



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 01:32 PM EDT

PDB ID : 5S58
Title : Tubulin-Z2856434826-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.30 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 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	:	2.20
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)	:	2.20

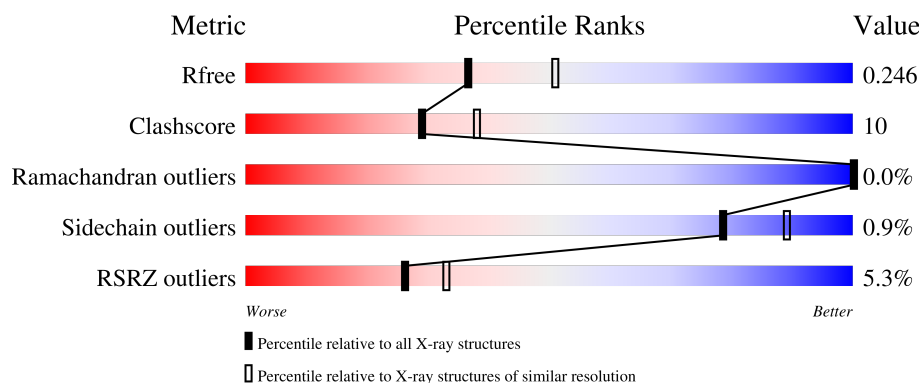
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	<div> <div>4%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	C	451	<div> <div>2%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
2	B	445	<div> <div>3%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	D	445	<div> <div>5%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
3	E	143	<div> <div>13%</div> <div>71%</div> <div>15%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div></div><div></div><div></div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17997 atoms, of which 18 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	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
2	B	425	Total	C	N	O	S	13	1	0
			3359	2109	577	646	27			
2	D	427	Total	C	N	O	S	5	0	0
			3348	2101	571	649	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	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
4	F	345	Total	C	N	O	S	0	0	0
			2830	1815	484	517	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
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
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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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		

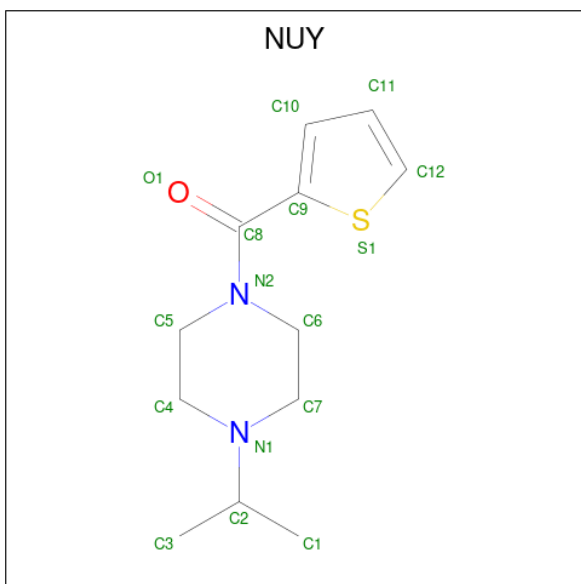
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





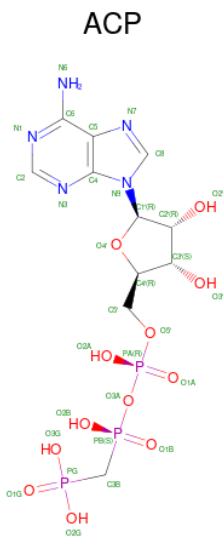
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is [4-(propan-2-yl)piperazin-1-yl](thiophen-2-yl)methanone (three-letter code: NUY) (formula: C₁₂H₁₈N₂OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	H	N	O	S	0
			34	12	18	2	1	1	

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

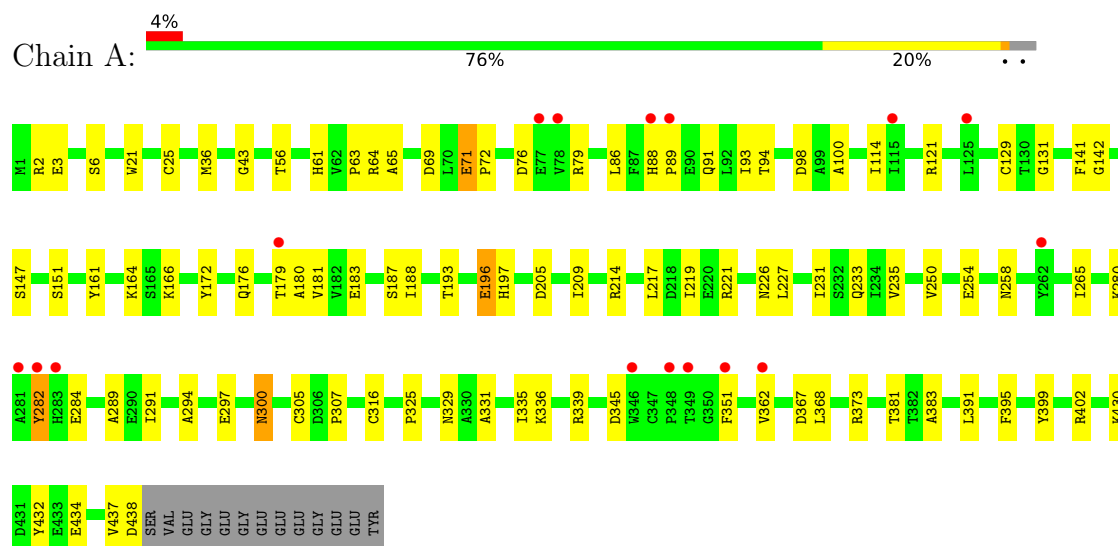
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	65	Total O 65 65	0	0
12	B	75	Total O 75 75	0	0
12	C	181	Total O 181 181	0	0
12	D	32	Total O 32 32	0	0
12	E	9	Total O 9 9	0	0
12	F	11	Total O 11 11	0	0

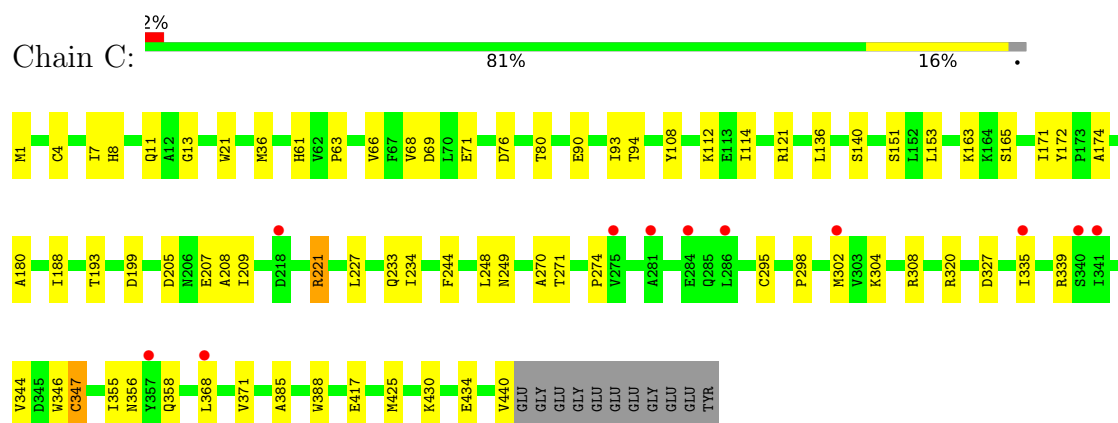
3 Residue-property plots

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.

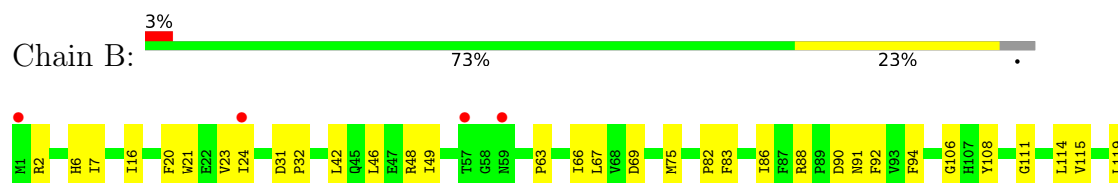
• Molecule 1: Tubulin alpha-1B chain

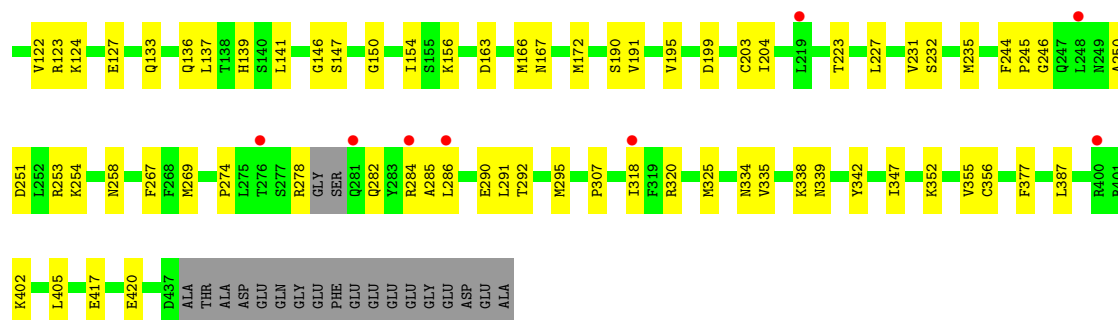


• Molecule 1: Tubulin alpha-1B chain

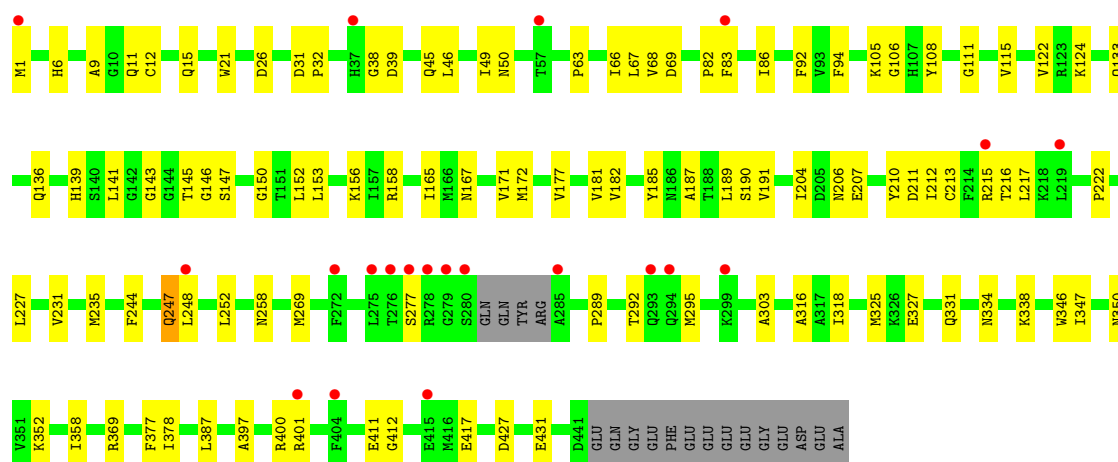
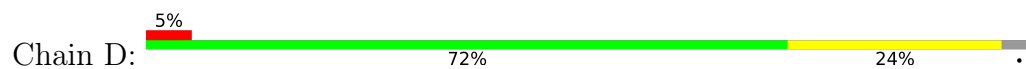


• Molecule 2: Tubulin beta-2B chain

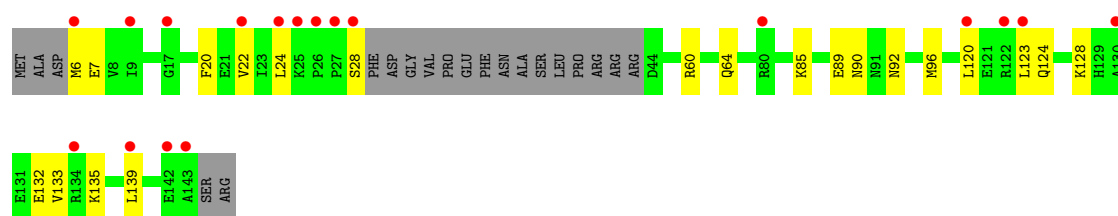




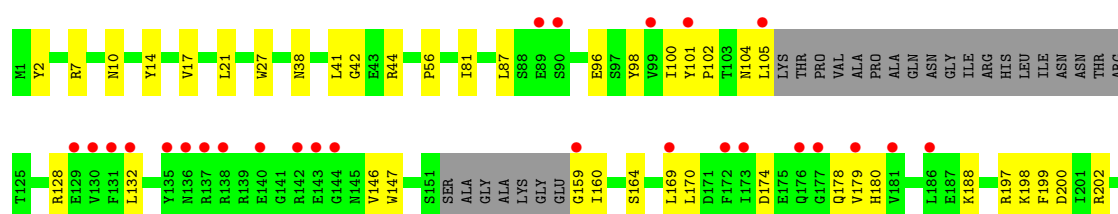
• Molecule 2: Tubulin beta-2B chain

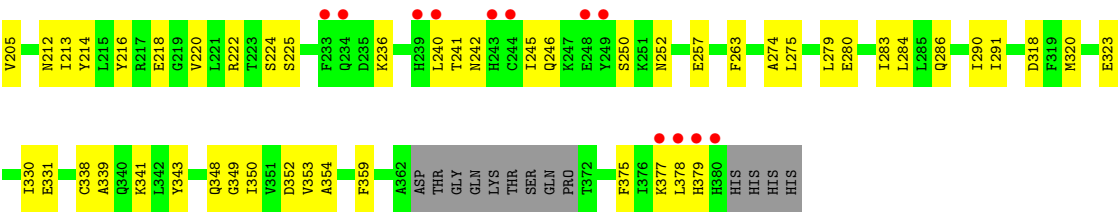


• Molecule 3: Stathmin-4



• 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	104.28Å 157.51Å 179.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.14 – 2.30 118.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.14-2.30) 99.9 (118.48-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.209 , 0.246 0.209 , 0.246	Depositor DCC
R_{free} test set	6534 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17997	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 2.73% 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: MES, GDP, CA, GTP, NUY, ACP, MG

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	0.43	0/4780
2	B	0.26	0/3433	0.41	0/4647
2	D	0.25	0/3421	0.42	0/4633
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2894	0.40	0/3910
All	All	0.25	0/17793	0.41	0/24080

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	63	0
1	C	3443	0	3352	57	0
2	B	3359	0	3235	76	0
2	D	3348	0	3227	73	0
3	E	1014	0	1029	16	0
4	F	2830	0	2799	63	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	0	0
8	D	28	0	12	3	0
9	B	12	0	12	1	0
10	D	16	18	0	0	0
11	F	31	0	14	5	0
12	A	65	0	0	2	0
12	B	75	0	0	4	0
12	C	181	0	0	3	0
12	D	32	0	0	0	0
12	E	9	0	0	0	0
12	F	11	0	0	0	0
All	All	17979	18	17050	333	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 10.

All (333) 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:102:PRO:HG2	4:F:105:LEU:HD13	1.48	0.96
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.54	0.88
1:A:381:THR:HG22	1:A:383:ALA:H	1.38	0.87
2:D:217:LEU:HA	2:D:277:SER:HB3	1.58	0.85
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.59	0.83
1:C:209:ILE:HD11	1:C:302:MET:CE	2.08	0.83
1:C:234:ILE:HD13	1:C:302:MET:HE1	1.59	0.82
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.63	0.81
1:C:234:ILE:HD13	1:C:302:MET:CE	2.12	0.79
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.48	0.77
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.68	0.76
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.67	0.75
1:C:76:ASP:O	1:C:80:THR:HG22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.68	0.74
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.71	0.73
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.22	0.73
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.07	0.71
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.55	0.69
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.74	0.69
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.22	0.69
2:B:83:PHE:O	2:B:86:ILE:HG22	1.93	0.69
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.73	0.69
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.11	0.68
1:C:270:ALA:O	1:C:302:MET:HG2	1.92	0.68
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.11	0.67
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.77	0.67
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.60	0.66
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.35	0.66
2:B:136:GLN:HA	2:B:167:ASN:O	1.95	0.66
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.31	0.66
2:B:278:ARG:HG2	2:B:282:GLN:NE2	2.11	0.65
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.79	0.65
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.79	0.65
2:B:82:PRO:O	12:B:601:HOH:O	2.14	0.65
2:B:147:SER:HG	2:B:190:SER:HG	1.42	0.65
3:E:120:LEU:O	3:E:124:GLN:HG3	1.97	0.65
2:D:83:PHE:O	2:D:86:ILE:HG22	1.97	0.65
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.12	0.65
2:D:136:GLN:HA	2:D:167:ASN:O	1.95	0.64
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.97	0.64
1:C:327:ASP:OD2	12:C:601:HOH:O	2.15	0.64
2:B:246:GLY:O	2:B:250:ALA:HB2	1.97	0.63
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.13	0.63
2:B:417:GLU:O	12:B:602:HOH:O	2.16	0.62
1:A:3:GLU:OE1	1:A:129:CYS:HB3	2.00	0.62
2:B:69:ASP:O	2:B:94:PHE:HA	2.00	0.62
4:F:188:LYS:HD3	4:F:323:GLU:OE2	2.00	0.62
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.82	0.62
1:A:280:LYS:HE2	1:A:282:TYR:O	1.99	0.62
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.81	0.62
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.66	0.61
1:A:297:GLU:HB2	1:A:300:ASN:HD21	1.65	0.61
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.83	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:C:163:LYS:HG3	3:E:90:ASN:OD1	2.00	0.60
1:A:179:THR:HA	2:B:352:LYS:HD2	1.82	0.60
3:E:85:LYS:O	3:E:89:GLU:HG3	2.00	0.60
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.83	0.60
2:D:69:ASP:O	2:D:94:PHE:HA	2.01	0.60
4:F:349:GLY:O	4:F:353:VAL:HG22	2.01	0.60
2:D:1:MET:CE	2:D:50:ASN:HB2	2.31	0.60
1:C:108:TYR:O	1:C:112:LYS:HG2	2.02	0.59
4:F:213:ILE:H	4:F:379:HIS:HB3	1.66	0.59
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.83	0.59
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.38	0.59
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.68	0.59
4:F:159:GLY:C	4:F:160:ILE:HD12	2.23	0.59
2:B:223:THR:O	2:B:227:LEU:HD13	2.03	0.59
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.85	0.59
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.33	0.58
2:D:152:LEU:O	2:D:156:LYS:HG2	2.03	0.58
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.38	0.58
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.39	0.58
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.85	0.58
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.38	0.58
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.04	0.58
1:C:165:SER:HA	1:C:199:ASP:OD2	2.04	0.58
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.85	0.58
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.04	0.58
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.19	0.57
1:C:417:GLU:OE2	12:C:602:HOH:O	2.18	0.57
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.04	0.57
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.69	0.57
2:D:11:GLN:O	2:D:15:GLN:HG2	2.05	0.57
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.34	0.57
1:A:151:SER:HB2	1:A:193:THR:OG1	2.05	0.57
1:C:234:ILE:HD13	1:C:302:MET:SD	2.45	0.57
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.32	0.56
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.03	0.56
2:D:397:ALA:O	2:D:401:ARG:NH1	2.38	0.56
2:B:191:VAL:O	2:B:195:VAL:HG23	2.06	0.56
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.56
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.41	0.56
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.36	0.55
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.06	0.55
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.89	0.55
4:F:212:ASN:HA	4:F:379:HIS:HB3	1.89	0.55
12:B:650:HOH:O	1:C:163:LYS:HD2	2.06	0.55
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.07	0.55
1:A:305:CYS:O	1:A:307:PRO:HD3	2.07	0.55
2:B:295:MET:CG	2:B:377:PHE:HB2	2.37	0.55
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.87	0.55
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.89	0.54
4:F:38:ASN:HB3	4:F:359:PHE:CE1	2.42	0.54
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.43	0.54
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.07	0.54
2:B:231:VAL:O	2:B:235:MET:HG3	2.08	0.54
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.90	0.54
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.90	0.54
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.38	0.53
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.22	0.53
2:B:334:ASN:ND2	2:B:338:LYS:HD2	2.23	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.53
4:F:320:MET:CG	4:F:330:ILE:HD11	2.39	0.53
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.39	0.53
4:F:246:GLN:O	4:F:250:SER:HB3	2.08	0.53
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.89	0.53
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.90	0.53
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.90	0.53
2:B:199:ASP:OD1	9:B:504:MES:H62	2.09	0.52
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.89	0.52
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.39	0.52
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.43	0.52
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.25	0.52
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.92	0.52
2:D:1:MET:HE3	2:D:50:ASN:HB2	1.90	0.52
1:A:294:ALA:O	1:A:300:ASN:ND2	2.43	0.52
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.44	0.52
4:F:198:LYS:O	4:F:199:PHE:HB3	2.09	0.52
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.90	0.52
4:F:198:LYS:HZ1	11:F:401:ACP:C2	2.22	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.51
2:D:211:ASP:O	2:D:215:ARG:HB2	2.10	0.51
2:D:124:LYS:C	2:D:124:LYS:HD3	2.31	0.51
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:O	1:A:235:VAL:HG23	2.11	0.51
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.11	0.51
3:E:128:LYS:O	3:E:128:LYS:HD3	2.10	0.51
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.93	0.51
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.26	0.50
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.41	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.46	0.50
2:D:248:LEU:HD21	2:D:352:LYS:CB	2.41	0.50
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.93	0.50
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.47	0.50
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.94	0.50
4:F:198:LYS:HG2	4:F:199:PHE:H	1.77	0.49
1:A:300:ASN:HB3	12:A:605:HOH:O	2.11	0.49
2:B:2:ARG:CB	2:B:133:GLN:HE21	2.24	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.49
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.10	0.49
2:D:248:LEU:CD2	2:D:352:LYS:HB3	2.42	0.49
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.47	0.49
2:D:1:MET:HG3	2:D:50:ASN:OD1	2.13	0.49
2:B:141:LEU:HD12	2:B:172:MET:SD	2.52	0.49
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
2:D:187:ALA:O	2:D:191:VAL:HG23	2.11	0.49
3:E:92:ASN:O	3:E:96:MET:HG2	2.11	0.49
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.35	0.49
1:A:71:GLU:HG2	1:A:72:PRO:N	2.27	0.49
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.94	0.49
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.95	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.94	0.49
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.43	0.49
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.48
4:F:202:ARG:HB3	4:F:220:VAL:HG23	1.95	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.48
1:C:271:THR:HG21	1:C:295:CYS:O	2.14	0.48
2:D:46:LEU:HA	2:D:49:ILE:HB	1.95	0.48
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.30	0.48
2:B:124:LYS:HD3	2:B:124:LYS:C	2.34	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.48
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.78	0.48
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.48	0.48
2:D:427:ASP:O	2:D:431:GLU:HG3	2.14	0.48
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:17:VAL:O	4:F:21:LEU:HG	2.13	0.48
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.95	0.48
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.36	0.48
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.96	0.48
2:B:46:LEU:HA	2:B:49:ILE:HB	1.95	0.48
2:D:181:VAL:HG13	2:D:182:VAL:HG13	1.96	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.48
2:B:163:ASP:O	2:B:253[B]:ARG:NH1	2.47	0.47
1:A:329:ASN:HB3	3:E:6:MET:CE	2.44	0.47
1:C:66:VAL:HG12	1:C:68:VAL:HG23	1.96	0.47
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.44	0.47
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.95	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.47
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.97	0.47
3:E:7:GLU:O	3:E:22:VAL:HA	2.13	0.47
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.47	0.47
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.45	0.47
4:F:197:ARG:HB2	4:F:224:SER:O	2.14	0.47
1:A:69:ASP:O	1:A:94:THR:HA	2.14	0.47
2:D:212:ILE:O	2:D:216:THR:HB	2.15	0.47
1:A:289:ALA:HA	1:A:331:ALA:CB	2.45	0.47
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.45	0.47
1:A:187:SER:CB	1:A:391:LEU:HD21	2.45	0.47
1:C:1:MET:O	12:C:603:HOH:O	2.20	0.47
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.47
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.24	0.46
2:D:9:ALA:HA	2:D:68:VAL:O	2.16	0.46
3:E:60:ARG:O	3:E:64:GLN:HG3	2.15	0.46
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.50	0.46
1:A:399:TYR:O	1:A:402:ARG:NH1	2.46	0.46
1:C:151:SER:HB2	1:C:193:THR:CG2	2.45	0.46
1:C:90:GLU:O	1:C:121:ARG:HD2	2.15	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.51	0.46
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.51	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.97	0.46
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.16	0.46
2:B:320:ARG:HA	2:B:356:CYS:O	2.15	0.46
2:D:145:THR:HB	8:D:501:GDP:O2B	2.16	0.46
2:D:147:SER:HB2	2:D:190:SER:OG	2.15	0.46
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.81	0.46
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.98	0.45
1:C:233:GLN:HG3	1:C:368:LEU:HD12	1.97	0.45
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.98	0.45
4:F:286:GLN:O	4:F:290:ILE:HG13	2.17	0.45
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.97	0.45
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.99	0.45
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.45
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.99	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.45
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.99	0.45
2:D:327:GLU:O	2:D:331:GLN:HG2	2.17	0.45
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.98	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.45
1:A:214:ARG:HG2	1:A:219:ILE:O	2.17	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.99	0.44
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.58	0.44
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.00	0.44
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.98	0.44
2:D:289:PRO:HD3	2:D:327:GLU:OE2	2.16	0.44
1:A:345:ASP:HB3	3:E:28:SER:HB2	2.00	0.44
3:E:135:LYS:O	3:E:139:LEU:HG	2.18	0.44
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.47	0.44
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.00	0.44
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.00	0.44
1:C:344:VAL:HG23	1:C:347:CYS:HB2	2.00	0.44
2:D:146:GLY:O	2:D:150:GLY:HA3	2.18	0.44
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.18	0.44
4:F:350:ILE:O	4:F:354:ALA:HB3	2.18	0.44
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.17	0.44
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.53	0.43
4:F:377:LYS:HB3	4:F:379:HIS:CE1	2.52	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.43
2:D:231:VAL:O	2:D:235:MET:HG3	2.18	0.43
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.37	0.43
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.00	0.43
2:B:325:MET:HE2	2:B:355:VAL:HG11	2.00	0.43
2:B:295:MET:HG3	2:B:377:PHE:HB2	2.00	0.43
1:C:8:HIS:HB3	1:C:13:GLY:O	2.18	0.43
2:D:141:LEU:HD12	2:D:172:MET:SD	2.58	0.43
2:B:114:LEU:O	2:B:114:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:CYS:SG	2:D:227:LEU:HD23	2.58	0.43
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.43
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.19	0.43
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.49	0.43
4:F:212:ASN:HA	4:F:379:HIS:CB	2.48	0.43
1:C:388:TRP:CE3	1:C:425:MET:HE1	2.53	0.43
2:B:115:VAL:HG21	2:B:156:LYS:HD2	2.00	0.43
1:C:234:ILE:CD1	1:C:302:MET:HE1	2.39	0.43
1:C:344:VAL:CG2	1:C:347:CYS:HB2	2.49	0.43
2:D:412:GLY:C	3:E:133:VAL:HG13	2.39	0.43
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.49	0.43
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.42
1:A:430:LYS:O	1:A:434:GLU:HG3	2.19	0.42
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.53	0.42
1:C:440:VAL:HG12	1:C:440:VAL:O	2.20	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.01	0.42
2:B:278:ARG:HG2	2:B:282:GLN:HE22	1.84	0.42
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.51	0.42
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.37	0.42
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.83	0.42
2:D:66:ILE:HD12	2:D:122:VAL:HG22	2.02	0.42
1:A:6:SER:O	1:A:65:ALA:HA	2.19	0.42
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.59	0.42
2:B:420:GLU:OE1	12:B:603:HOH:O	2.21	0.42
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.54	0.42
2:D:105:LYS:HE2	2:D:411:GLU:OE2	2.19	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.54	0.42
4:F:341:LYS:HG2	4:F:341:LYS:O	2.19	0.42
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.01	0.42
2:D:185:TYR:O	2:D:189:LEU:HG	2.20	0.42
2:D:295:MET:CE	2:D:377:PHE:HB2	2.49	0.42
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.55	0.42
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.55	0.42
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.19	0.42
1:A:437:VAL:HG12	1:A:438:ASP:N	2.35	0.41
4:F:225:SER:O	4:F:252:ASN:HB2	2.20	0.41
1:A:2:ARG:HB3	1:A:131:GLY:O	2.20	0.41
1:A:181:VAL:HG12	1:A:181:VAL:O	2.19	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.41
2:B:42:LEU:N	2:B:42:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLY:O	2:B:150:GLY:HA3	2.20	0.41
1:C:69:ASP:O	1:C:94:THR:HA	2.19	0.41
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.41
2:B:318:ILE:N	2:B:318:ILE:HD12	2.36	0.41
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.41
2:B:42:LEU:HD12	2:B:42:LEU:H	1.86	0.41
1:A:114:ILE:O	1:A:114:ILE:HG12	2.21	0.41
1:A:181:VAL:HG11	2:B:347:ILE:CG2	2.51	0.41
2:B:2:ARG:CG	2:B:133:GLN:HE21	2.33	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.41
4:F:178:GLN:NE2	4:F:180:HIS:HE1	2.19	0.41
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.02	0.41
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.48	0.41
2:B:284:ARG:HG2	2:B:285:ALA:O	2.21	0.41
2:B:387:LEU:HD23	2:B:387:LEU:C	2.41	0.41
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.19	0.41
4:F:240:LEU:HD12	4:F:240:LEU:N	2.36	0.41
2:D:66:ILE:CD1	2:D:122:VAL:HG22	2.50	0.41
1:A:176:GLN:HG3	4:F:56:PRO:CG	2.51	0.41
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.01	0.41
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.95	0.41
2:D:292:THR:O	2:D:295:MET:HG2	2.21	0.41
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.55	0.41
1:A:43:GLY:HA2	1:A:56:THR:O	2.21	0.41
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.56	0.41
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.03	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.40
2:D:295:MET:HE2	2:D:295:MET:HB2	1.75	0.40
1:A:362:VAL:HG22	12:A:602:HOH:O	2.21	0.40
1:C:174:ALA:HB2	1:C:207:GLU:N	2.37	0.40
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.04	0.40
4:F:274:ALA:C	4:F:275:LEU:HD22	2.42	0.40
3:E:132:GLU:HA	3:E:135:LYS:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	423 (97%)	13 (3%)	0	100	100
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	422/445 (95%)	405 (96%)	17 (4%)	0	100	100
2	D	423/445 (95%)	409 (97%)	13 (3%)	1 (0%)	47	58
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	337/384 (88%)	323 (96%)	14 (4%)	0	100	100
All	All	2176/2319 (94%)	2104 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	82	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	362 (98%)	7 (2%)	57	73
1	C	372/379 (98%)	369 (99%)	3 (1%)	81	91
2	B	368/383 (96%)	366 (100%)	2 (0%)	88	95
2	D	368/383 (96%)	363 (99%)	5 (1%)	67	81
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	311/342 (91%)	310 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1898/1993 (95%)	1880 (99%)	18 (1%)	78	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	196	GLU
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
1	A	316	CYS
2	B	48	ARG
2	B	139	HIS
1	C	71	GLU
1	C	221	ARG
1	C	347	CYS
2	D	39	ASP
2	D	133	GLN
2	D	139	HIS
2	D	207	GLU
2	D	247	GLN
4	F	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	HIS
1	A	128	GLN
1	A	283	HIS
1	A	300	ASN
2	B	15	GLN
2	B	282	GLN
2	B	294	GLN
1	C	11	GLN
1	C	300	ASN
2	D	167	ASN
2	D	294	GLN
2	D	300	ASN
2	D	394	GLN

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Mol	Chain	Res	Type
4	F	180	HIS
4	F	229	ASN
4	F	242	ASN
4	F	269	GLN
4	F	333	ASN
4	F	348	GLN
4	F	379	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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
8	GDP	B	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.88	7 (22%)
10	NUY	D	503	-	16,17,17	0.33	0	18,23,23	0.80	0
9	MES	B	504	-	12,12,12	2.36	1 (8%)	14,16,16	1.93	3 (21%)
11	ACP	F	401	6	27,33,33	1.41	5 (18%)	32,52,52	1.48	4 (12%)
8	GDP	D	501	6	24,30,30	1.16	2 (8%)	31,47,47	1.94	8 (25%)
5	GTP	C	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.71	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.67	6 (18%)

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
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
10	NUY	D	503	-	-	1/8/22/22	0/2/2/2
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
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	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	-7.90	1.66	1.77
8	B	501	GDP	C6-C5	4.13	1.48	1.41
8	D	501	GDP	C6-C5	4.03	1.48	1.41
5	A	501	GTP	C6-N1	3.10	1.38	1.33
5	C	501	GTP	C6-N1	3.07	1.38	1.33
11	F	401	ACP	PG-O3G	2.99	1.61	1.54
11	F	401	ACP	PG-O2G	2.98	1.61	1.54
11	F	401	ACP	PB-O3A	2.91	1.61	1.58
11	F	401	ACP	C5-C4	2.57	1.47	1.40
8	D	501	GDP	C5-C4	2.47	1.47	1.40
8	B	501	GDP	C5-C4	2.38	1.47	1.40
11	F	401	ACP	PB-O2B	2.23	1.61	1.56

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.27	120.20	127.22
5	C	501	GTP	N3-C2-N1	-5.16	120.33	127.22
8	B	501	GDP	C2-N3-C4	4.96	121.03	115.36
8	D	501	GDP	C2-N3-C4	4.94	121.00	115.36
8	D	501	GDP	C6-N1-C2	4.17	122.55	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PA-O3A-PB	-4.10	119.57	132.56
5	C	501	GTP	C2-N3-C4	4.08	120.01	115.36
8	D	501	GDP	C5-C6-N1	-4.05	117.89	123.43
8	B	501	GDP	C6-C5-C4	-4.03	116.95	120.80
8	B	501	GDP	C6-N1-C2	4.00	122.29	115.93
5	A	501	GTP	C2-N3-C4	3.91	119.82	115.36
8	B	501	GDP	C5-C6-N1	-3.85	118.17	123.43
9	B	504	MES	C5-N4-C3	3.82	117.43	108.83
8	D	501	GDP	C6-C5-C4	-3.77	117.19	120.80
11	F	401	ACP	C3'-C2'-C1'	3.49	106.24	100.98
8	D	501	GDP	N3-C2-N1	-3.43	122.65	127.22
8	B	501	GDP	N3-C2-N1	-3.33	122.78	127.22
11	F	401	ACP	N3-C2-N1	-3.16	123.73	128.68
5	C	501	GTP	PB-O3B-PG	-3.14	122.07	132.83
5	A	501	GTP	C5-C6-N1	-3.10	119.19	123.43
9	B	504	MES	C6-C5-N4	-3.10	105.41	110.10
5	A	501	GTP	PA-O3A-PB	-3.00	122.54	132.83
5	C	501	GTP	PA-O3A-PB	-2.99	122.57	132.83
5	C	501	GTP	C5-C6-N1	-2.94	119.42	123.43
8	D	501	GDP	PA-O3A-PB	-2.93	122.77	132.83
8	B	501	GDP	C4-C5-N7	-2.76	106.53	109.40
5	A	501	GTP	C6-N1-C2	2.67	120.17	115.93
9	B	504	MES	O3S-S-C8	2.62	110.00	105.77
8	B	501	GDP	PA-O3A-PB	-2.60	123.89	132.83
8	D	501	GDP	C4-C5-N7	-2.58	106.71	109.40
11	F	401	ACP	C4-C5-N7	-2.56	106.73	109.40
5	C	501	GTP	C6-N1-C2	2.55	119.97	115.93
5	A	501	GTP	PB-O3B-PG	-2.28	124.99	132.83
8	D	501	GDP	C3'-C2'-C1'	2.28	104.41	100.98

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
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	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
10	D	503	NUY	O1-C8-N2-C6
9	B	504	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A

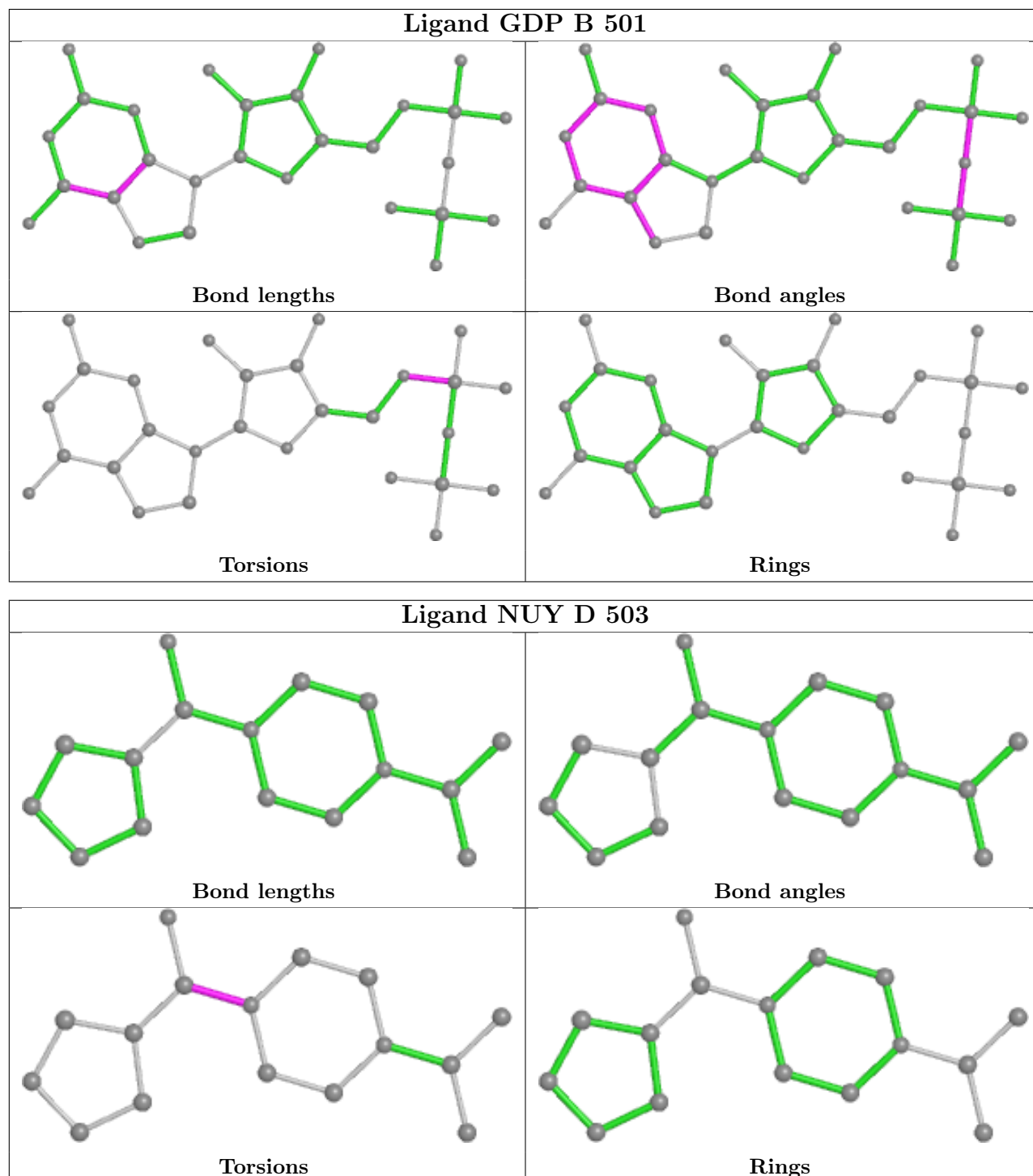
There are no ring outliers.

4 monomers are involved in 10 short contacts:

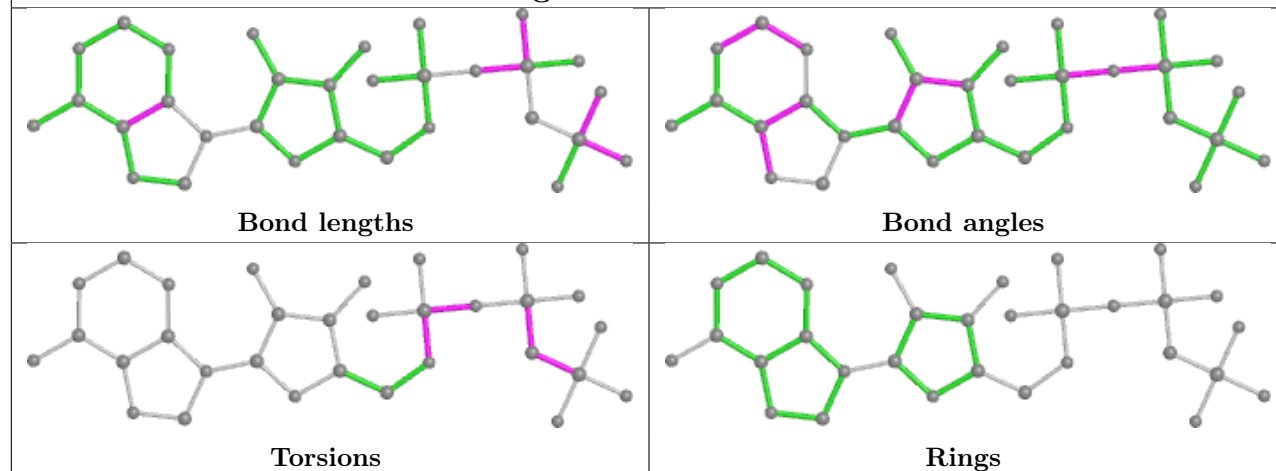
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	MES	1	0
11	F	401	ACP	5	0
8	D	501	GDP	3	0
5	A	501	GTP	1	0

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.

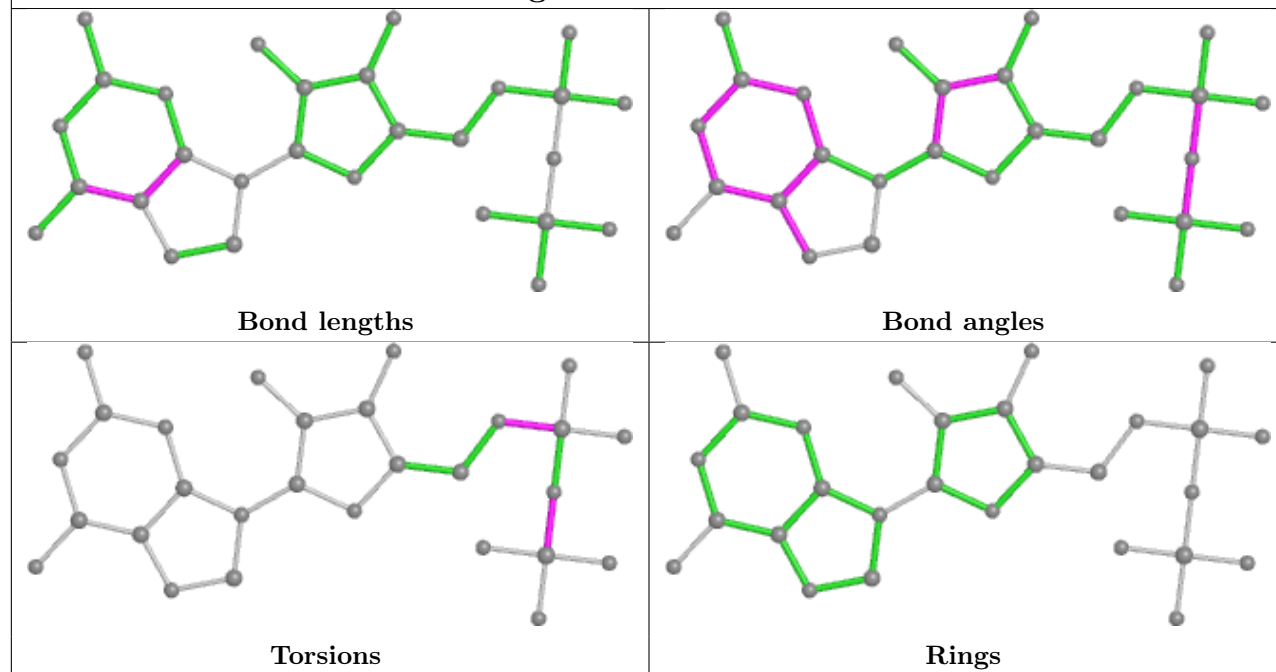
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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



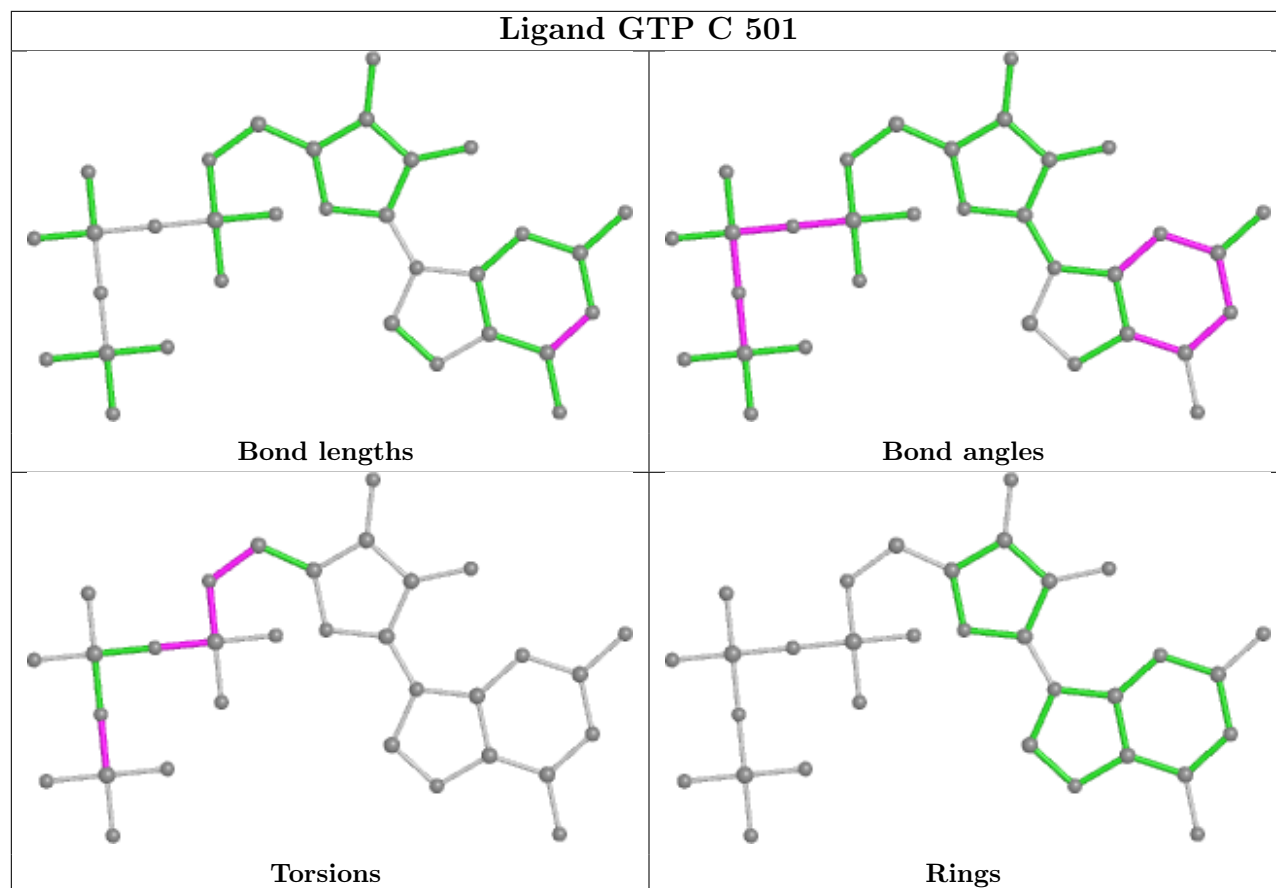
Ligand ACP F 401



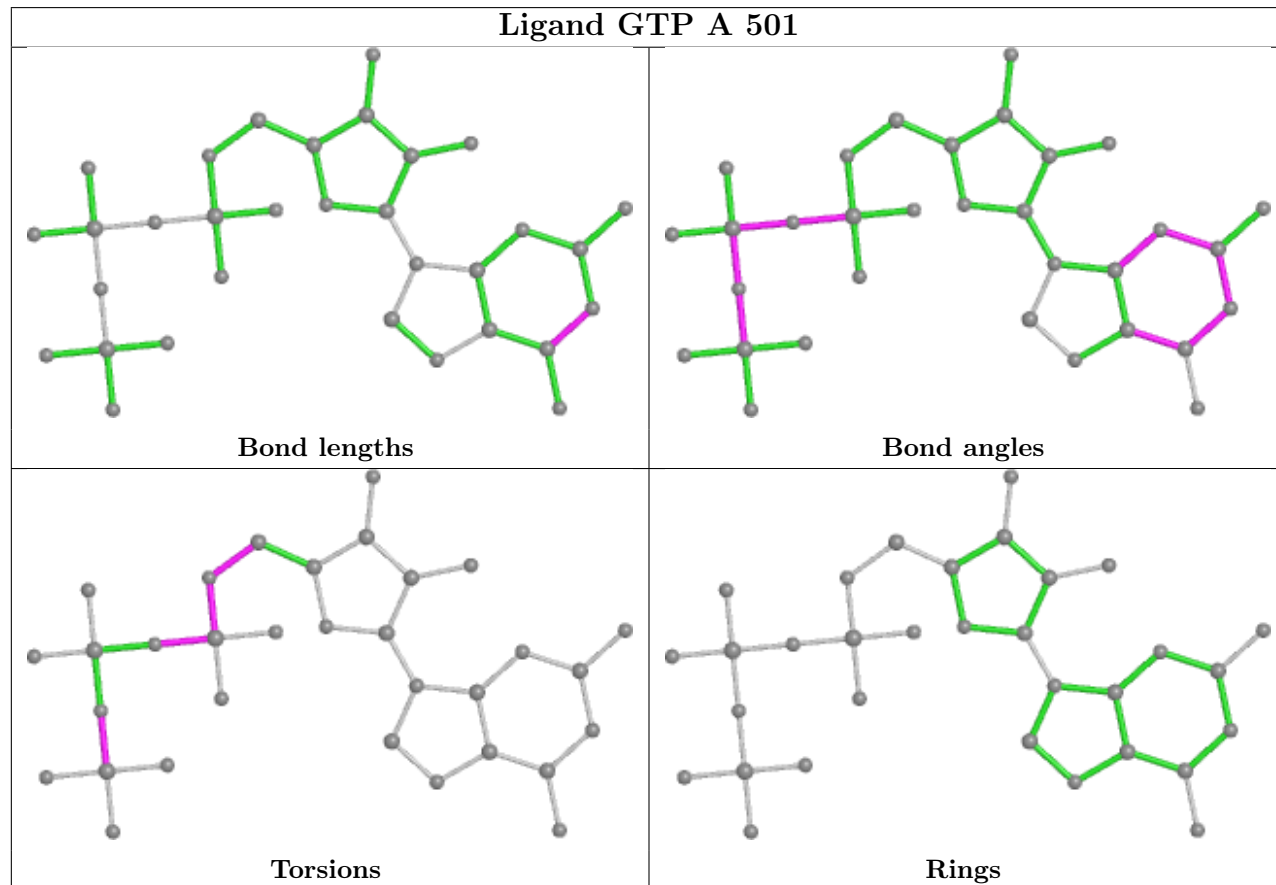
Ligand GDP D 501



Ligand GTP C 501



Ligand GTP A 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.42	16 (3%) 41 48	47, 67, 101, 156	0
1	C	440/451 (97%)	0.35	11 (2%) 57 64	41, 53, 79, 109	0
2	B	425/445 (95%)	0.45	12 (2%) 53 60	42, 63, 103, 149	2 (0%)
2	D	427/445 (95%)	0.44	21 (4%) 29 36	47, 70, 104, 155	4 (0%)
3	E	123/143 (86%)	0.90	18 (14%) 2 3	52, 76, 124, 158	0
4	F	345/384 (89%)	0.66	38 (11%) 5 7	58, 90, 159, 198	0
All	All	2198/2319 (94%)	0.48	116 (5%) 26 33	41, 67, 120, 198	6 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	276	THR	8.3
1	A	282	TYR	6.4
3	E	6	MET	5.8
4	F	143	GLU	5.7
2	D	278	ARG	5.4
2	B	1	MET	5.3
2	B	281	GLN	5.3
3	E	24	LEU	4.9
1	C	340	SER	4.8
4	F	379	HIS	4.7
2	D	279	GLY	4.6
3	E	26	PRO	4.5
4	F	137	ARG	4.5
4	F	169	LEU	4.4
3	E	143	ALA	4.4
4	F	173	ILE	4.3
1	A	179	THR	4.3
2	D	1	MET	4.3
4	F	131	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
4	F	136	ASN	4.2
3	E	27	PRO	4.2
4	F	135	TYR	4.2
3	E	25	LYS	4.1
4	F	99	VAL	4.1
4	F	140	GLU	4.0
2	B	57	THR	3.9
4	F	240	LEU	3.8
1	C	286	LEU	3.8
1	A	351	PHE	3.6
1	C	341	ILE	3.6
2	D	401	ARG	3.6
4	F	89	GLU	3.6
2	B	284	ARG	3.6
2	B	248	LEU	3.5
2	D	277	SER	3.5
4	F	144	GLY	3.5
1	A	125	LEU	3.5
2	B	276	THR	3.4
1	C	357	TYR	3.4
1	A	88	HIS	3.4
3	E	142	GLU	3.3
4	F	130	VAL	3.3
2	D	275	LEU	3.3
4	F	142	ARG	3.2
4	F	249	TYR	3.2
2	D	272	PHE	3.2
3	E	122	ARG	3.2
3	E	139	LEU	3.1
4	F	132	LEU	3.1
2	D	37	HIS	3.0
4	F	233	PHE	3.0
4	F	138	ARG	3.0
4	F	234	GLN	2.9
4	F	239	HIS	2.9
1	A	262	TYR	2.9
2	D	248	LEU	2.9
4	F	129	GLU	2.9
1	C	218	ASP	2.9
2	D	294	GLN	2.8
4	F	176	GLN	2.8
4	F	179	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	120	LEU	2.7
4	F	90	SER	2.7
1	C	302	MET	2.6
3	E	130	ALA	2.6
4	F	248	GLU	2.6
2	D	215	ARG	2.6
2	D	293	GLN	2.6
2	D	280	SER	2.6
1	C	368	LEU	2.6
4	F	380	HIS	2.6
2	D	299	LYS	2.6
3	E	134	ARG	2.5
2	D	404	PHE	2.5
4	F	243	HIS	2.5
1	A	77	GLU	2.5
2	B	24	ILE	2.5
3	E	123	LEU	2.5
4	F	377	LYS	2.4
2	D	57	THR	2.4
4	F	378	LEU	2.4
2	D	285	ALA	2.4
3	E	17	GLY	2.4
4	F	105	LEU	2.4
2	B	318	ILE	2.3
1	A	89	PRO	2.3
4	F	181	VAL	2.3
4	F	177	GLY	2.3
1	A	78	VAL	2.3
1	A	349	THR	2.2
4	F	244	CYS	2.2
4	F	186	LEU	2.2
1	C	335	ILE	2.2
1	A	346	TRP	2.2
1	A	283	HIS	2.2
1	A	281	ALA	2.2
3	E	9	ILE	2.2
2	D	219	LEU	2.2
3	E	22	VAL	2.1
2	D	415	GLU	2.1
4	F	159	GLY	2.1
2	B	286	LEU	2.1
1	C	275	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	115	ILE	2.1
4	F	172	PHE	2.1
1	A	362	VAL	2.1
3	E	28	SER	2.1
1	C	284	GLU	2.0
2	B	219	LEU	2.0
2	B	400	ARG	2.0
2	B	59	ASN	2.0
1	A	348	PRO	2.0
2	D	83	PHE	2.0
4	F	101	TYR	2.0
3	E	80	ARG	2.0
1	C	281	ALA	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
11	ACP	F	401	31/31	0.79	0.15	98,105,115,119	0
9	MES	B	504	12/12	0.83	0.22	84,92,112,127	0
7	CA	B	503	1/1	0.84	0.11	106,106,106,106	0
7	CA	A	503	1/1	0.94	0.14	96,96,96,96	0
7	CA	A	504	1/1	0.95	0.09	92,92,92,92	0
10	NUY	D	503	16/16	0.95	0.15	57,69,81,81	34
6	MG	D	502	1/1	0.95	0.17	68,68,68,68	0
6	MG	A	502	1/1	0.96	0.15	51,51,51,51	0
6	MG	B	502	1/1	0.96	0.14	41,41,41,41	0
8	GDP	D	501	28/28	0.96	0.16	63,66,79,83	0

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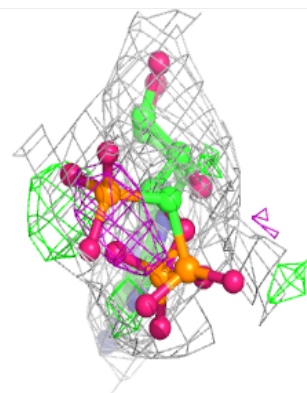
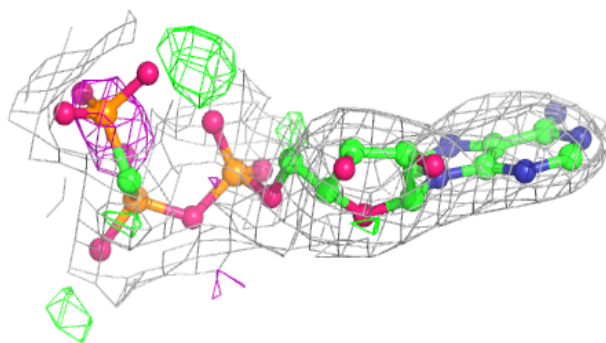
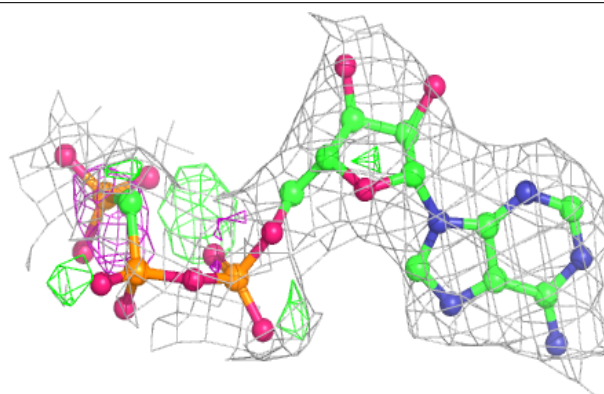
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	F	402	1/1	0.97	0.08	100,100,100,100	0
5	GTP	A	501	32/32	0.98	0.15	45,51,56,58	0
5	GTP	C	501	32/32	0.98	0.17	33,45,49,53	0
6	MG	C	502	1/1	0.98	0.13	42,42,42,42	0
7	CA	C	503	1/1	0.99	0.08	73,73,73,73	0
8	GDP	B	501	28/28	0.99	0.16	42,47,51,54	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.

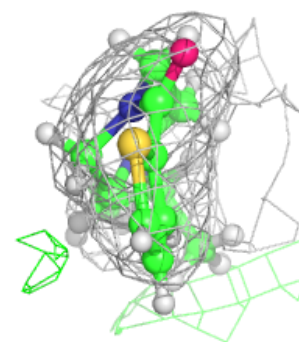
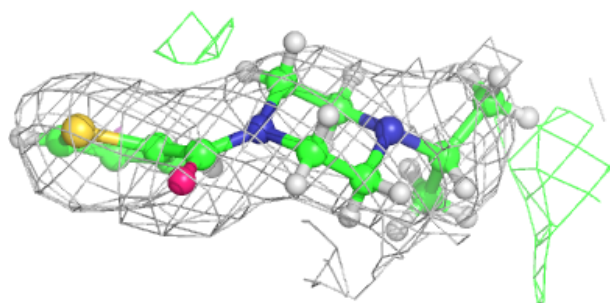
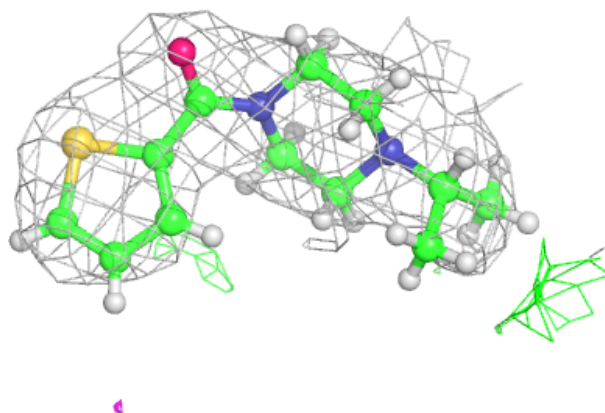
Electron density around ACP F 401:

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



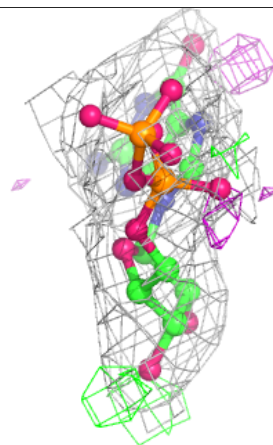
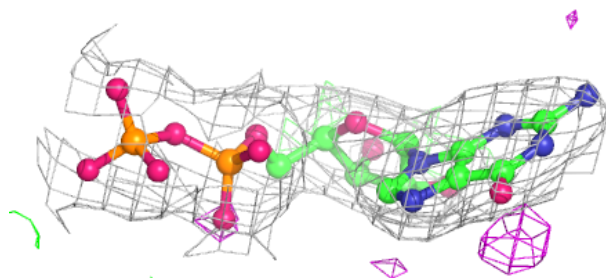
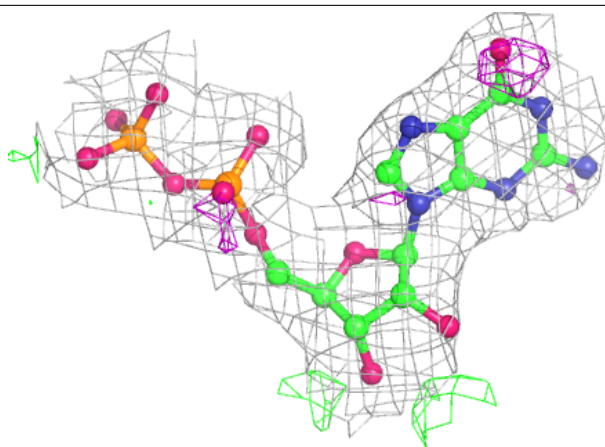
Electron density around NUY D 503:

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

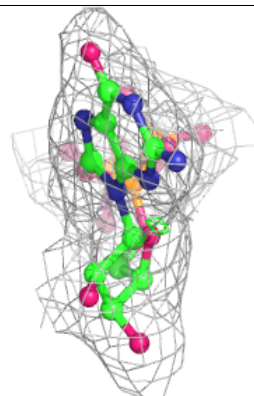
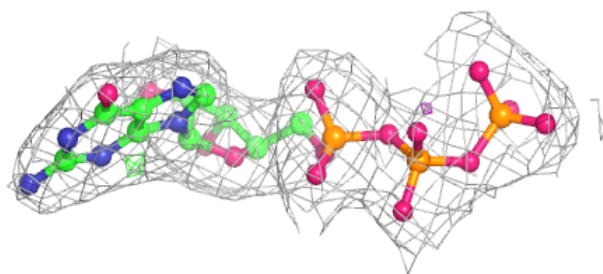
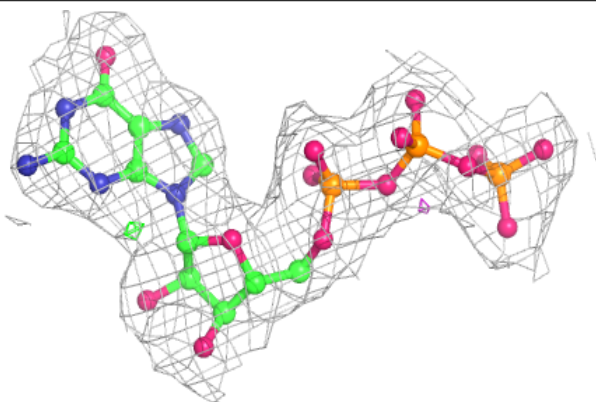


Electron density around GDP D 501:

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

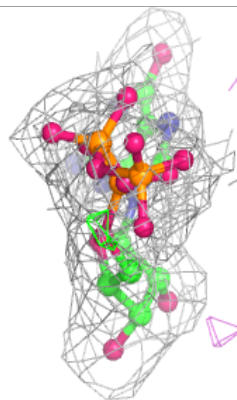
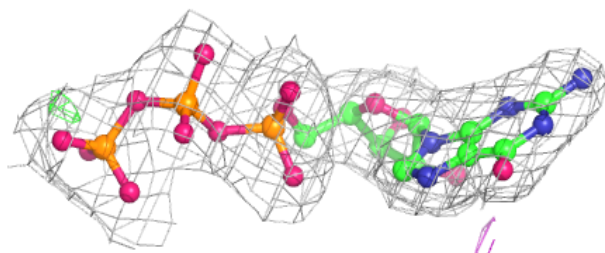
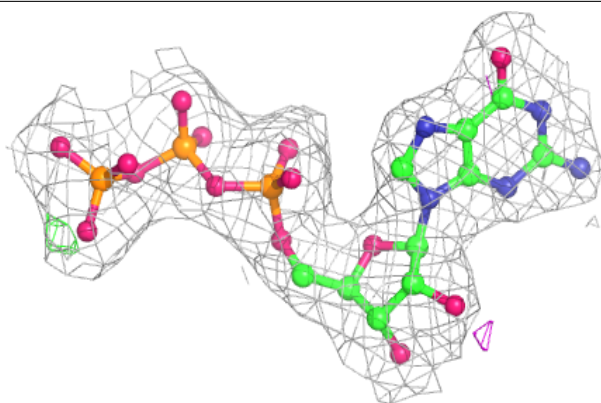
**Electron density around GTP A 501:**

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

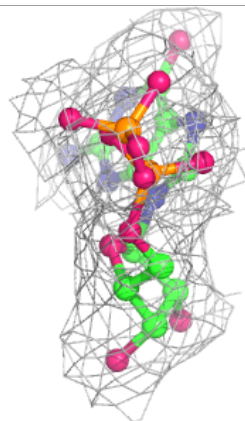
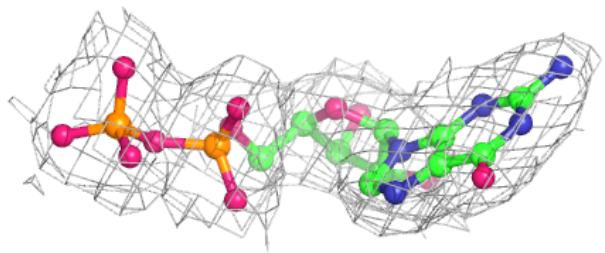
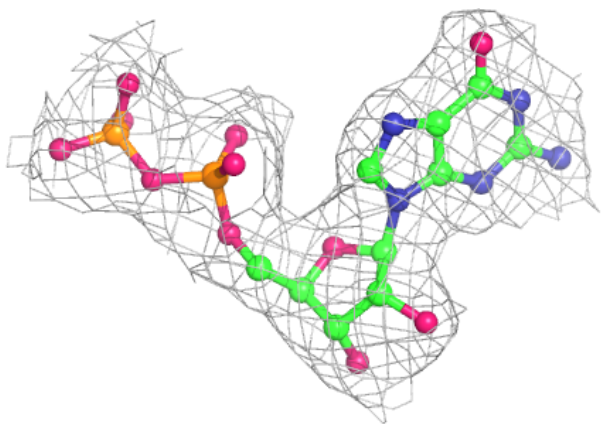


Electron density around GTP C 501:

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

**Electron density around 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.