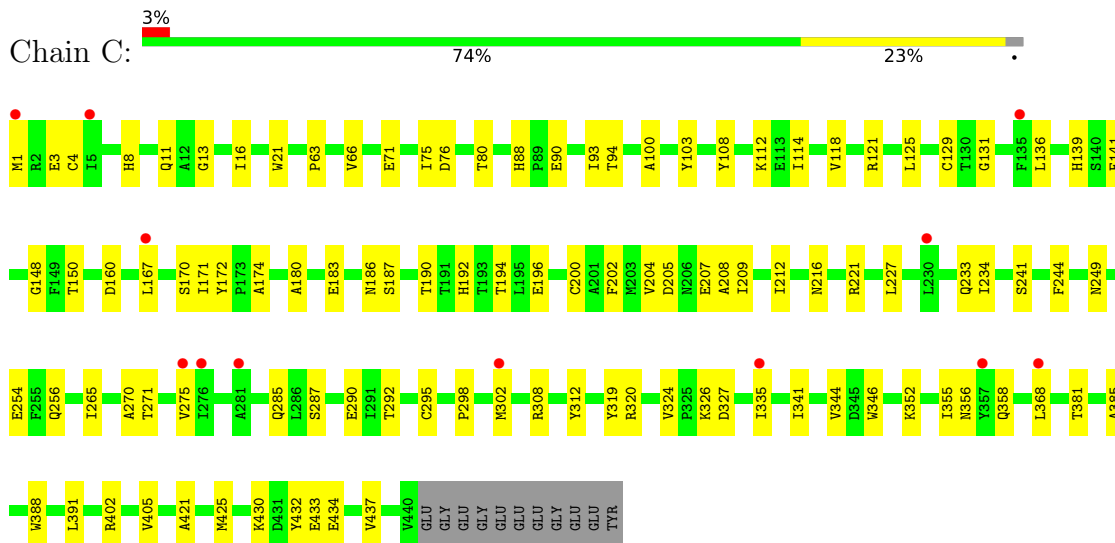
3 Residue-property plots

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.

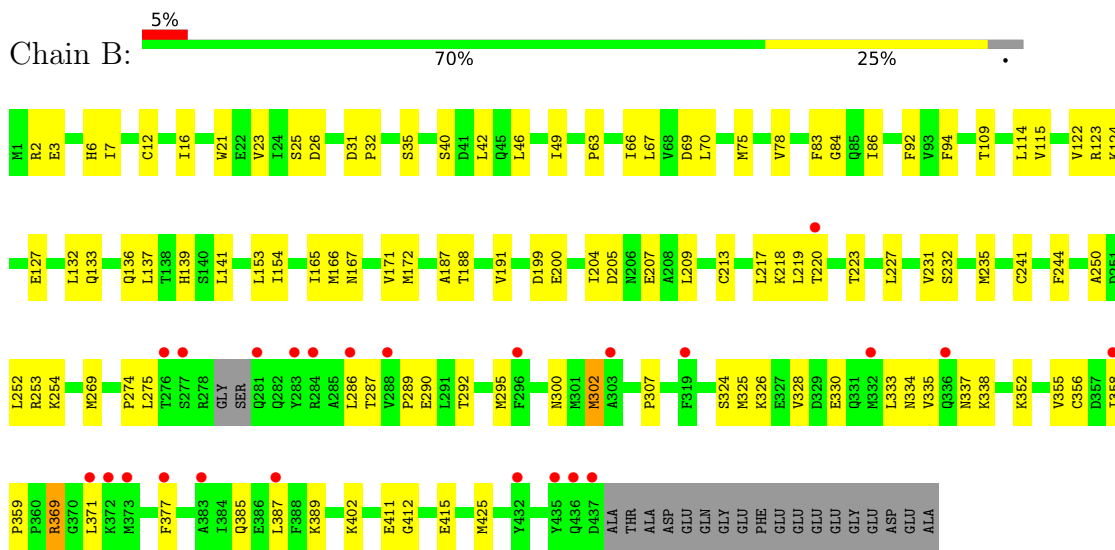
- Molecule 1: Tubulin alpha-1B chain



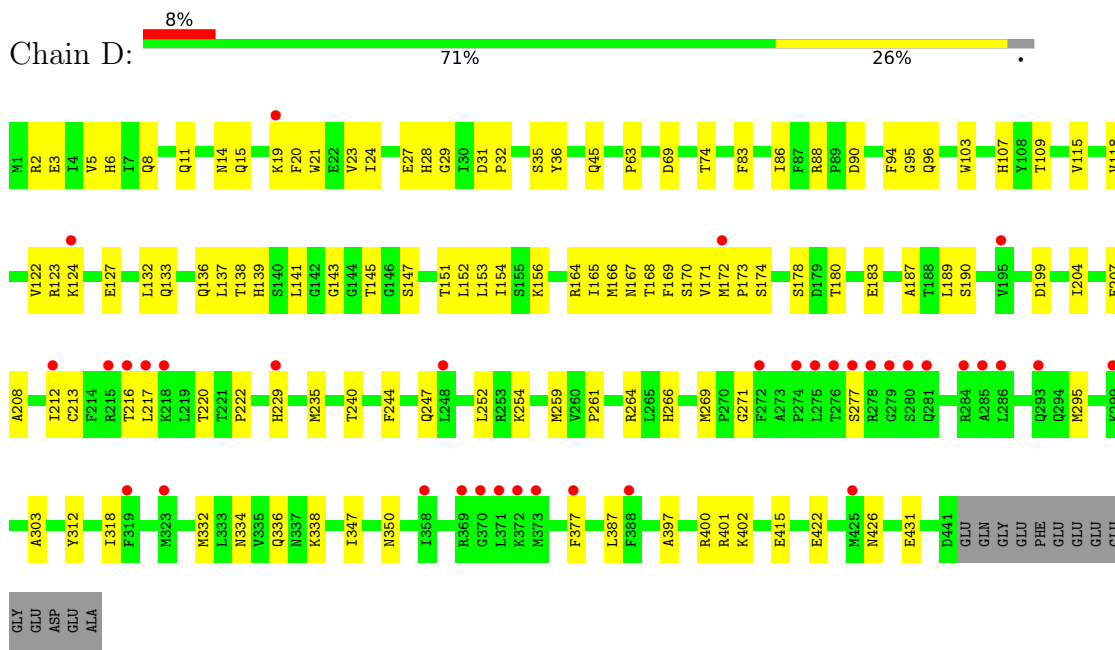
- Molecule 1: Tubulin alpha-1B chain



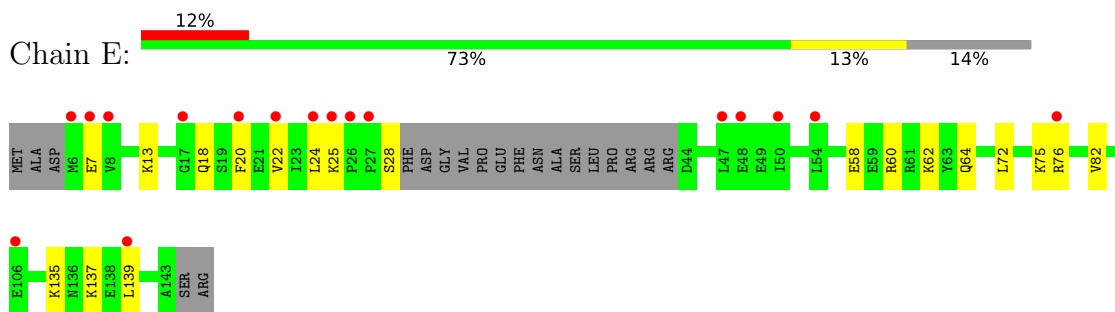
- Molecule 2: Tubulin beta-2B chain



• Molecule 2: Tubulin beta-2B chain

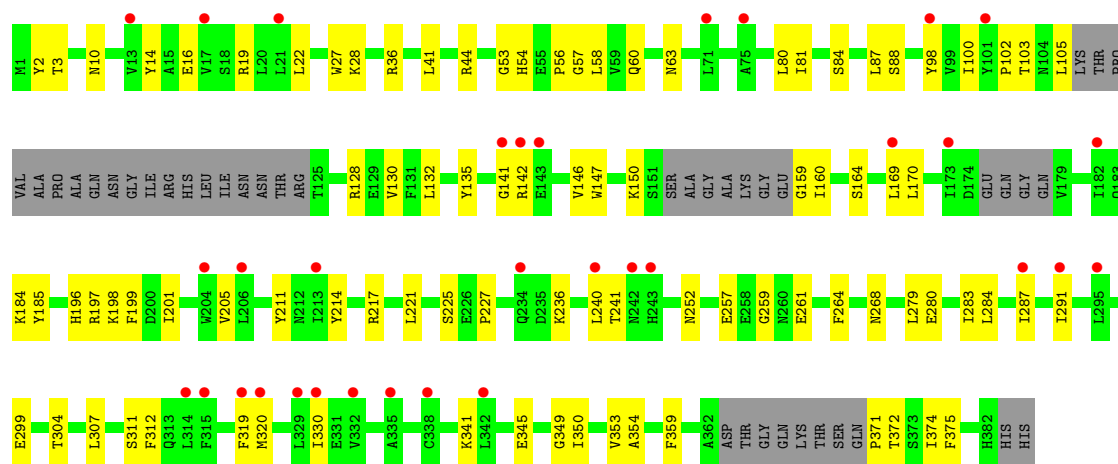


• Molecule 3: Stathmin-4



• 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	105.66Å 159.80Å 179.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.92 – 2.70 119.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (55.92-2.70) 99.3 (119.24-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.215 , 0.269 0.216 , 0.269	Depositor DCC
R_{free} test set	4079 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtrriage
Anisotropy	0.421	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, MG, CA, GTP, GDP, XOS, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/3502	0.41	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.26	0/3433	0.42	0/4647
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2892	0.39	0/3907
All	All	0.25	0/17812	0.41	0/24108

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	3424	0	3334	87	0
1	C	3443	0	3352	78	1
2	B	3359	0	3235	86	0
2	D	3368	0	3236	81	0
3	E	1014	0	1029	15	0
4	F	2826	0	2795	71	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	1	0
9	B	12	0	12	0	0
10	B	12	8	0	0	0
10	C	12	8	0	2	0
11	F	31	0	14	3	0
12	A	13	0	0	2	0
12	B	25	0	0	1	0
12	C	48	0	0	3	0
12	D	9	0	0	0	0
12	E	3	0	0	0	0
All	All	17728	16	17055	399	1

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 12.

All (399) 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)
1:C:136:LEU:HD22	1:C:167:LEU:HD22	1.48	0.92
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.53	0.89
1:C:200:CYS:HB2	1:C:256:GLN:HE22	1.37	0.88
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.39	0.88
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.62	0.82
2:B:136:GLN:HA	2:B:167:ASN:O	1.80	0.81
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.63	0.79
2:D:217:LEU:HA	2:D:277:SER:HB3	1.64	0.78
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.67	0.76
1:A:179:THR:HA	2:B:352:LYS:HD2	1.68	0.75
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.03	0.74
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.32	0.74
2:D:174:SER:OG	2:D:207:GLU:OE1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.73
1:A:381:THR:HG22	1:A:383:ALA:H	1.52	0.73
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.88	0.73
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.71	0.71
1:C:271:THR:HG21	1:C:295:CYS:O	1.89	0.71
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.71	0.71
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.72	0.71
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.73	0.70
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.26	0.70
2:B:220:THR:HG21	1:C:326:LYS:HE3	1.73	0.70
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.25	0.69
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.69
2:D:83:PHE:O	2:D:86:ILE:HG22	1.91	0.69
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.76	0.68
1:C:1:MET:N	12:C:601:HOH:O	2.25	0.68
1:C:76:ASP:O	1:C:80:THR:HG22	1.94	0.68
1:C:136:LEU:CD2	1:C:167:LEU:HD22	2.21	0.68
1:C:241:SER:HA	1:C:249:ASN:OD1	1.95	0.66
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.77	0.66
2:D:220:THR:O	2:D:222:PRO:HD3	1.96	0.65
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.78	0.65
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.32	0.65
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.22	0.65
2:D:152:LEU:O	2:D:156:LYS:HG2	1.97	0.64
1:A:166:LYS:HE2	1:A:197:HIS:O	1.98	0.64
2:B:69:ASP:O	2:B:94:PHE:HA	1.98	0.64
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.79	0.64
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.80	0.64
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.81	0.63
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.64	0.63
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.34	0.63
1:A:336:LYS:NZ	1:A:341:ILE:HB	2.14	0.62
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.81	0.62
2:B:209:LEU:HD21	2:B:302:MET:HG2	1.81	0.62
1:C:209:ILE:HD11	1:C:302:MET:CE	2.28	0.62
1:A:141:PHE:HB3	1:A:187:SER:OG	2.00	0.62
2:B:325:MET:HG3	2:B:355:VAL:HG21	1.80	0.62
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.81	0.62
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.82	0.62
2:B:167:ASN:OD1	2:B:200:GLU:HB2	1.99	0.61
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.30	0.61
1:C:256:GLN:HG2	10:C:504:XOS:C7	2.29	0.61
1:A:318:LEU:HD13	12:A:601:HOH:O	1.99	0.61
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.16	0.61
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.82	0.61
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.36	0.61
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.65	0.60
2:B:141:LEU:HD12	2:B:172:MET:SD	2.41	0.60
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.31	0.60
1:C:3:GLU:OE1	1:C:129:CYS:HB3	2.01	0.60
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.17	0.60
4:F:371:PRO:HA	4:F:372:THR:C	2.21	0.59
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.84	0.59
1:A:227:LEU:O	1:A:231:ILE:HG13	2.02	0.59
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.85	0.59
2:D:145:THR:HB	8:D:501:GDP:O2B	2.03	0.59
4:F:198:LYS:HG2	4:F:199:PHE:H	1.67	0.59
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.84	0.58
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.44	0.58
1:C:196:GLU:HG2	12:C:615:HOH:O	2.03	0.58
2:D:69:ASP:O	2:D:94:PHE:HA	2.04	0.58
2:B:218:LYS:O	2:B:219:LEU:HD23	2.04	0.58
1:A:311:LYS:HA	1:A:342:GLN:O	2.04	0.58
2:D:332:MET:O	2:D:336:GLN:HG3	2.03	0.58
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.39	0.57
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.18	0.57
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.34	0.57
4:F:371:PRO:HA	4:F:372:THR:HB	1.85	0.57
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.40	0.57
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.34	0.57
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.87	0.57
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.85	0.57
2:B:324:SER:O	2:B:328:VAL:HG23	2.05	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.87	0.56
2:B:231:VAL:O	2:B:235:MET:HG3	2.04	0.56
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.39	0.56
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.34	0.56
2:B:187:ALA:O	2:B:191:VAL:HG23	2.05	0.56
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.05	0.56
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:225:SER:O	4:F:252:ASN:HB2	2.05	0.56
2:D:212:ILE:O	2:D:216:THR:HB	2.05	0.56
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.88	0.55
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.89	0.55
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.89	0.55
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.89	0.55
4:F:371:PRO:CA	4:F:372:THR:HB	2.37	0.55
4:F:159:GLY:C	4:F:160:ILE:HD12	2.27	0.55
4:F:304:THR:HG21	4:F:311:SER:OG	2.07	0.55
2:B:209:LEU:CD2	2:B:302:MET:HG2	2.36	0.55
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.89	0.55
2:B:205:ASP:OD1	2:B:207:GLU:N	2.36	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.42	0.55
2:D:95:GLY:O	2:D:96:GLN:NE2	2.39	0.54
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.41	0.54
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.72	0.54
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.89	0.54
2:D:11:GLN:HA	2:D:74:THR:HG21	1.89	0.54
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.89	0.54
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.90	0.54
3:E:72:LEU:O	3:E:76:ARG:HG2	2.07	0.54
2:D:141:LEU:HA	2:D:147:SER:HB3	1.90	0.54
4:F:150:LYS:HD2	11:F:401:ACP:O2A	2.08	0.54
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.43	0.54
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.07	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
3:E:75:LYS:HD3	3:E:76:ARG:NH2	2.23	0.54
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.23	0.54
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.41	0.54
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.89	0.54
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.37	0.54
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.32	0.53
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.20	0.53
3:E:13:LYS:HG2	3:E:18:GLN:OE1	2.08	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.43	0.53
1:C:186:ASN:O	1:C:190:THR:HG22	2.07	0.53
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.90	0.53
1:A:328:VAL:O	1:A:332:ILE:HG13	2.09	0.53
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.91	0.53
4:F:320:MET:CG	4:F:330:ILE:HD11	2.38	0.53
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:MET:CG	2:B:377:PHE:HB2	2.39	0.52
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.43	0.52
1:A:419:SER:O	1:A:423:GLU:HG3	2.10	0.52
2:D:147:SER:HB2	2:D:190:SER:OG	2.08	0.52
1:A:70:LEU:HD22	1:A:110:ILE:CG2	2.39	0.52
2:B:223:THR:O	2:B:227:LEU:HD13	2.09	0.52
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.92	0.52
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.09	0.52
2:B:325:MET:HE2	2:B:355:VAL:HG11	1.89	0.52
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.92	0.52
1:A:315:CYS:HG	1:A:351:PHE:HD2	1.56	0.52
2:D:397:ALA:O	2:D:401:ARG:NH1	2.43	0.52
1:A:114:ILE:HG12	1:A:114:ILE:O	2.10	0.52
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.92	0.52
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.35	0.52
1:A:207:GLU:OE2	4:F:54:HIS:ND1	2.42	0.51
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.44	0.51
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.92	0.51
2:D:199:ASP:O	2:D:266:HIS:HB2	2.10	0.51
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.40	0.51
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.45	0.51
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.45	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.10	0.51
4:F:350:ILE:O	4:F:354:ALA:HB3	2.10	0.51
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.29	0.51
1:C:287:SER:OG	1:C:290:GLU:HG3	2.11	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.51
2:D:123:ARG:O	2:D:127:GLU:HG3	2.11	0.51
2:D:109:THR:HG21	3:E:137:LYS:HZ2	1.76	0.51
1:A:336:LYS:HZ3	1:A:341:ILE:HB	1.76	0.50
2:D:318:ILE:N	2:D:318:ILE:HD12	2.26	0.50
2:B:21:TRP:O	2:B:25:SER:OG	2.21	0.50
4:F:128:ARG:NH1	4:F:170:LEU:HD22	2.26	0.50
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.46	0.50
1:A:115:ILE:O	1:A:119:LEU:HG	2.12	0.50
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.42	0.50
2:B:333:LEU:O	2:B:337:ASN:ND2	2.44	0.50
3:E:60:ARG:O	3:E:64:GLN:HG3	2.12	0.50
1:C:216:ASN:HB3	1:C:275:VAL:O	2.12	0.50
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.47	0.50
1:A:100:ALA:CB	2:B:253[B]:ARG:HG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:HIS:HB3	1:C:13:GLY:O	2.11	0.50
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.94	0.49
2:D:8:GLN:HB3	2:D:138:THR:OG1	2.12	0.49
1:A:320:ARG:HA	1:A:356:ASN:O	2.12	0.49
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.42	0.49
2:D:11:GLN:O	2:D:15:GLN:HG2	2.12	0.49
1:A:10:GLY:O	1:A:14:VAL:HG23	2.13	0.49
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.45	0.49
4:F:63:ASN:HA	4:F:312:PHE:O	2.12	0.49
2:B:3:GLU:O	2:B:132:LEU:HD12	2.13	0.49
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.78	0.49
1:A:2:ARG:HB3	1:A:131:GLY:O	2.13	0.49
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.49
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.48	0.49
1:A:33:ASP:OD1	1:A:33:ASP:N	2.45	0.49
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.94	0.49
4:F:141:GLY:O	4:F:142:ARG:HB2	2.12	0.49
1:A:141:PHE:O	1:A:147:SER:HB3	2.13	0.49
1:A:200:CYS:HA	1:A:266:HIS:HB2	1.95	0.49
2:D:2:ARG:CB	2:D:133:GLN:HE21	2.24	0.49
2:B:46:LEU:HA	2:B:49:ILE:HB	1.94	0.49
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.48
2:B:412:GLY:C	3:E:82:VAL:HG13	2.34	0.48
1:A:291:ILE:HG13	1:A:292:THR:N	2.28	0.48
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.49	0.48
2:D:124:LYS:C	2:D:124:LYS:HD3	2.33	0.48
2:B:69:ASP:OD1	2:B:70:LEU:N	2.46	0.48
2:D:109:THR:HG21	3:E:137:LYS:NZ	2.28	0.48
1:A:408:TYR:HB3	1:A:413:MET:HE1	1.96	0.48
2:B:31:ASP:OD1	2:B:35:SER:N	2.38	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.48
3:E:7:GLU:O	3:E:22:VAL:HA	2.12	0.48
2:B:109:THR:HG21	2:B:411:GLU:OE1	2.14	0.48
1:C:234:ILE:HD12	1:C:234:ILE:N	2.28	0.48
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.44	0.48
2:B:42:LEU:H	2:B:42:LEU:HD12	1.78	0.48
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.14	0.48
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.39	0.48
2:B:67:LEU:N	2:B:67:LEU:HD12	2.29	0.48
1:C:11:GLN:HE22	2:D:247:GLN:HE22	1.61	0.48
4:F:80:LEU:HD12	4:F:84:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.49	0.47
4:F:349:GLY:O	4:F:353:VAL:HG22	2.13	0.47
1:C:114:ILE:O	1:C:118:VAL:HG23	2.14	0.47
1:A:284:GLU:CD	1:A:284:GLU:H	2.18	0.47
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.41	0.47
2:D:31:ASP:OD1	2:D:35:SER:N	2.47	0.47
4:F:259:GLY:O	4:F:261:GLU:HG3	2.15	0.47
4:F:371:PRO:HA	4:F:372:THR:O	2.14	0.47
1:A:431:ASP:O	1:A:435:VAL:HG23	2.14	0.47
1:A:70:LEU:HD12	1:A:145:THR:OG1	2.14	0.47
1:A:6:SER:O	1:A:65:ALA:HA	2.14	0.47
1:A:70:LEU:HD22	1:A:110:ILE:HG21	1.95	0.47
2:D:180:THR:O	2:D:183:GLU:HG3	2.15	0.47
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.44	0.47
1:C:270:ALA:O	1:C:302:MET:HG2	2.14	0.47
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.50	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
1:C:192:HIS:CG	1:C:421:ALA:HA	2.49	0.47
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.30	0.47
2:B:40:SER:OG	2:B:42:LEU:HD13	2.14	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.96	0.47
2:D:32:PRO:HA	2:D:83:PHE:CD2	2.50	0.47
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.97	0.47
4:F:198:LYS:HG2	4:F:199:PHE:N	2.29	0.47
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.45	0.47
2:D:143:GLY:O	2:D:147:SER:OG	2.33	0.46
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.46	0.46
2:D:240:THR:HG23	2:D:244:PHE:HD2	1.81	0.46
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.51	0.46
1:C:75:ILE:HB	1:C:94:THR:HG21	1.98	0.46
2:D:5:VAL:HG23	2:D:132:LEU:CD1	2.45	0.46
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.97	0.46
2:B:359:PRO:HB2	2:B:371:LEU:O	2.14	0.46
1:A:12:ALA:HB2	5:A:501:GTP:C8	2.50	0.46
2:B:275:LEU:HD12	2:B:300:ASN:ND2	2.31	0.46
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.98	0.46
2:D:259:MET:O	2:D:261:PRO:HD3	2.16	0.46
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.50	0.46
1:A:136:LEU:HD21	1:A:252:LEU:HD21	1.97	0.46
1:C:75:ILE:HB	1:C:94:THR:CG2	2.46	0.46
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:THR:HG23	2:B:425:MET:HE2	1.97	0.45
2:D:107:HIS:O	2:D:152:LEU:HD22	2.16	0.45
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.48	0.45
2:B:114:LEU:O	2:B:114:LEU:HG	2.16	0.45
1:A:103:TYR:CD1	1:A:189:LEU:HD13	2.51	0.45
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.52	0.45
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.51	0.45
1:A:320:ARG:HD2	12:A:609:HOH:O	2.17	0.45
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.46	0.45
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.97	0.45
1:A:336:LYS:HZ2	1:A:341:ILE:HB	1.81	0.45
2:B:165:ILE:HA	2:B:199:ASP:OD2	2.17	0.45
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.99	0.45
1:C:167:LEU:C	1:C:167:LEU:HD23	2.37	0.45
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.52	0.45
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.32	0.44
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.99	0.44
1:C:108:TYR:O	1:C:112:LYS:HG2	2.18	0.44
2:B:124:LYS:HD3	2:B:124:LYS:C	2.37	0.44
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.98	0.44
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.99	0.44
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.99	0.44
1:A:248:LEU:HD23	1:A:354:GLY:HA3	1.99	0.44
2:D:23:VAL:O	2:D:27:GLU:HG3	2.18	0.44
2:B:241:CYS:HB3	2:B:250:ALA:HB3	1.99	0.44
2:B:287:THR:HB	2:B:289:PRO:HD2	2.00	0.44
3:E:135:LYS:O	3:E:139:LEU:HG	2.17	0.44
1:A:315:CYS:SG	1:A:351:PHE:HD2	2.41	0.44
1:C:136:LEU:HD23	1:C:167:LEU:HB3	1.99	0.44
4:F:87:LEU:O	4:F:88:SER:OG	2.19	0.44
1:A:187:SER:CB	1:A:391:LEU:HD21	2.48	0.44
2:D:180:THR:HB	2:D:183:GLU:HG3	1.99	0.44
4:F:98:TYR:CE1	4:F:130:VAL:HG12	2.53	0.44
4:F:196:HIS:O	4:F:227:PRO:HA	2.18	0.44
1:A:3:GLU:OE1	1:A:129:CYS:HB3	2.18	0.44
1:A:179:THR:O	2:B:352:LYS:HG3	2.18	0.44
2:B:326:LYS:O	2:B:330:GLU:HG3	2.18	0.44
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.32	0.43
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.99	0.43
2:D:271:GLY:HA3	2:D:377:PHE:HB3	1.99	0.43
1:A:266:HIS:O	1:A:268:PRO:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ALA:HB3	1:C:302:MET:CG	2.47	0.43
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.53	0.43
2:B:334:ASN:O	2:B:338:LYS:HG3	2.18	0.43
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.83	0.43
1:C:167:LEU:HD11	1:C:202:PHE:HE2	1.83	0.43
1:C:265:ILE:HG23	1:C:432:TYR:CZ	2.53	0.43
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.00	0.43
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.20	0.43
2:B:292:THR:HG22	2:B:335:VAL:HG21	2.00	0.43
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.01	0.43
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.54	0.43
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.01	0.43
2:D:3:GLU:O	2:D:132:LEU:HD12	2.18	0.43
2:D:220:THR:C	2:D:222:PRO:HD3	2.38	0.43
4:F:240:LEU:HD12	4:F:240:LEU:N	2.34	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.53	0.43
4:F:184:LYS:NZ	4:F:185:TYR:O	2.51	0.43
1:A:71:GLU:HG2	1:A:73:THR:H	1.83	0.43
1:C:433:GLU:O	1:C:437:VAL:HG23	2.18	0.43
4:F:211:TYR:CE2	4:F:299:GLU:HB2	2.54	0.43
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.48	0.43
2:B:7:ILE:O	2:B:137:LEU:HA	2.19	0.43
1:C:204:VAL:HG13	1:C:302:MET:HE3	2.01	0.43
1:A:176:GLN:HG3	4:F:56:PRO:HG3	2.01	0.42
4:F:22:LEU:HD23	4:F:27:TRP:O	2.19	0.42
1:A:69:ASP:O	1:A:94:THR:HA	2.19	0.42
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.49	0.42
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.49	0.42
2:B:371:LEU:HD23	2:B:371:LEU:HA	1.88	0.42
1:A:349:THR:HB	3:E:25:LYS:HB3	2.00	0.42
1:C:174:ALA:HB2	1:C:207:GLU:H	1.84	0.42
2:D:178:SER:HB3	2:D:183:GLU:OE2	2.19	0.42
4:F:19:ARG:HD2	4:F:19:ARG:C	2.39	0.42
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.54	0.42
2:B:69:ASP:OD1	12:B:601:HOH:O	2.22	0.42
2:B:123:ARG:O	2:B:127:GLU:HG3	2.19	0.42
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.00	0.42
2:B:295:MET:HG3	2:B:377:PHE:HB2	2.01	0.42
1:C:208:ALA:O	1:C:212:ILE:HG13	2.19	0.42
2:D:147:SER:O	2:D:151:THR:HG23	2.20	0.42
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:THR:HA	4:F:28:LYS:O	2.18	0.42
1:A:317:LEU:CD2	1:A:377:MET:HG3	2.50	0.42
2:B:78:VAL:O	2:B:84:GLY:HA3	2.19	0.42
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.54	0.42
2:D:312:TYR:HE1	2:D:377:PHE:HZ	1.67	0.42
2:D:115:VAL:HG23	2:D:153:LEU:HD23	2.02	0.42
3:E:22:VAL:HG13	3:E:22:VAL:O	2.19	0.42
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.50	0.42
2:B:355:VAL:HG12	2:B:356:CYS:N	2.35	0.42
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.50	0.41
1:C:71:GLU:HG2	12:C:620:HOH:O	2.20	0.41
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.02	0.41
4:F:225:SER:HB2	4:F:252:ASN:O	2.20	0.41
4:F:372:THR:O	4:F:372:THR:HG22	2.19	0.41
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.20	0.41
2:D:28:HIS:HA	2:D:45:GLN:HB3	2.02	0.41
2:D:132:LEU:O	2:D:164:ARG:HD3	2.20	0.41
4:F:341:LYS:HG2	4:F:341:LYS:O	2.21	0.41
4:F:198:LYS:O	4:F:199:PHE:HB3	2.20	0.41
2:B:2:ARG:HB2	2:B:133:GLN:HG3	2.03	0.41
2:B:75:MET:CE	2:B:92:PHE:HB3	2.51	0.41
2:B:115:VAL:HG23	2:B:153:LEU:HD23	2.02	0.41
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.21	0.41
1:C:425:MET:HE3	1:C:425:MET:HB3	1.89	0.41
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.19	0.41
4:F:146:VAL:HG22	4:F:164:SER:HB3	2.01	0.41
2:D:295:MET:HB2	2:D:295:MET:HE3	1.81	0.41
1:C:402:ARG:HA	1:C:405:VAL:HG21	2.01	0.41
10:C:504:XOS:O1	10:C:504:XOS:CL1	2.76	0.41
2:B:387:LEU:HD23	2:B:387:LEU:C	2.41	0.41
1:C:194:THR:O	1:C:194:THR:HG22	2.20	0.41
4:F:53:GLY:N	4:F:60:GLN:OE1	2.43	0.41
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.20	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.03	0.41
1:A:72:PRO:HD3	1:A:95:GLY:O	2.21	0.41
1:A:312:TYR:CE2	1:A:341:ILE:HG23	2.56	0.41
2:D:29:GLY:O	2:D:36:TYR:HA	2.21	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.03	0.41
4:F:160:ILE:HD12	4:F:160:ILE:N	2.36	0.41
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.50	0.41
2:D:208:ALA:O	2:D:212:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:264:PHE:O	4:F:268:ASN:HB2	2.20	0.41
1:A:54:SER:O	1:A:61:HIS:HA	2.21	0.40
2:B:171:VAL:HA	2:B:204:ILE:O	2.21	0.40
2:B:220:THR:HG21	1:C:326:LYS:CE	2.45	0.40
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.56	0.40
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.02	0.40
2:D:173:PRO:HG3	2:D:187:ALA:HB2	2.03	0.40
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.21	0.40
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.03	0.40
2:D:118:VAL:O	2:D:122:VAL:HG23	2.21	0.40
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.04	0.40
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.37	0.40
4:F:199:PHE:CE1	4:F:221:LEU:HD23	2.56	0.40
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.87	0.40
2:D:2:ARG:HB3	2:D:133:GLN:HG2	2.03	0.40
2:D:387:LEU:C	2:D:387:LEU:HD23	2.42	0.40
4:F:307:LEU:HD12	4:F:307:LEU:HA	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ASP:O	1:C:285:GLN:NE2[4_555]	2.12	0.08

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	436/451 (97%)	420 (96%)	14 (3%)	2 (0%)	29	54
1	C	439/451 (97%)	426 (97%)	13 (3%)	0	100	100
2	B	422/445 (95%)	399 (94%)	23 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	429/445 (96%)	414 (96%)	15 (4%)	0	100	100
3	E	119/143 (83%)	116 (98%)	3 (2%)	0	100	100
4	F	334/384 (87%)	314 (94%)	20 (6%)	0	100	100
All	All	2179/2319 (94%)	2089 (96%)	88 (4%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA
1	A	98	ASP

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	369/379 (97%)	365 (99%)	4 (1%)	73	90
1	C	372/379 (98%)	370 (100%)	2 (0%)	88	96
2	B	368/383 (96%)	365 (99%)	3 (1%)	81	93
2	D	368/383 (96%)	366 (100%)	2 (0%)	88	96
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	311/342 (91%)	311 (100%)	0	100	100
All	All	1898/1993 (95%)	1887 (99%)	11 (1%)	86	95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
1	A	282	TYR
1	A	300	ASN
1	A	361	THR
2	B	139	HIS
2	B	302	MET

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Mol	Chain	Res	Type
2	B	369	ARG
1	C	221	ARG
1	C	381	THR
2	D	139	HIS
2	D	229	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	133	GLN
2	B	15	GLN
2	B	294	GLN
2	B	300	ASN
1	C	11	GLN
1	C	15	GLN
1	C	85	GLN
1	C	256	GLN
1	C	372	GLN
2	D	247	GLN
2	D	294	GLN
4	F	229	ASN
4	F	269	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MES	B	504	-	12,12,12	2.20	1 (8%)	14,16,16	1.99	6 (42%)
11	ACP	F	401	6	27,33,33	1.37	5 (18%)	32,52,52	1.55	4 (12%)
10	XOS	C	504	-	11,12,12	0.30	0	16,17,17	0.41	0
5	GTP	C	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.43	6 (18%)
10	XOS	B	505	-	11,12,12	0.28	0	16,17,17	0.45	0
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.42	5 (15%)
8	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.27	4 (13%)
8	GDP	B	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.20	3 (10%)

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	MES	B	504	-	-	4/6/14/14	0/1/1/1
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
10	XOS	C	504	-	-	7/9/9/9	0/1/1/1
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
10	XOS	B	505	-	-	4/9/9/9	0/1/1/1
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.31	1.67	1.77
5	C	501	GTP	C5-C6	-4.07	1.39	1.47
5	A	501	GTP	C5-C6	-3.82	1.39	1.47
11	F	401	ACP	PG-O3G	2.92	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PG-O2G	2.91	1.61	1.54
11	F	401	ACP	C5-C4	2.54	1.47	1.40
11	F	401	ACP	PB-O3A	2.50	1.61	1.58
8	B	501	GDP	C6-N1	-2.39	1.34	1.37
8	D	501	GDP	C6-N1	-2.35	1.34	1.37
11	F	401	ACP	PB-O2B	2.20	1.61	1.56
5	C	501	GTP	C2-N3	2.12	1.38	1.33
5	A	501	GTP	C2-N3	2.07	1.38	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-4.78	117.40	132.56
9	B	504	MES	C5-N4-C3	3.68	117.11	108.83
8	D	501	GDP	PA-O3A-PB	-3.55	120.66	132.83
11	F	401	ACP	C3'-C2'-C1'	3.52	106.28	100.98
5	C	501	GTP	PA-O3A-PB	-3.52	120.76	132.83
5	A	501	GTP	C8-N7-C5	3.15	109.00	102.99
9	B	504	MES	C6-C5-N4	-3.14	105.34	110.10
11	F	401	ACP	N3-C2-N1	-3.06	123.90	128.68
5	A	501	GTP	PA-O3A-PB	-3.05	122.35	132.83
5	A	501	GTP	C5-C6-N1	3.04	119.33	113.95
5	C	501	GTP	C5-C6-N1	2.96	119.18	113.95
5	C	501	GTP	C8-N7-C5	2.93	108.58	102.99
8	B	501	GDP	PA-O3A-PB	-2.82	123.15	132.83
5	A	501	GTP	C2-N1-C6	-2.75	120.03	125.10
5	C	501	GTP	C2-N1-C6	-2.71	120.10	125.10
5	A	501	GTP	PB-O3B-PG	-2.66	123.69	132.83
9	B	504	MES	O2S-S-C8	2.66	110.12	106.92
11	F	401	ACP	C4-C5-N7	-2.66	106.63	109.40
8	D	501	GDP	C3'-C2'-C1'	2.63	104.94	100.98
9	B	504	MES	O1S-S-C8	2.57	110.01	106.92
8	B	501	GDP	C8-N7-C5	2.53	107.82	102.99
8	D	501	GDP	C8-N7-C5	2.37	107.50	102.99
8	B	501	GDP	C5-C6-N1	2.33	118.06	113.95
5	C	501	GTP	O6-C6-C5	-2.28	119.92	124.37
8	D	501	GDP	C5-C6-N1	2.20	117.83	113.95
9	B	504	MES	C7-N4-C5	2.19	116.84	111.23
9	B	504	MES	O3S-S-C8	2.16	109.26	105.77
5	C	501	GTP	PB-O3B-PG	-2.16	125.43	132.83

There are no chirality outliers.

All (46) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
10	B	505	XOS	C6-C5-S1-N1
10	B	505	XOS	C6-C5-S1-O2
10	C	504	XOS	C6-C5-S1-N1
10	C	504	XOS	C6-C5-S1-O2
10	C	504	XOS	C7-N1-S1-C5
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
10	C	504	XOS	C4-C5-S1-O2
10	B	505	XOS	C4-C5-S1-N1
10	C	504	XOS	C4-C5-S1-N1
10	B	505	XOS	C4-C5-S1-O2
10	C	504	XOS	C6-C5-S1-O1
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	PG-C3B-PB-O3A
5	A	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
10	C	504	XOS	C7-N1-S1-O1
8	D	501	GDP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A

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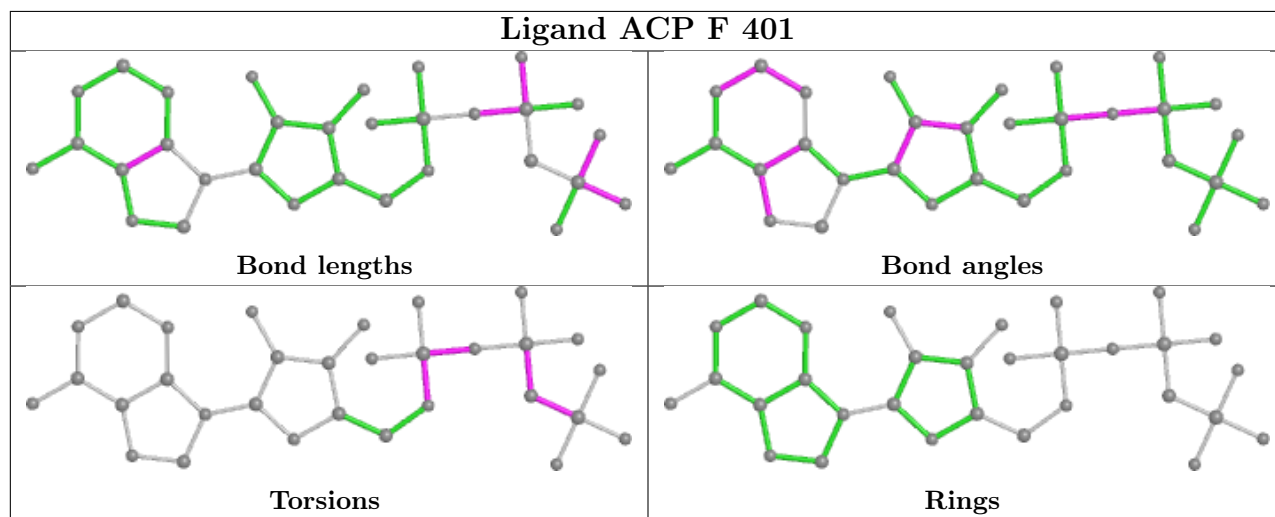
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A

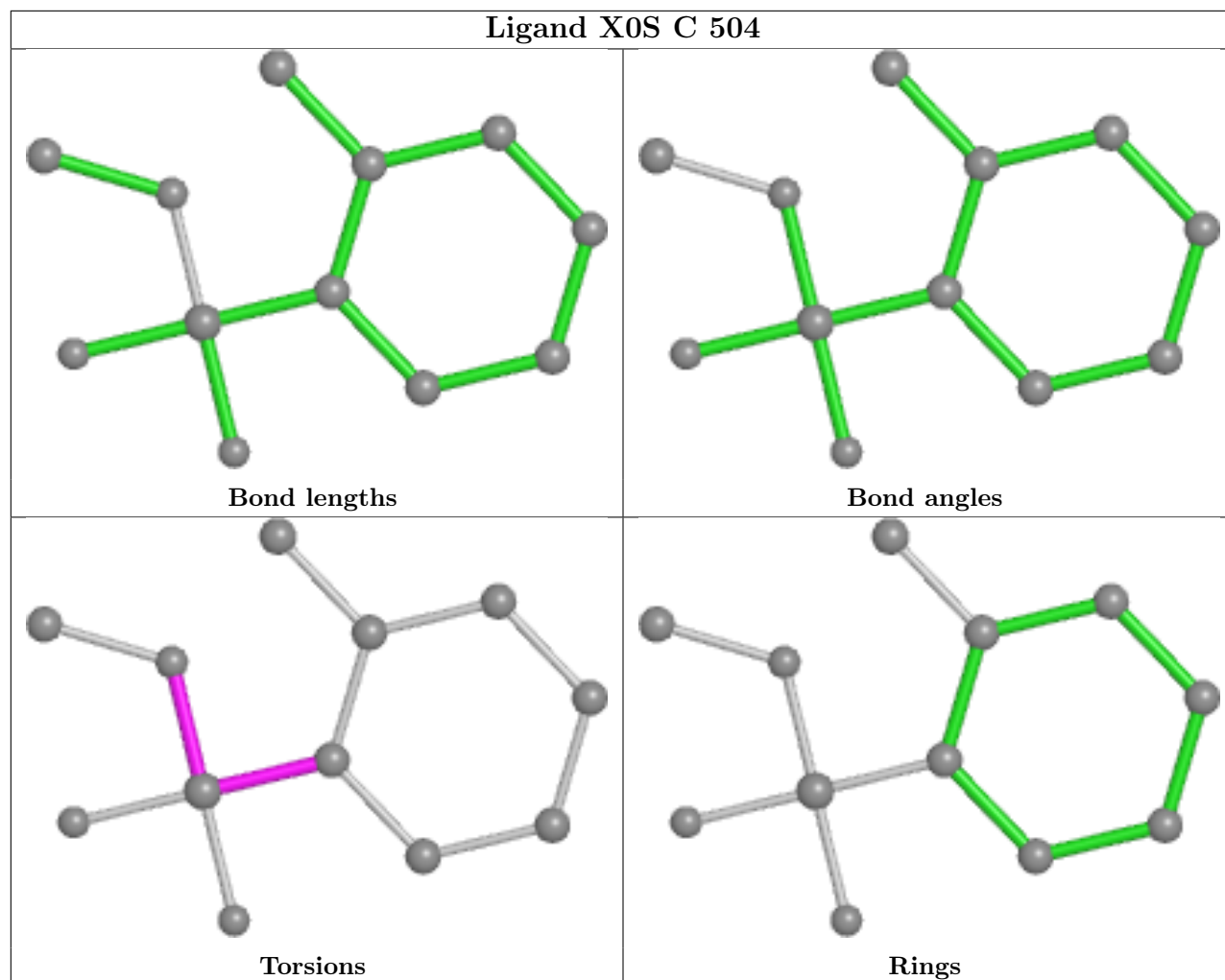
There are no ring outliers.

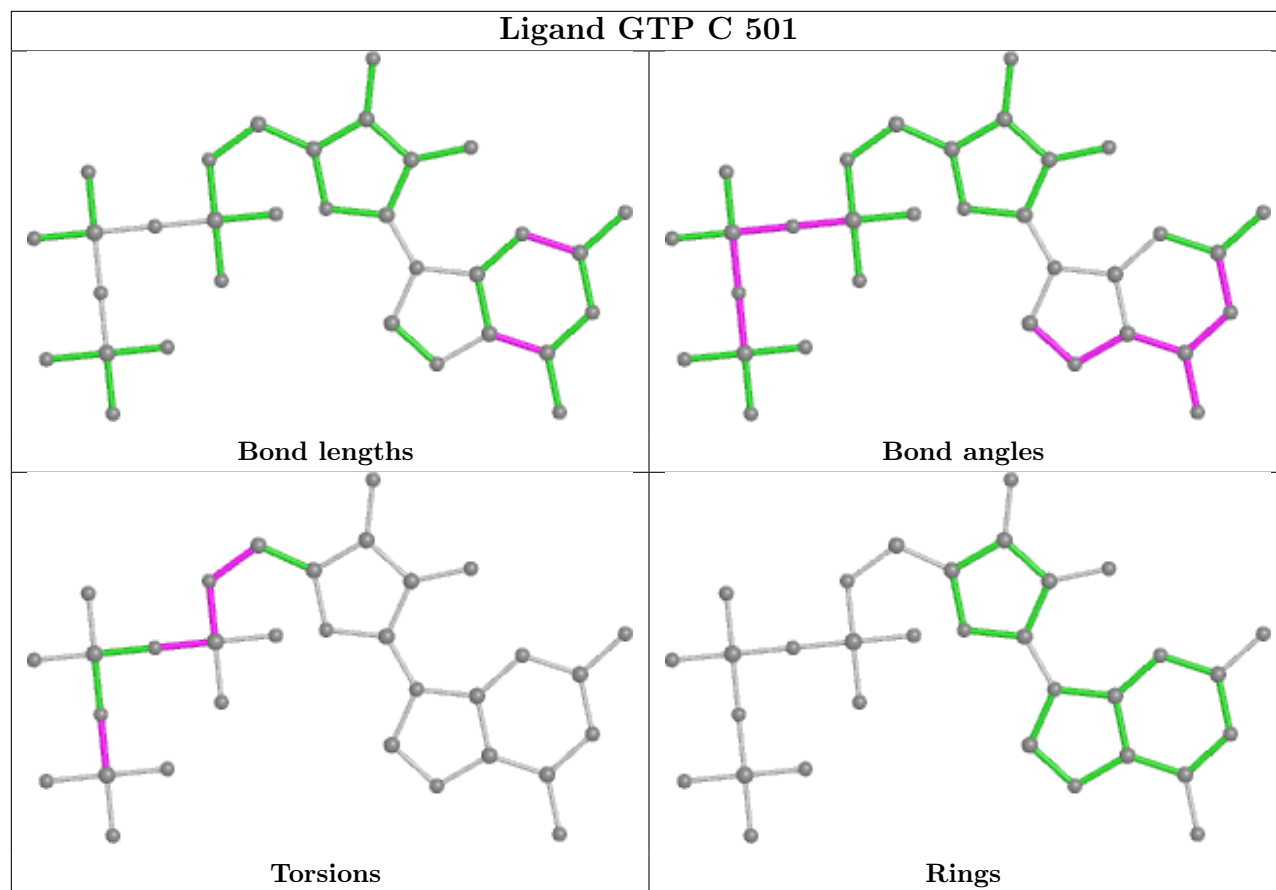
5 monomers are involved in 8 short contacts:

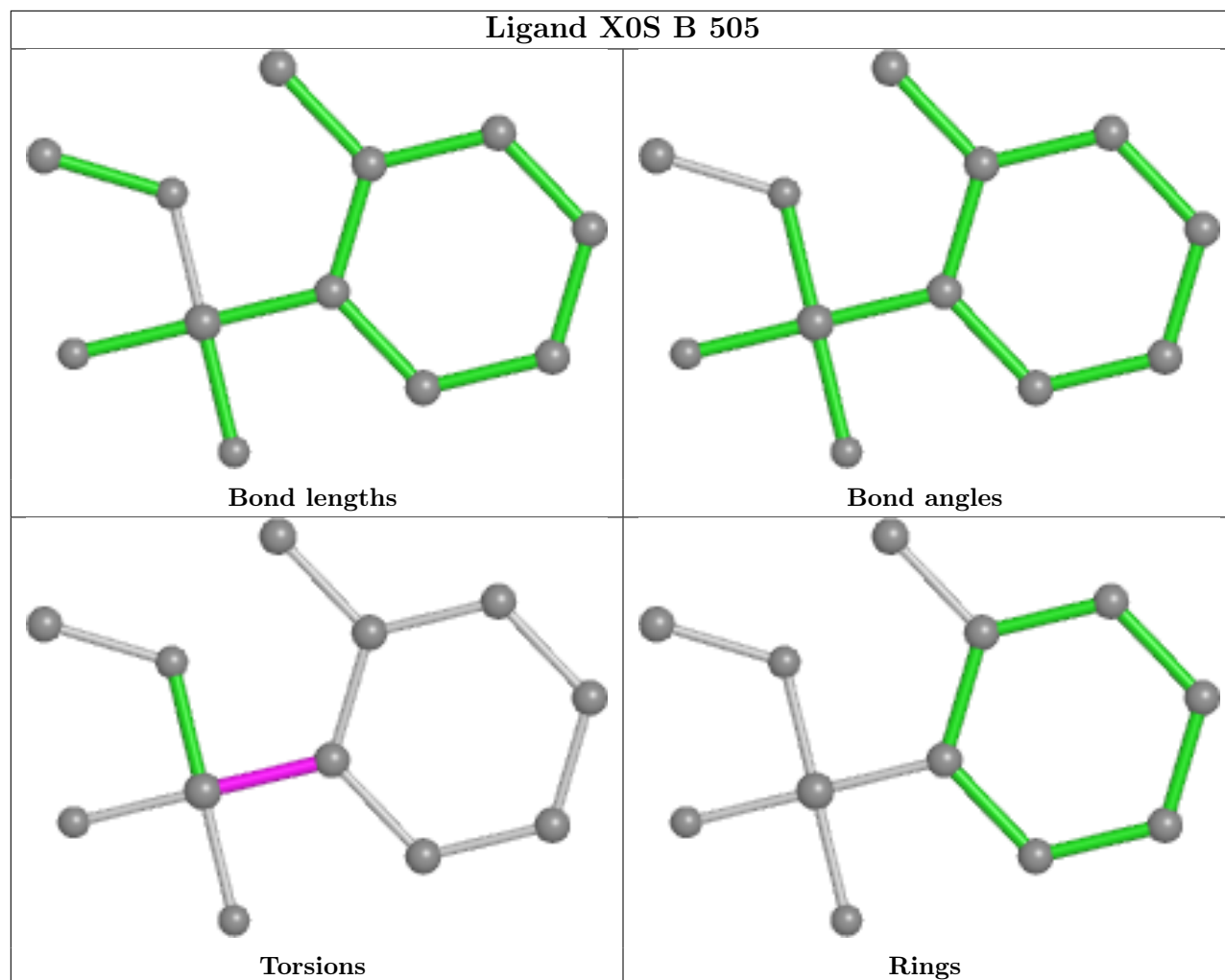
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	3	0
10	C	504	X0S	2	0
5	A	501	GTP	1	0
8	D	501	GDP	1	0
8	B	501	GDP	1	0

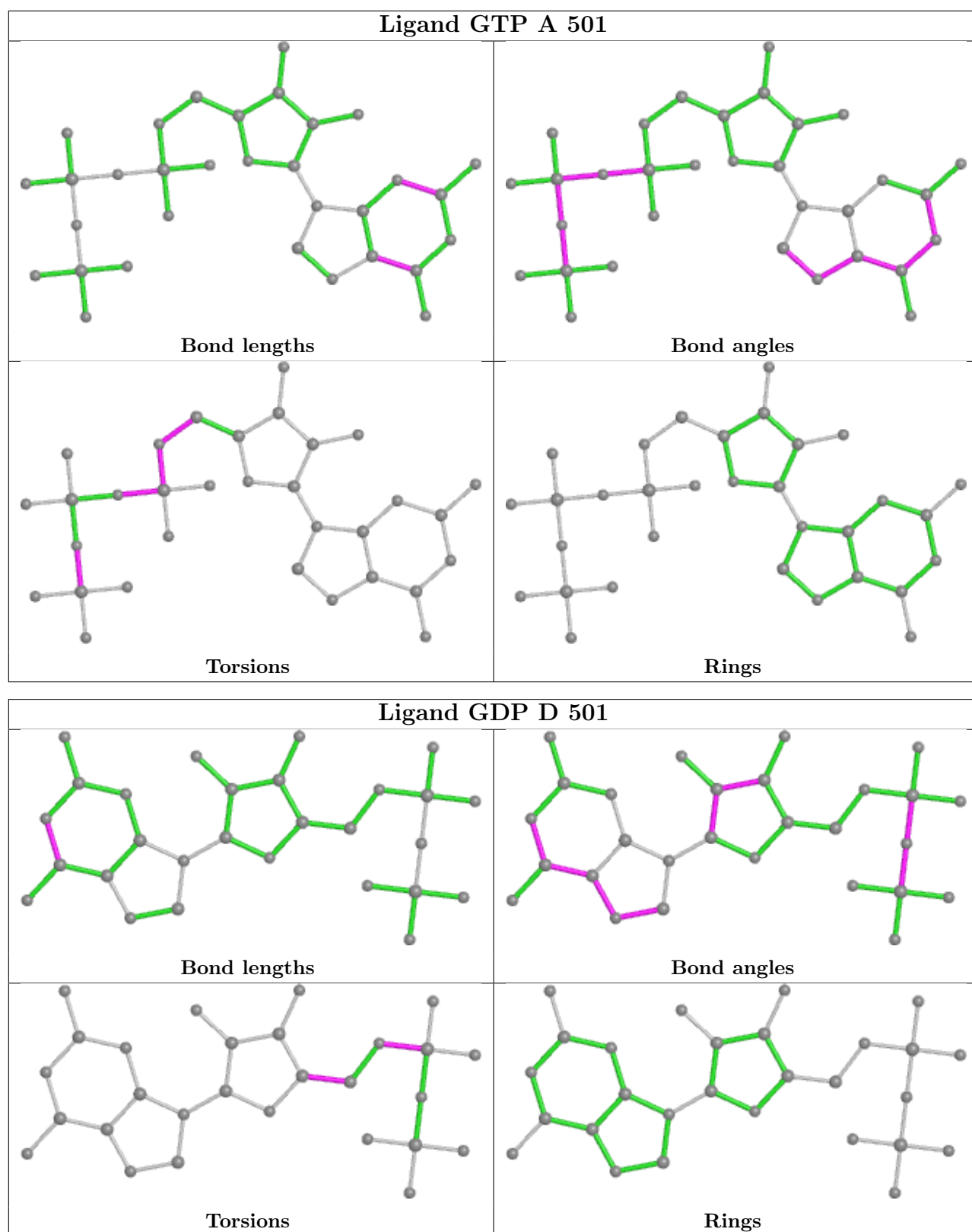
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

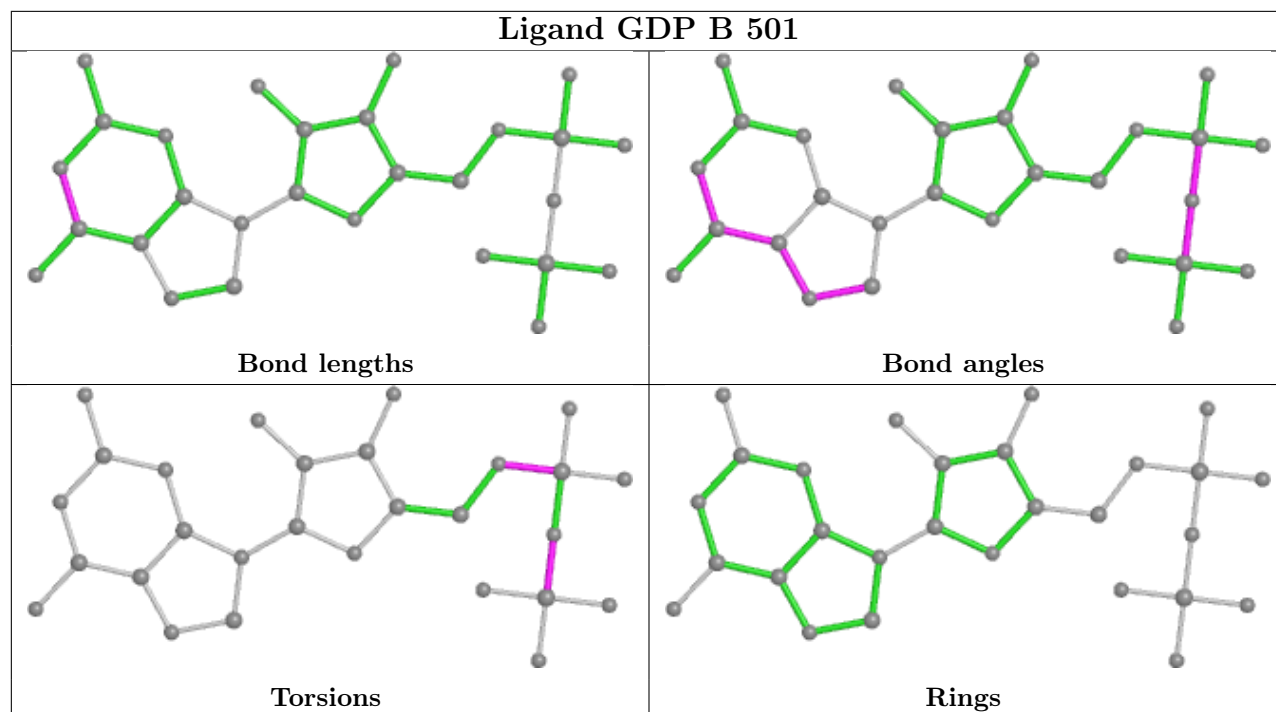












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.57	38 (8%) 10 8	70, 92, 138, 220	0
1	C	440/451 (97%)	0.42	12 (2%) 54 55	61, 77, 113, 146	0
2	B	425/445 (95%)	0.55	24 (5%) 24 23	61, 86, 143, 195	3 (0%)
2	D	431/445 (96%)	0.56	36 (8%) 11 9	77, 104, 153, 195	5 (1%)
3	E	123/143 (86%)	0.82	17 (13%) 2 2	78, 113, 168, 199	0
4	F	344/384 (89%)	0.64	33 (9%) 8 6	90, 130, 198, 225	0
All	All	2201/2319 (94%)	0.56	160 (7%) 15 13	61, 97, 162, 225	8 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	7.3
3	E	24	LEU	6.8
4	F	240	LEU	6.8
2	D	276	THR	6.8
2	D	284	ARG	6.1
2	D	217	LEU	5.8
2	D	277	SER	5.6
1	A	351	PHE	5.5
3	E	22	VAL	5.3
3	E	6	MET	5.1
3	E	25	LYS	5.0
3	E	26	PRO	4.7
2	D	299	LYS	4.6
2	B	283	TYR	4.6
4	F	315	PHE	4.4
2	B	281	GLN	4.4
2	D	275	LEU	4.4
4	F	314	LEU	4.3
2	D	371	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	279	GLY	4.2
2	D	215	ARG	4.1
2	D	218	LYS	4.0
2	D	285	ALA	3.9
2	D	280	SER	3.8
3	E	27	PRO	3.8
4	F	320	MET	3.8
4	F	330	ILE	3.7
4	F	71	LEU	3.7
3	E	50	ILE	3.7
2	B	276	THR	3.6
4	F	319	PHE	3.6
1	A	326	LYS	3.6
2	D	323	MET	3.5
4	F	243	HIS	3.5
2	D	278	ARG	3.5
2	B	286	LEU	3.4
3	E	7	GLU	3.4
1	C	368	LEU	3.3
2	D	274	PRO	3.3
2	D	216	THR	3.3
1	A	66	VAL	3.2
1	A	317	LEU	3.2
2	D	286	LEU	3.2
2	D	272	PHE	3.2
2	D	248	LEU	3.1
4	F	234	GLN	3.1
1	C	1	MET	3.1
1	A	341	ILE	3.0
4	F	206	LEU	3.0
1	A	350	GLY	3.0
2	D	229	HIS	3.0
2	D	370	GLY	3.0
2	D	372	LYS	2.9
4	F	291	ILE	2.9
2	B	332	MET	2.9
2	D	281	GLN	2.9
1	C	302	MET	2.9
4	F	13	VAL	2.9
1	A	115	ILE	2.9
1	C	276	ILE	2.9
1	A	136	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	213	ILE	2.9
1	A	348	PRO	2.8
3	E	47	LEU	2.8
2	D	195	VAL	2.8
1	A	349	THR	2.8
1	A	86	LEU	2.8
4	F	173	ILE	2.8
2	D	369	ARG	2.8
4	F	332	VAL	2.7
2	B	284	ARG	2.7
4	F	141	GLY	2.7
4	F	182	ILE	2.7
4	F	17	VAL	2.7
3	E	76	ARG	2.7
1	A	344	VAL	2.7
1	A	328	VAL	2.6
3	E	8	VAL	2.6
4	F	287	ILE	2.6
4	F	338	CYS	2.6
4	F	169	LEU	2.6
2	D	319	PHE	2.6
2	B	288	VAL	2.6
4	F	295	LEU	2.6
1	A	169	PHE	2.6
2	B	432	TYR	2.5
4	F	98	TYR	2.5
2	B	373	MET	2.5
2	D	293	GLN	2.4
3	E	54	LEU	2.4
2	B	319	PHE	2.4
1	A	335	ILE	2.4
1	A	149	PHE	2.4
1	A	332	ILE	2.4
1	A	88	HIS	2.4
1	C	167	LEU	2.4
2	B	303	ALA	2.4
1	A	93	ILE	2.4
2	B	358	ILE	2.4
1	A	202	PHE	2.4
2	D	172	MET	2.4
1	A	167	LEU	2.4
1	A	255	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	20	PHE	2.4
2	B	220	THR	2.3
2	B	383	ALA	2.3
1	A	315	CYS	2.3
2	B	437	ASP	2.3
2	D	373	MET	2.3
1	A	119	LEU	2.3
1	A	230	LEU	2.3
1	A	269	LEU	2.3
1	A	141	PHE	2.3
4	F	21	LEU	2.3
4	F	143	GLU	2.3
2	D	425	MET	2.3
4	F	342	LEU	2.3
4	F	101	TYR	2.3
2	D	388	PHE	2.3
1	A	68	VAL	2.3
1	A	112	LYS	2.3
2	B	336	GLN	2.3
2	B	372	LYS	2.2
1	A	135	PHE	2.2
4	F	204	TRP	2.2
1	A	435	VAL	2.2
2	B	277	SER	2.2
4	F	75	ALA	2.2
3	E	48	GLU	2.2
1	C	335	ILE	2.2
2	B	435	TYR	2.1
1	A	204	VAL	2.1
1	A	196	GLU	2.1
1	A	137	VAL	2.1
1	C	230	LEU	2.1
3	E	106	GLU	2.1
1	A	176	GLN	2.1
1	A	288	VAL	2.1
3	E	17	GLY	2.1
2	B	377	PHE	2.1
4	F	242	ASN	2.1
4	F	329	LEU	2.1
1	C	5	ILE	2.1
2	B	436	GLN	2.1
1	C	281	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	357	TYR	2.1
2	D	377	PHE	2.1
2	B	371	LEU	2.0
2	B	387	LEU	2.0
1	A	156	ARG	2.0
3	E	139	LEU	2.0
1	C	275	VAL	2.0
4	F	335	ALA	2.0
2	D	19	LYS	2.0
2	D	124	LYS	2.0
1	C	135	PHE	2.0
2	B	296	PHE	2.0
2	D	212	ILE	2.0
2	D	358	ILE	2.0
1	A	89	PRO	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 monosaccharides 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.

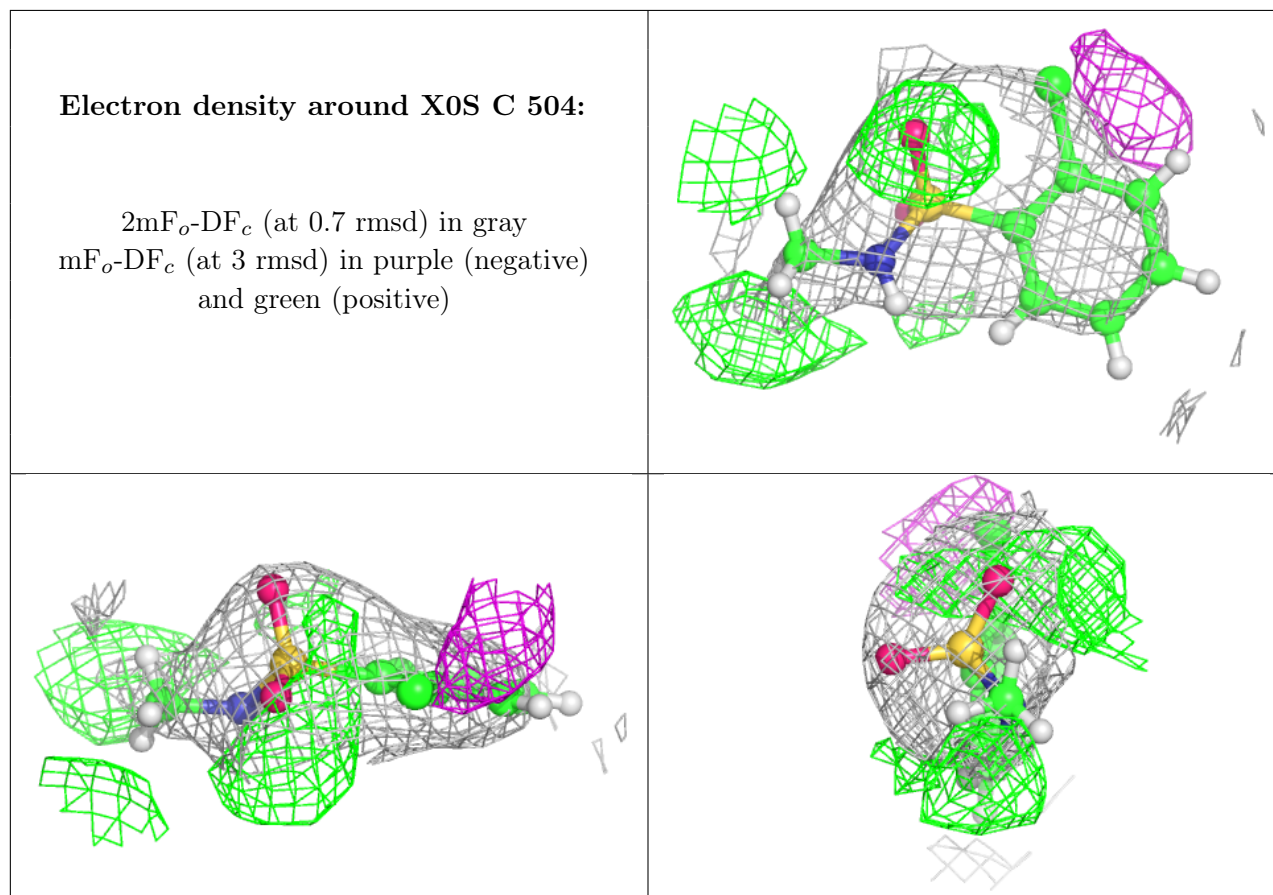
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.60	0.15	140,140,140,140	0
7	CA	A	504	1/1	0.80	0.13	111,111,111,111	0
6	MG	D	502	1/1	0.85	0.15	95,95,95,95	0
10	X0S	C	504	12/12	0.87	0.33	68,84,95,110	20
11	ACP	F	401	31/31	0.89	0.15	128,141,154,158	0
10	X0S	B	505	12/12	0.90	0.28	75,92,112,112	20
7	CA	A	503	1/1	0.92	0.14	124,124,124,124	0
8	GDP	D	501	28/28	0.95	0.20	90,99,109,110	0

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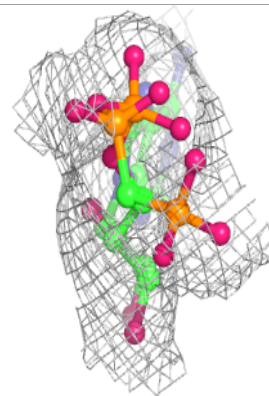
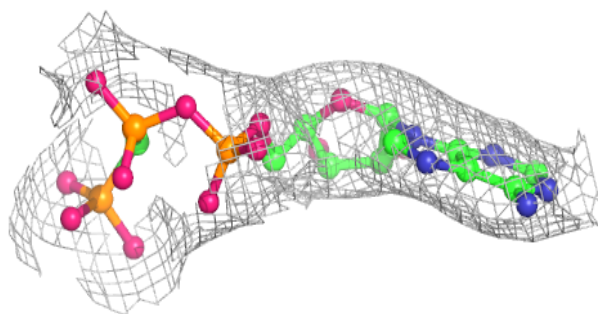
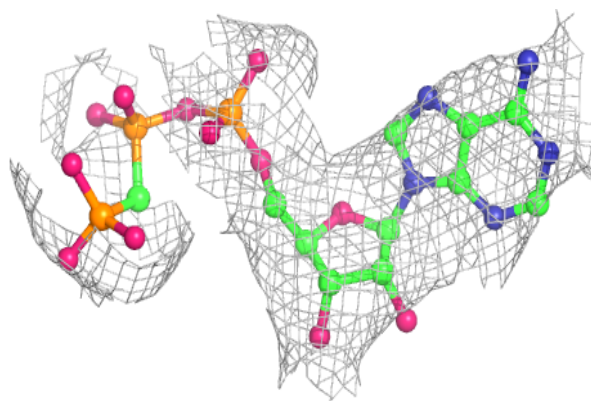
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	C	503	1/1	0.95	0.17	100,100,100,100	0
9	MES	B	504	12/12	0.97	0.16	75,82,92,93	0
5	GTP	A	501	32/32	0.97	0.17	68,73,80,82	0
6	MG	B	502	1/1	0.97	0.21	63,63,63,63	0
6	MG	C	502	1/1	0.97	0.17	70,70,70,70	0
6	MG	F	402	1/1	0.98	0.15	135,135,135,135	0
6	MG	A	502	1/1	0.98	0.20	71,71,71,71	0
8	GDP	B	501	28/28	0.98	0.19	52,66,72,74	0
5	GTP	C	501	32/32	0.98	0.19	60,69,78,81	0

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

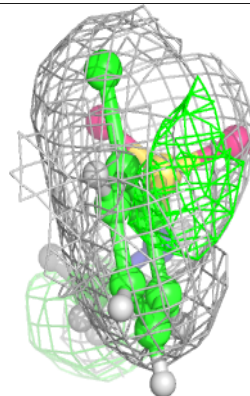
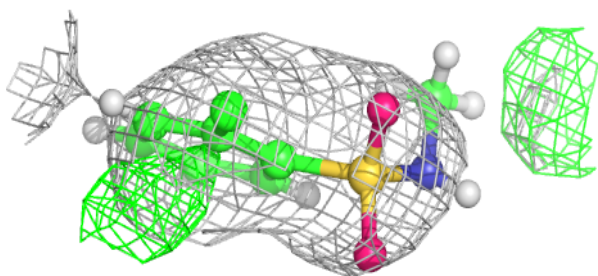
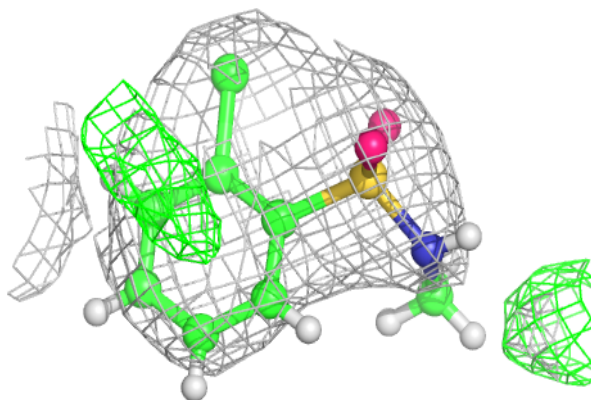


Electron density around ACP F 401:

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

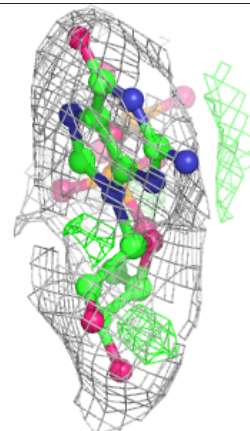
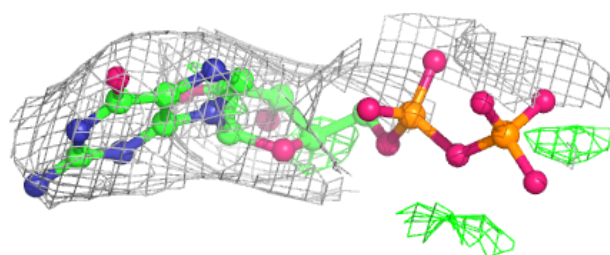
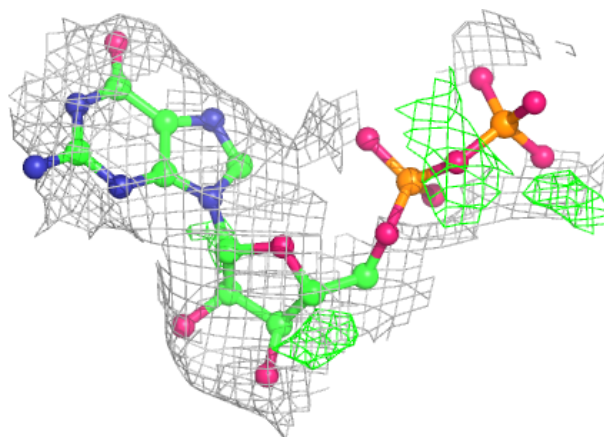
**Electron density around X0S B 505:**

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

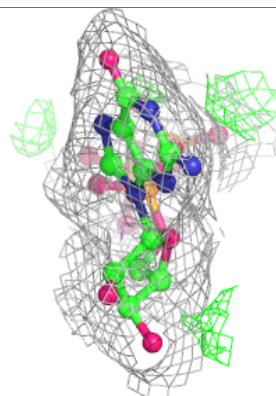
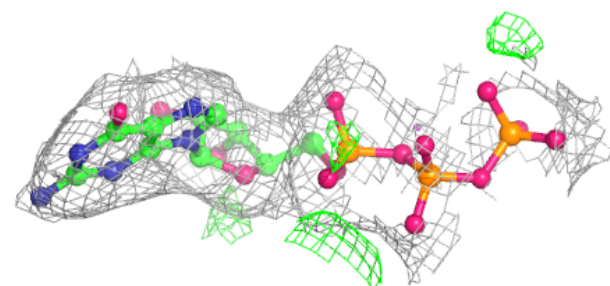
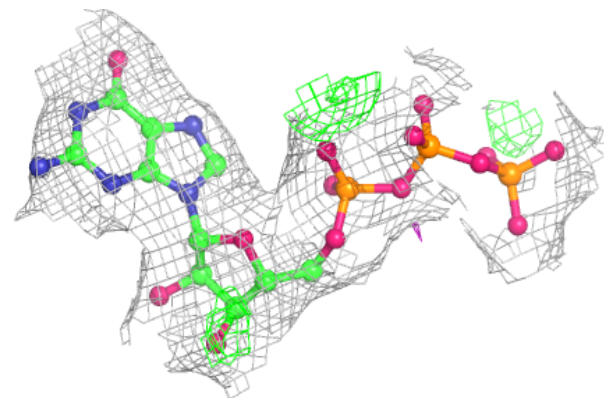


Electron density around GDP D 501:

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

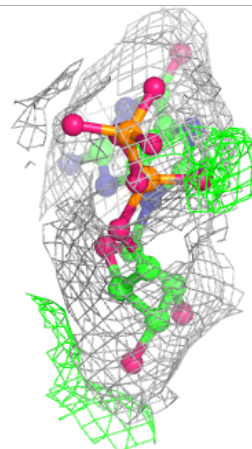
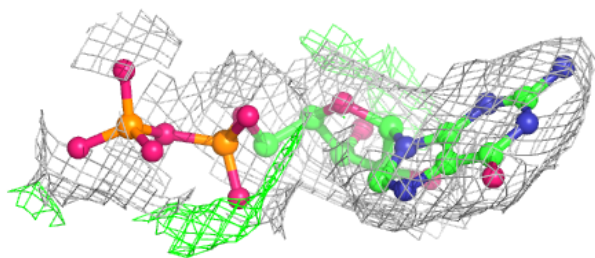
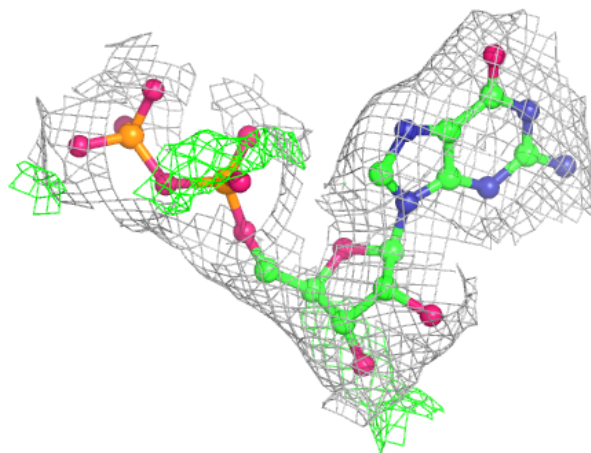
**Electron density around GTP A 501:**

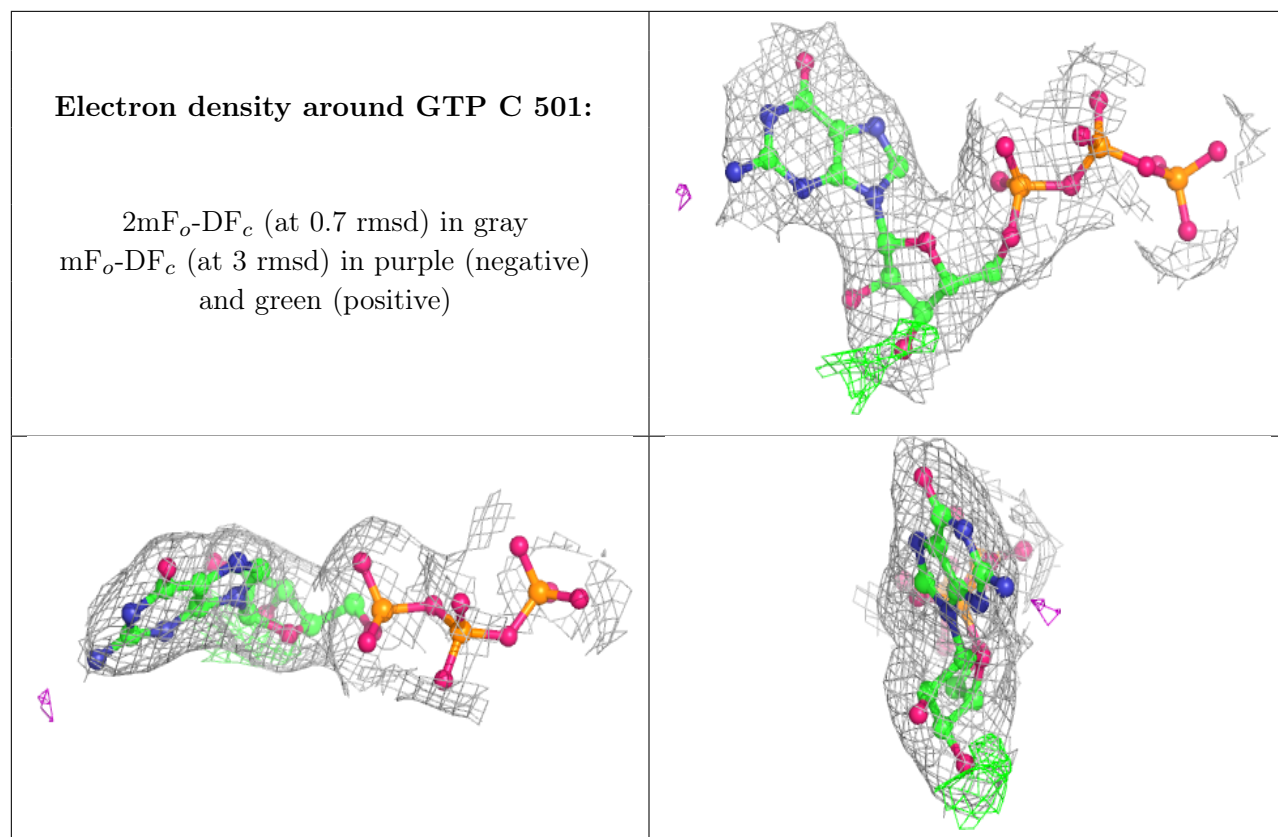
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.