



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 01:09 PM EDT

PDB ID : 5S5T
Title : Tubulin-Z198194394-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.53 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

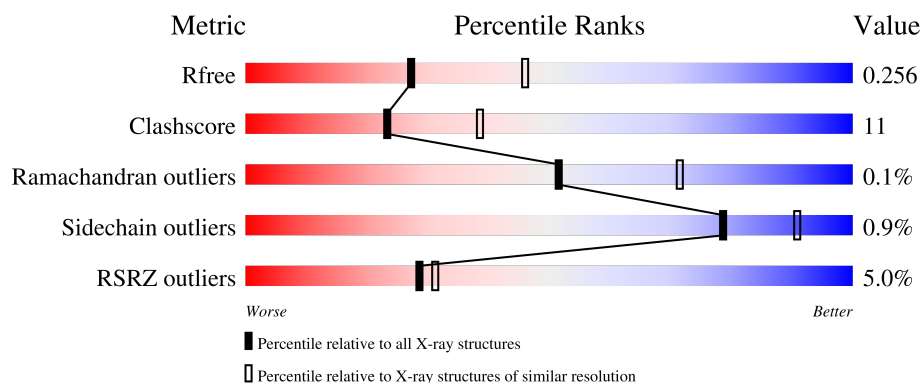
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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>2%</div> <div>76%</div> <div>20%</div> <div>••</div> </div>
1	C	451	<div> <div>%</div> <div>74%</div> <div>24%</div> <div>•</div> </div>
2	B	445	<div> <div>3%</div> <div>68%</div> <div>27%</div> <div>5%</div> </div>
2	D	445	<div> <div>3%</div> <div>71%</div> <div>26%</div> <div>•</div> </div>
3	E	143	<div> <div>8%</div> <div>70%</div> <div>16%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>15%</div><div></div><div>66%</div><div>25%</div><div>8%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18030 atoms, of which 14 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	421	Total	C	N	O	S	2	1	0
			3336	2096	572	641	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
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

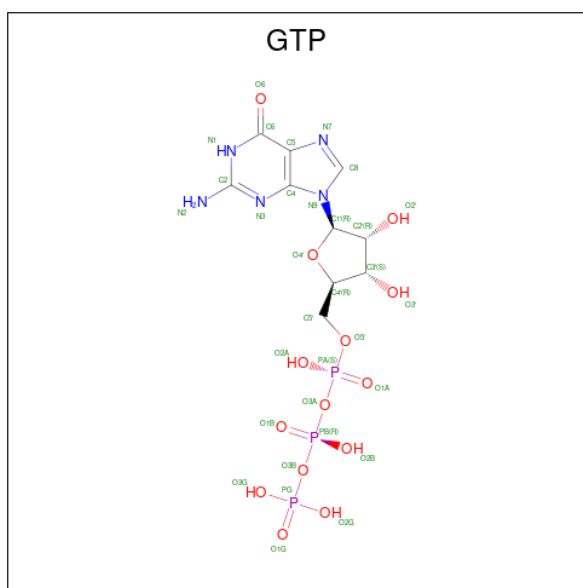
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	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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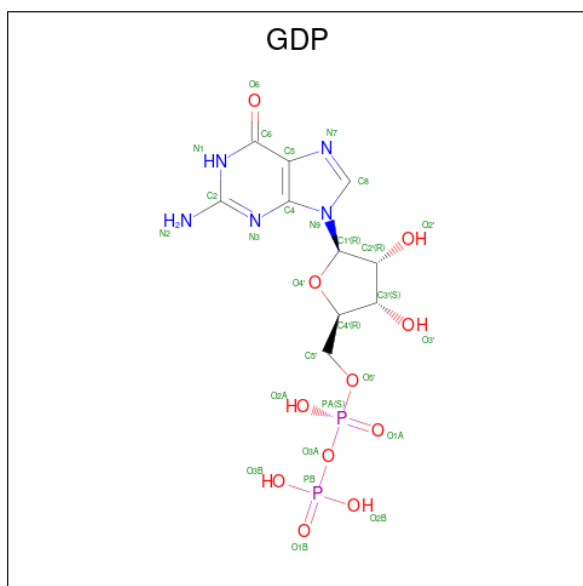
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

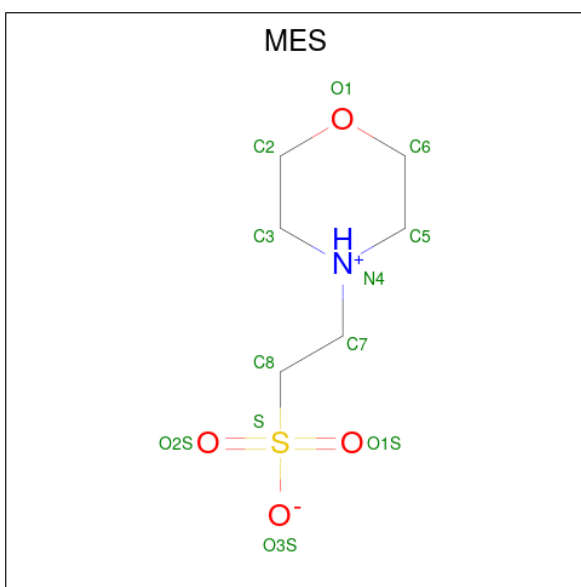
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

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



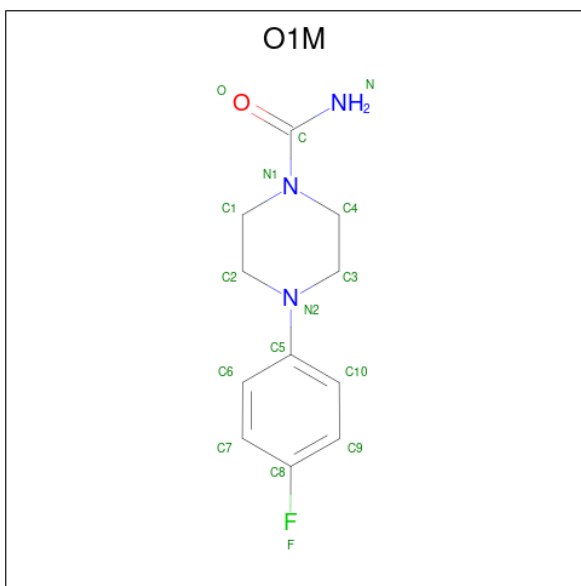
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



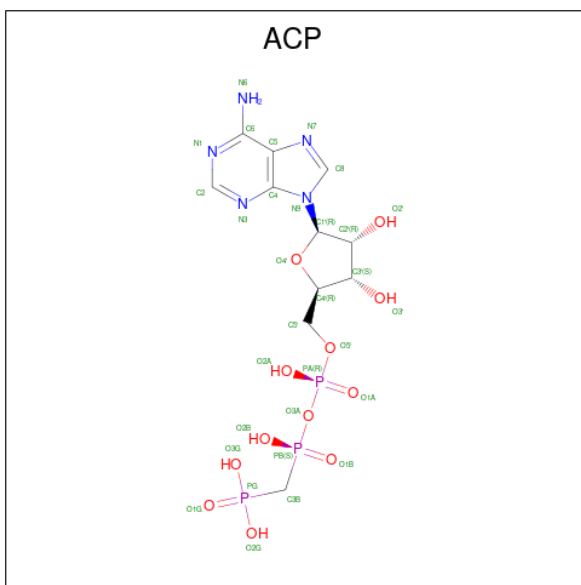
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 4-(4-fluorophenyl)piperazine-1-carboxamide (three-letter code: O1M) (formula: $C_{11}H_{14}FN_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	F	H	N	O	0	0
			30	11	1	14	3	1		

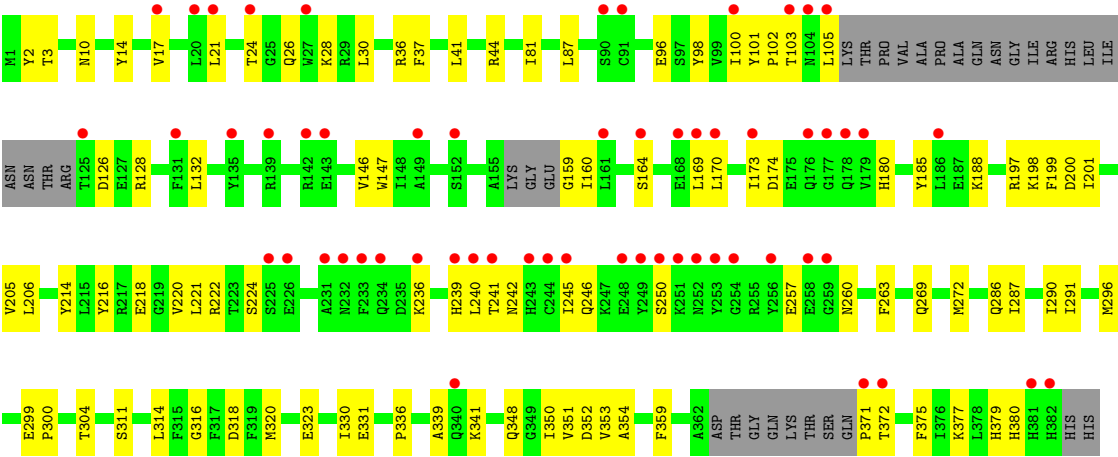
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	70	Total O 70 70	0	0
12	B	80	Total O 80 80	0	0
12	C	169	Total O 169 169	0	0
12	D	31	Total O 31 31	0	0
12	E	7	Total O 7 7	0	0
12	F	9	Total O 9 9	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.83Å 158.22Å 178.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.32 – 2.53 72.32 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.7 (72.32-2.53) 97.7 (72.32-2.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.211 , 0.256 0.211 , 0.256	Depositor DCC
R_{free} test set	1962 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.5	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	0.94	EDS
Total number of atoms	18030	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: GTP, MES, O1M, ACP, MG, GDP, CA

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	0.26	0/3502	0.42	0/4754
1	C	0.27	0/3521	0.43	0/4780
2	B	0.25	0/3409	0.42	0/4613
2	D	0.25	0/3442	0.42	0/4664
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17840	0.41	0/24145

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	76	0
1	C	3443	0	3353	72	0
2	B	3336	0	3219	87	0
2	D	3368	0	3236	80	0
3	E	1014	0	1029	17	0
4	F	2877	0	2839	74	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	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	3	0
9	B	12	0	12	3	0
10	B	16	14	0	0	0
11	F	31	0	14	4	0
12	A	70	0	0	5	1
12	B	80	0	0	3	0
12	C	169	0	0	4	1
12	D	31	0	0	2	0
12	E	7	0	0	0	0
12	F	9	0	0	0	0
All	All	18016	14	17084	393	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 11.

All (393) 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:221:ARG:HG3	2:D:325:MET:HG2	1.44	0.99
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.55	0.88
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.56	0.87
2:B:253[A]:ARG:NH1	9:B:504:MES:O3S	2.09	0.86
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.59	0.85
4:F:241:THR:OG1	11:F:401:ACP:O3'	1.95	0.84
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.60	0.83
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.60	0.82
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.63	0.80
2:D:217:LEU:HA	2:D:277:SER:HB3	1.64	0.79
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.45	0.79
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.67	0.77
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.67	0.77
2:D:136:GLN:HA	2:D:167:ASN:O	1.83	0.76
1:A:179:THR:HA	2:B:352:LYS:HD2	1.66	0.76
2:B:83:PHE:O	2:B:86:ILE:HG22	1.87	0.75
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.69	0.73
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.72	0.72
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.53	0.72
2:D:83:PHE:O	2:D:86:ILE:HG22	1.89	0.71
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.23	0.71
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.90	0.71
1:C:76:ASP:O	1:C:80:THR:HG22	1.90	0.71
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.34	0.68
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.24	0.68
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.09	0.67
2:B:136:GLN:HA	2:B:167:ASN:O	1.95	0.67
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.25	0.67
2:B:69:ASP:O	2:B:94:PHE:HA	1.95	0.66
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.30	0.66
2:B:209:LEU:HD23	2:B:302:MET:HG2	1.75	0.66
1:C:320:ARG:HA	1:C:356:ASN:O	1.94	0.66
1:C:270:ALA:O	1:C:302:MET:HG2	1.94	0.66
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.76	0.65
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.79	0.65
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.79	0.65
1:C:341:ILE:HD12	1:C:341:ILE:O	1.97	0.65
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.79	0.64
2:D:432:TYR:OH	12:D:601:HOH:O	2.12	0.64
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.62	0.64
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.79	0.63
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.80	0.63
4:F:371:PRO:HA	4:F:372:THR:HB	1.80	0.63
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.30	0.62
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.81	0.62
2:B:295:MET:CG	2:B:377:PHE:HB2	2.30	0.62
4:F:371:PRO:HA	4:F:372:THR:O	2.00	0.62
2:D:46:LEU:HA	2:D:49:ILE:HB	1.82	0.61
1:A:75:ILE:HD12	1:A:94:THR:CG2	2.30	0.61
2:D:152:LEU:O	2:D:156:LYS:HG2	1.99	0.61
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.16	0.61
1:A:69:ASP:O	1:A:94:THR:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.33	0.61
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.19	0.60
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.83	0.60
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.32	0.60
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.00	0.60
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.83	0.59
1:A:356:ASN:HB2	12:A:633:HOH:O	2.01	0.59
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.85	0.59
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.37	0.59
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.30	0.59
1:C:165:SER:HA	1:C:199:ASP:OD2	2.02	0.59
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.84	0.59
2:D:11:GLN:O	2:D:15:GLN:HG2	2.03	0.58
1:A:430:LYS:HE2	1:A:434:GLU:OE2	2.02	0.58
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.32	0.58
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.39	0.58
1:C:241:SER:HA	1:C:249:ASN:OD1	2.04	0.58
1:C:308:ARG:HD2	12:C:719:HOH:O	2.04	0.58
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.85	0.58
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.20	0.57
2:D:427:ASP:O	2:D:431:GLU:HG3	2.04	0.57
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.39	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.35	0.57
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.39	0.57
2:B:164:ARG:HD2	12:B:660:HOH:O	2.02	0.57
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.87	0.57
2:B:187:ALA:O	2:B:191:VAL:HG23	2.05	0.57
2:D:295:MET:CE	2:D:377:PHE:HB2	2.33	0.57
1:A:234:ILE:O	1:A:238:ILE:HG13	2.04	0.56
3:E:60:ARG:O	3:E:64:GLN:HG3	2.05	0.56
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.39	0.56
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.05	0.56
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.87	0.56
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.87	0.56
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.41	0.56
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.88	0.56
1:A:166:LYS:HE2	1:A:197:HIS:O	2.06	0.56
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.06	0.56
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.33	0.56
1:C:214:ARG:HG2	1:C:219:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.56
4:F:246:GLN:O	4:F:250:SER:HB3	2.06	0.56
2:B:188:THR:HG23	2:B:425:MET:HE2	1.87	0.55
4:F:320:MET:CG	4:F:330:ILE:HD11	2.36	0.55
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.55
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.87	0.55
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.71	0.55
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.89	0.55
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.41	0.55
2:D:332:MET:O	2:D:336:GLN:HG3	2.06	0.55
1:A:431:ASP:O	1:A:435:VAL:HG23	2.07	0.55
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.42	0.55
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.55
1:A:75:ILE:HB	1:A:94:THR:HG21	1.88	0.55
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.35	0.54
2:B:324:SER:O	2:B:328:VAL:HG23	2.07	0.54
2:D:223:THR:O	2:D:227:LEU:HG	2.08	0.54
4:F:159:GLY:C	4:F:160:ILE:HD12	2.28	0.54
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.89	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.42	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.54
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.43	0.54
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.42	0.54
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.90	0.54
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.27	0.54
2:B:209:LEU:CD2	2:B:302:MET:HG2	2.38	0.54
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.90	0.54
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.89	0.53
1:C:271:THR:HG21	1:C:295:CYS:O	2.07	0.53
2:D:145:THR:HB	8:D:501:GDP:O2B	2.09	0.53
4:F:197:ARG:HB2	4:F:224:SER:O	2.07	0.53
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.72	0.53
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.90	0.53
1:C:235:VAL:O	1:C:239:THR:HG23	2.09	0.53
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.91	0.53
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.90	0.53
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.89	0.53
4:F:371:PRO:HA	4:F:372:THR:C	2.29	0.53
1:A:227:LEU:O	1:A:231:ILE:HG13	2.09	0.53
1:A:289:ALA:HA	1:A:331:ALA:CB	2.38	0.53
2:B:199:ASP:OD1	9:B:504:MES:H62	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.91	0.52
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.24	0.52
1:A:298:PRO:HA	1:A:301:GLN:NE2	2.24	0.52
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.74	0.52
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.74	0.52
2:B:141:LEU:HD12	2:B:172:MET:SD	2.50	0.52
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.91	0.52
1:C:209:ILE:HD11	1:C:302:MET:CE	2.36	0.52
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.25	0.52
2:B:253[B]:ARG:O	2:B:257:VAL:HG23	2.10	0.51
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.91	0.51
2:D:208:ALA:O	2:D:212:ILE:HG13	2.10	0.51
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.45	0.51
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.46	0.51
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.45	0.51
2:D:141:LEU:HD12	2:D:172:MET:SD	2.51	0.51
2:D:142:GLY:O	2:D:183:GLU:HG2	2.11	0.51
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.93	0.51
1:A:187:SER:CB	1:A:391:LEU:HD21	2.40	0.51
2:D:69:ASP:O	2:D:94:PHE:HA	2.10	0.51
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.10	0.51
2:B:124:LYS:HD3	2:B:124:LYS:C	2.31	0.51
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.92	0.51
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.92	0.51
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.40	0.50
1:C:287:SER:OG	1:C:290:GLU:HG3	2.11	0.50
1:C:312:TYR:CE1	1:C:341:ILE:HG22	2.46	0.50
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.44	0.50
1:A:136:LEU:HD21	1:A:252:LEU:HD21	1.94	0.50
1:A:320:ARG:HD2	12:A:647:HOH:O	2.12	0.50
1:C:108:TYR:O	1:C:112:LYS:HG2	2.11	0.50
1:C:271:THR:HG23	1:C:300:ASN:O	2.11	0.50
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.94	0.49
2:D:1:MET:CE	2:D:50:ASN:HB2	2.42	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.46	0.49
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.77	0.49
2:B:114:LEU:O	2:B:114:LEU:HG	2.11	0.49
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.47	0.49
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.49
4:F:101:TYR:N	4:F:126:ASP:OD1	2.36	0.49
2:B:305:CYS:O	2:B:307:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253[A]:ARG:O	2:B:257:VAL:HG23	2.12	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.47	0.49
2:D:147:SER:HB2	2:D:190:SER:OG	2.12	0.49
3:E:72:LEU:O	3:E:76:ARG:HG2	2.13	0.49
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.31	0.49
1:A:298:PRO:HA	1:A:301:GLN:CD	2.33	0.48
2:B:431:GLU:O	2:B:434:GLN:HG2	2.12	0.48
1:C:252:LEU:HD12	1:C:252:LEU:O	2.13	0.48
2:D:163:ASP:O	2:D:253:ARG:NH2	2.36	0.48
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.95	0.48
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.48
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.95	0.48
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.13	0.48
1:C:192:HIS:CG	1:C:421:ALA:HA	2.48	0.48
2:D:11:GLN:HA	2:D:74:THR:HG21	1.94	0.48
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.47	0.48
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.96	0.48
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.48
2:B:48:ARG:HB2	2:B:243:ARG:O	2.14	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.48
3:E:120:LEU:O	3:E:124:GLN:HG3	2.13	0.48
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.44	0.48
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.95	0.48
2:B:46:LEU:HA	2:B:49:ILE:HB	1.95	0.47
2:B:191:VAL:O	2:B:195:VAL:HG23	2.13	0.47
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.96	0.47
4:F:188:LYS:HD3	4:F:323:GLU:OE2	2.14	0.47
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.47
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.44	0.47
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.96	0.47
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.95	0.47
1:A:351:PHE:HE1	3:E:24:LEU:CD1	2.28	0.47
2:D:286:LEU:HD23	2:D:291:LEU:HD13	1.97	0.47
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.97	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.44	0.47
1:C:166:LYS:HE2	1:C:197:HIS:O	2.15	0.47
2:D:327:GLU:O	2:D:331:GLN:HG2	2.14	0.47
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.96	0.47
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.97	0.47
1:A:234:ILE:HD12	1:A:234:ILE:N	2.30	0.47
1:A:294:ALA:O	1:A:300:ASN:ND2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.48	0.46
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.98	0.46
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.38	0.46
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.15	0.46
4:F:350:ILE:O	4:F:354:ALA:HB3	2.14	0.46
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.81	0.46
2:D:325:MET:CE	2:D:355:VAL:HG21	2.46	0.46
4:F:17:VAL:O	4:F:21:LEU:HG	2.16	0.46
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.15	0.46
1:A:136:LEU:HD21	1:A:252:LEU:CD2	2.45	0.46
1:C:74:VAL:HB	12:C:615:HOH:O	2.14	0.46
1:C:196:GLU:HG2	12:C:654:HOH:O	2.14	0.46
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.45	0.46
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.98	0.46
2:D:318:ILE:N	2:D:318:ILE:HD12	2.30	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.35	0.46
1:C:187:SER:CB	1:C:391:LEU:HD21	2.46	0.46
2:B:67:LEU:N	2:B:67:LEU:HD12	2.30	0.46
2:D:15:GLN:NE2	2:D:74:THR:HG23	2.30	0.46
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.21	0.46
1:A:176:GLN:HB2	12:A:624:HOH:O	2.16	0.46
2:B:179:ASP:N	2:B:183:GLU:OE2	2.45	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.97	0.46
1:C:433:GLU:O	1:C:437:VAL:HG23	2.15	0.46
2:D:272:PHE:HE2	12:D:628:HOH:O	1.99	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.46
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.98	0.46
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.45	0.46
2:B:1:MET:HB2	2:B:130:ASP:OD2	2.16	0.46
4:F:198:LYS:HG2	4:F:199:PHE:H	1.80	0.46
2:B:417:GLU:O	12:B:601:HOH:O	2.20	0.46
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.98	0.46
1:A:75:ILE:HB	1:A:94:THR:CG2	2.46	0.45
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.14	0.45
4:F:246:GLN:HB3	4:F:260:ASN:ND2	2.31	0.45
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.99	0.45
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.99	0.45
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.97	0.45
2:D:295:MET:HE2	2:D:295:MET:HB2	1.83	0.45
2:B:123:ARG:O	2:B:127:GLU:HG3	2.16	0.45
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:ARG:NH1	2:D:436:GLN:O	2.49	0.45
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.52	0.45
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.17	0.45
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.47	0.45
2:D:191:VAL:O	2:D:195:VAL:HG23	2.16	0.45
1:A:292:THR:HG22	1:A:335:ILE:HD12	1.99	0.45
2:B:231:VAL:O	2:B:235:MET:HG3	2.17	0.45
2:D:124:LYS:C	2:D:124:LYS:HD3	2.38	0.45
4:F:316:GLY:N	4:F:336:PRO:HG3	2.32	0.45
2:D:1:MET:HG3	2:D:50:ASN:CB	2.47	0.44
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.18	0.44
2:D:253:ARG:O	2:D:257:VAL:HG23	2.17	0.44
3:E:70:LYS:O	3:E:74:GLU:HG3	2.17	0.44
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.52	0.44
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.17	0.44
2:B:173:PRO:HG3	2:B:187:ALA:HB2	2.00	0.44
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.17	0.44
4:F:3:THR:OG1	4:F:37:PHE:HA	2.16	0.44
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.44	0.44
4:F:286:GLN:O	4:F:290:ILE:HG13	2.17	0.44
1:A:181:VAL:HG11	2:B:347:ILE:CG2	2.47	0.44
2:B:63:PRO:HD3	2:B:86:ILE:HG12	2.00	0.44
4:F:371:PRO:HA	4:F:372:THR:CB	2.43	0.44
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.51	0.44
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.44
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.48	0.44
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.47	0.44
3:E:135:LYS:O	3:E:139:LEU:HG	2.18	0.44
4:F:198:LYS:O	4:F:199:PHE:HB3	2.17	0.44
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.47	0.44
4:F:304:THR:HG21	4:F:311:SER:OG	2.18	0.44
2:B:318:ILE:N	2:B:318:ILE:HD12	2.32	0.44
2:B:323:MET:HB3	2:B:373:MET:CE	2.48	0.44
1:C:271:THR:HG21	1:C:295:CYS:HA	1.99	0.44
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.99	0.44
1:C:14:VAL:HG11	1:C:74:VAL:HG12	2.00	0.43
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.53	0.43
4:F:296:MET:SD	4:F:380:HIS:HB2	2.58	0.43
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.99	0.43
2:B:290:GLU:O	2:B:294:GLN:HG3	2.18	0.43
2:D:349:ASN:O	2:D:352:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.48	0.43
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.00	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
2:D:2:ARG:CB	2:D:133:GLN:HE21	2.29	0.43
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.00	0.43
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.00	0.43
4:F:341:LYS:HG2	4:F:341:LYS:O	2.18	0.43
4:F:17:VAL:HG13	4:F:351:VAL:HG22	2.00	0.43
1:A:2:ARG:HB3	1:A:133:GLN:HG3	2.00	0.43
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.48	0.43
2:B:413:MET:HE1	2:B:418:PHE:CE1	2.54	0.43
4:F:2:TYR:CD1	4:F:359:PHE:HB3	2.54	0.43
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.54	0.43
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.54	0.43
2:D:146:GLY:O	2:D:150:GLY:HA3	2.18	0.43
2:B:28:HIS:HB3	2:B:49:ILE:HD13	2.01	0.43
2:B:181:VAL:HG22	1:C:258:ASN:OD1	2.19	0.43
2:D:173:PRO:HG3	2:D:187:ALA:HB2	1.99	0.43
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.51	0.43
2:B:390:ARG:O	2:B:394:GLN:HG3	2.18	0.43
1:C:311:LYS:HD2	1:C:436:GLY:O	2.19	0.43
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.19	0.43
1:A:66:VAL:HG23	1:A:125:LEU:CD1	2.49	0.42
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.19	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.42
2:D:320:ARG:O	2:D:373:MET:HA	2.19	0.42
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.19	0.42
2:B:83:PHE:HA	12:B:605:HOH:O	2.18	0.42
2:B:213:CYS:HB3	2:B:219:LEU:HD12	2.02	0.42
2:B:270:PRO:HA	2:B:377:PHE:O	2.19	0.42
1:C:296:PHE:CD1	1:C:335:ILE:HD13	2.54	0.42
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.59	0.42
4:F:200:ASP:O	4:F:221:LEU:HA	2.19	0.42
1:A:74:VAL:HB	12:A:622:HOH:O	2.19	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.42
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.52	0.42
2:B:158:ARG:NH1	2:B:196:GLU:O	2.53	0.42
1:C:150:THR:O	1:C:154:MET:HG2	2.20	0.42
4:F:24:THR:O	4:F:26:GLN:HG3	2.20	0.42
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.01	0.42
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.54	0.42
4:F:287:ILE:O	4:F:291:ILE:HG13	2.19	0.42
1:A:284:GLU:CD	1:A:284:GLU:H	2.23	0.42
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.54	0.42
2:B:119:LEU:HD11	2:B:156:LYS:HB3	2.01	0.42
1:C:151:SER:HB2	1:C:193:THR:CG2	2.49	0.42
2:D:141:LEU:HD22	2:D:190:SER:HB3	2.01	0.42
2:B:105:LYS:HA	2:B:109:THR:OG1	2.19	0.42
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.42
4:F:160:ILE:HD12	4:F:160:ILE:N	2.34	0.42
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.01	0.42
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.20	0.41
4:F:269:GLN:HA	4:F:272:MET:HE2	2.02	0.41
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.51	0.41
1:A:289:ALA:HA	1:A:331:ALA:HB2	2.00	0.41
4:F:3:THR:HA	4:F:28:LYS:O	2.20	0.41
1:C:208:ALA:O	1:C:212:ILE:HG13	2.20	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.56	0.41
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.33	0.41
1:A:153:LEU:O	1:A:157:LEU:HG	2.20	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.41
2:B:86:ILE:HG12	2:B:86:ILE:O	2.19	0.41
4:F:206:LEU:HD23	4:F:353:VAL:CG2	2.50	0.41
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.38	0.41
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.35	0.41
3:E:67:GLU:OE1	3:E:67:GLU:HA	2.21	0.41
1:A:42:ILE:HA	12:A:601:HOH:O	2.20	0.41
1:A:43:GLY:HA2	1:A:56:THR:O	2.21	0.41
2:B:137:LEU:HB3	2:B:168:THR:HG22	2.03	0.41
1:C:46:ASP:N	1:C:46:ASP:OD1	2.53	0.41
1:A:275:VAL:HG13	1:A:368:LEU:HD22	2.02	0.41
2:B:9:ALA:HA	2:B:68:VAL:O	2.21	0.41
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.56	0.41
4:F:377:LYS:HD3	4:F:379:HIS:NE2	2.36	0.41
4:F:3:THR:HB	4:F:30:LEU:HD11	2.03	0.41
1:A:1:MET:HE2	1:A:46:ASP:HA	2.03	0.40
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.56	0.40
1:C:6:SER:O	1:C:65:ALA:HA	2.21	0.40
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.56	0.40
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:504:MES:H51	9:B:504:MES:H81	1.71	0.40
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.22	0.40
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.40
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.02	0.40
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.03	0.40
1:C:325:PRO:HD2	12:C:644:HOH:O	2.21	0.40
3:E:7:GLU:O	3:E:22:VAL:HA	2.20	0.40
1:C:419:SER:O	1:C:423:GLU:HG3	2.22	0.40
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.03	0.40
2:D:248:LEU:HD11	2:D:352:LYS:HB3	2.02	0.40
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.57	0.40
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.57	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)
12:A:656:HOH:O	12:C:719:HOH:O[3_555]	1.92	0.28

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%)	427 (98%)	8 (2%)	1 (0%)	47	67
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	416/445 (94%)	403 (97%)	12 (3%)	1 (0%)	47	67
2	D	429/445 (96%)	416 (97%)	12 (3%)	1 (0%)	47	67
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	328 (95%)	16 (5%)	0	100	100
All	All	2183/2319 (94%)	2122 (97%)	58 (3%)	3 (0%)	51	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	281	GLN
1	A	282	TYR
2	B	82	PRO

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%)	362 (98%)	7 (2%)	57	79
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	88
2	B	367/383 (96%)	365 (100%)	2 (0%)	88	95
2	D	368/383 (96%)	363 (99%)	5 (1%)	67	85
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1901/1993 (95%)	1883 (99%)	18 (1%)	78	91

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	176	GLN
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
1	A	381	THR
2	B	139	HIS
2	B	241	CYS
1	C	71	GLU
1	C	221	ARG
1	C	251	ASP
1	C	381	THR
2	D	39	ASP

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Mol	Chain	Res	Type
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN
2	D	325	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	101	ASN
1	A	128	GLN
1	A	301	GLN
2	B	15	GLN
2	B	294	GLN
1	C	11	GLN
1	C	300	ASN
2	D	294	GLN
4	F	180	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN
4	F	348	GLN
4	F	380	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
9	MES	B	504	-	12,12,12	2.21	1 (8%)	14,16,16	2.01	5 (35%)
8	GDP	B	501	6	24,30,30	1.13	2 (8%)	31,47,47	1.87	7 (22%)
5	GTP	C	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.69	6 (18%)
5	GTP	A	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.73	7 (21%)
8	GDP	D	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.96	8 (25%)
11	ACP	F	401	6	27,33,33	1.42	5 (18%)	32,52,52	1.49	4 (12%)
10	O1M	B	505	-	16,17,17	0.42	0	21,23,23	0.94	1 (4%)

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
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
11	ACP	F	401	6	-	12/15/38/38	0/3/3/3
10	O1M	B	505	-	-	0/8/18/18	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.40	1.67	1.77
8	D	501	GDP	C6-C5	4.24	1.48	1.41
8	B	501	GDP	C6-C5	3.86	1.48	1.41
5	A	501	GTP	C6-N1	3.08	1.38	1.33
5	C	501	GTP	C6-N1	3.02	1.38	1.33
11	F	401	ACP	PG-O2G	3.01	1.61	1.54
11	F	401	ACP	PG-O3G	2.97	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	2.95	1.61	1.58
11	F	401	ACP	C5-C4	2.54	1.47	1.40
8	D	501	GDP	C5-C4	2.40	1.47	1.40
8	B	501	GDP	C5-C4	2.37	1.47	1.40
11	F	401	ACP	PB-O2B	2.28	1.61	1.56

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.41	120.01	127.22
5	C	501	GTP	N3-C2-N1	-5.22	120.26	127.22
8	D	501	GDP	C2-N3-C4	4.95	121.01	115.36
8	B	501	GDP	C2-N3-C4	4.83	120.87	115.36
8	D	501	GDP	C5-C6-N1	-4.19	117.70	123.43
5	A	501	GTP	C2-N3-C4	4.19	120.14	115.36
8	D	501	GDP	C6-N1-C2	4.18	122.57	115.93
5	C	501	GTP	C2-N3-C4	4.12	120.06	115.36
11	F	401	ACP	PA-O3A-PB	-4.04	119.75	132.56
8	B	501	GDP	C6-N1-C2	4.04	122.35	115.93
8	B	501	GDP	C6-C5-C4	-3.95	117.02	120.80
8	D	501	GDP	C6-C5-C4	-3.82	117.15	120.80
8	B	501	GDP	C5-C6-N1	-3.77	118.28	123.43
9	B	504	MES	C5-N4-C3	3.69	117.14	108.83
11	F	401	ACP	C3'-C2'-C1'	3.58	106.36	100.98
8	B	501	GDP	N3-C2-N1	-3.42	122.67	127.22
8	D	501	GDP	N3-C2-N1	-3.39	122.70	127.22
9	B	504	MES	C6-C5-N4	-3.26	105.16	110.10
11	F	401	ACP	N3-C2-N1	-3.14	123.77	128.68
5	C	501	GTP	C5-C6-N1	-3.06	119.24	123.43
5	A	501	GTP	PA-O3A-PB	-3.06	122.33	132.83
5	A	501	GTP	C5-C6-N1	-2.99	119.34	123.43
8	B	501	GDP	PA-O3A-PB	-2.92	122.80	132.83
8	D	501	GDP	PA-O3A-PB	-2.88	122.95	132.83
8	D	501	GDP	C4-C5-N7	-2.86	106.42	109.40
9	B	504	MES	O1S-S-C8	2.75	110.23	106.92
5	A	501	GTP	C6-N1-C2	2.69	120.21	115.93
5	C	501	GTP	C6-N1-C2	2.66	120.16	115.93
5	C	501	GTP	PA-O3A-PB	-2.60	123.90	132.83
11	F	401	ACP	C4-C5-N7	-2.56	106.73	109.40
8	B	501	GDP	C4-C5-N7	-2.56	106.73	109.40
9	B	504	MES	O3S-S-C8	2.47	109.76	105.77
9	B	504	MES	C7-N4-C5	2.43	117.46	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	PB-O3B-PG	-2.35	124.75	132.83
10	B	505	O1M	C3-N2-C2	2.20	116.38	111.52
5	A	501	GTP	PB-O3B-PG	-2.14	125.48	132.83
5	A	501	GTP	N2-C2-N1	2.03	120.41	117.25
8	D	501	GDP	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (34) 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
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
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-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C3'-C4'-C5'-O5'
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
9	B	504	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A

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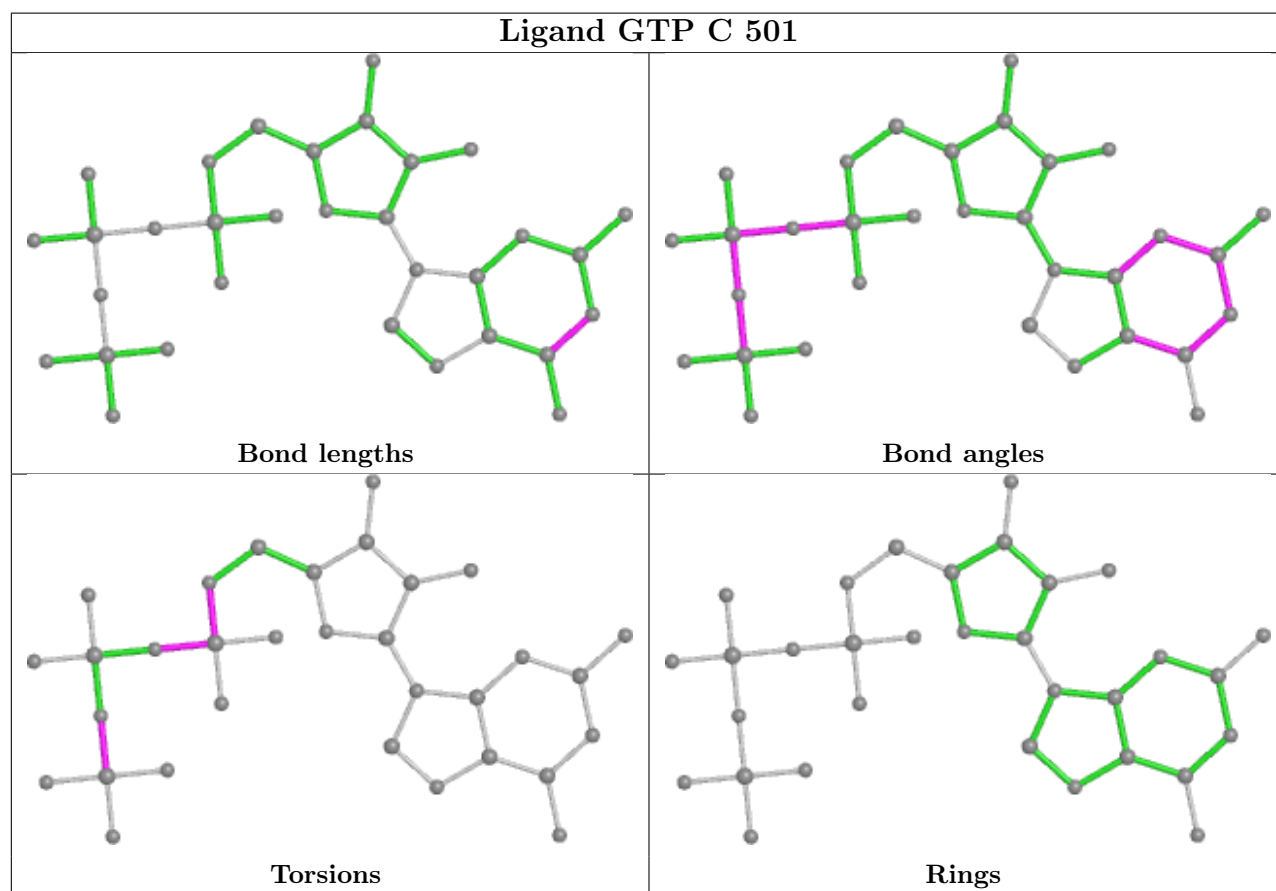
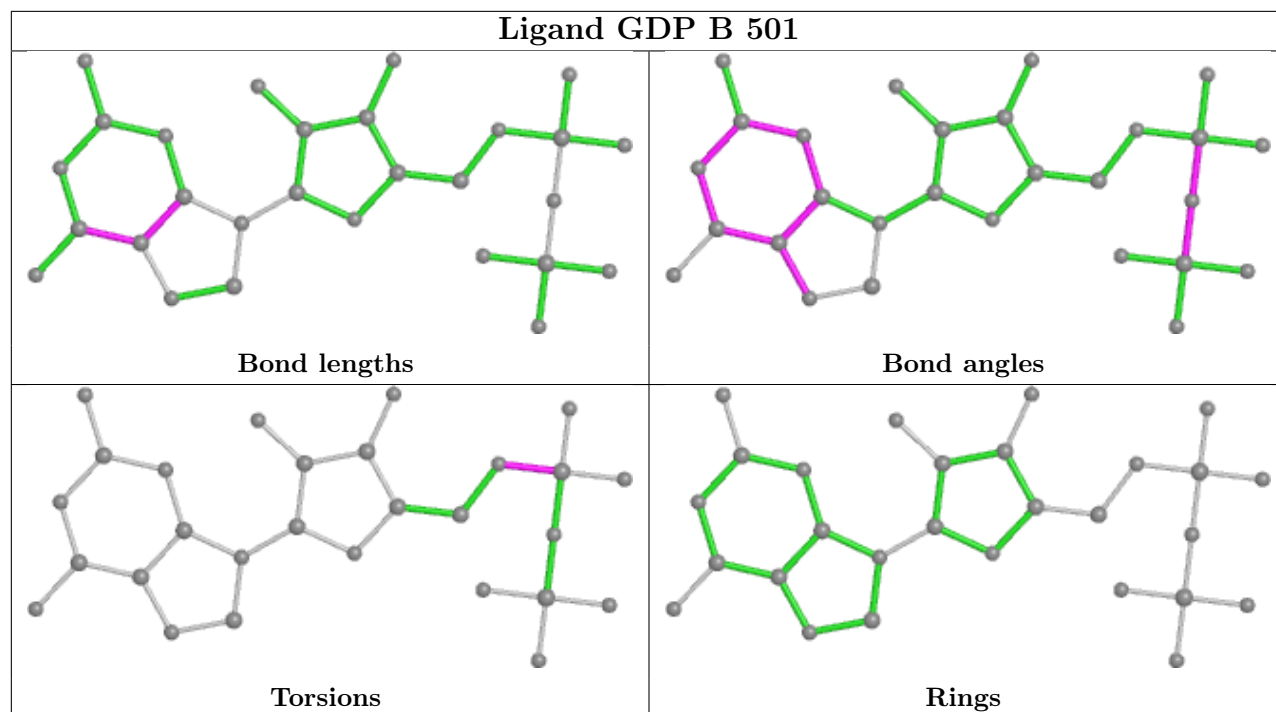
Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A

There are no ring outliers.

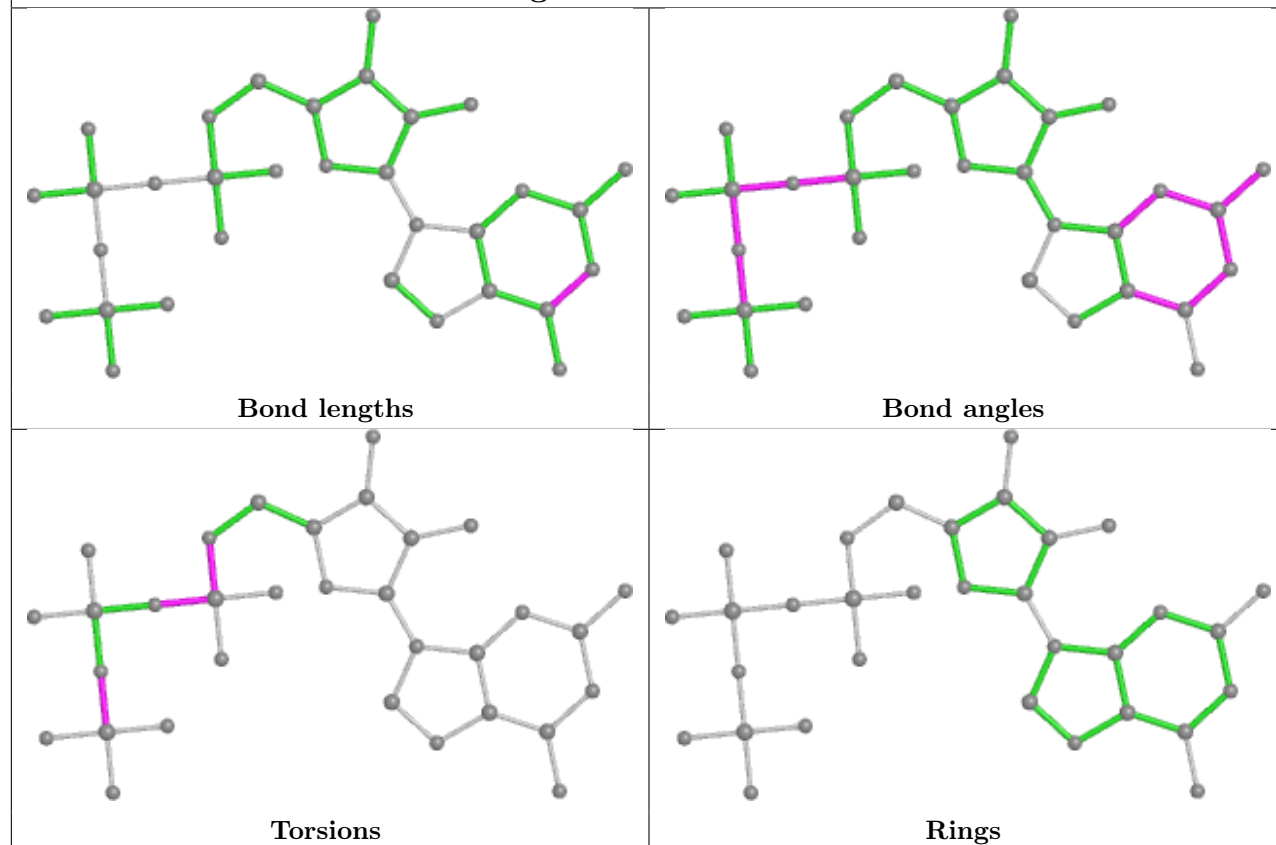
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	MES	3	0
8	B	501	GDP	1	0
5	A	501	GTP	1	0
8	D	501	GDP	3	0
11	F	401	ACP	4	0

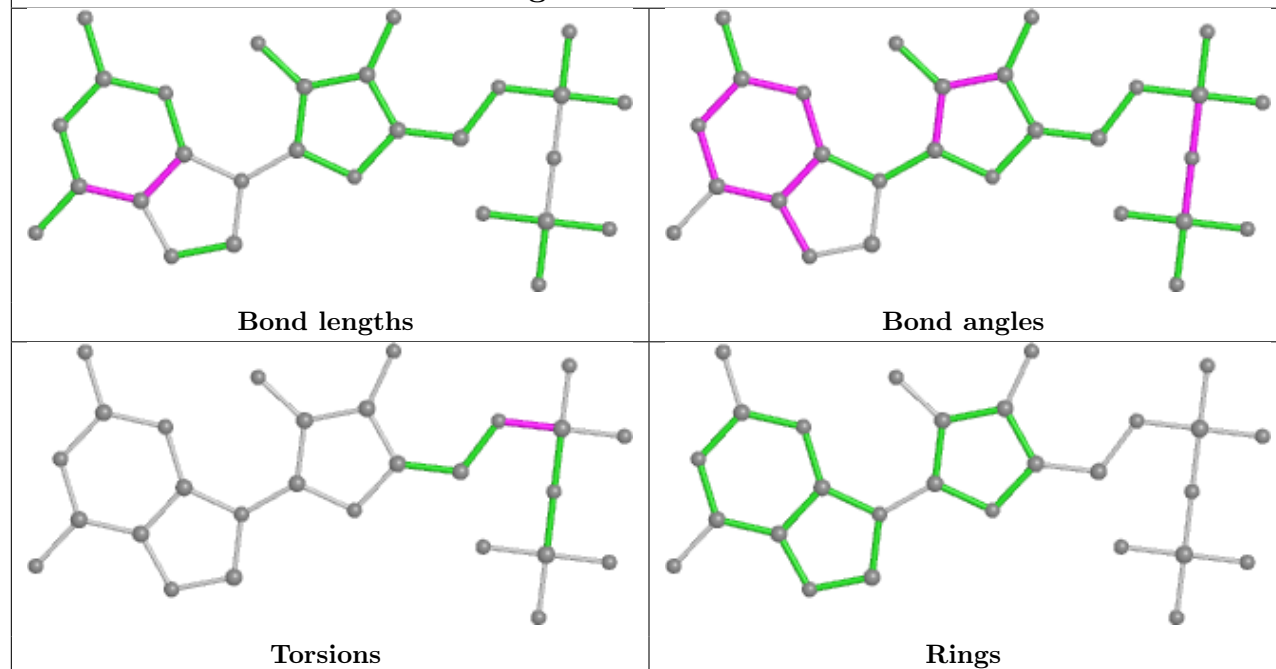
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

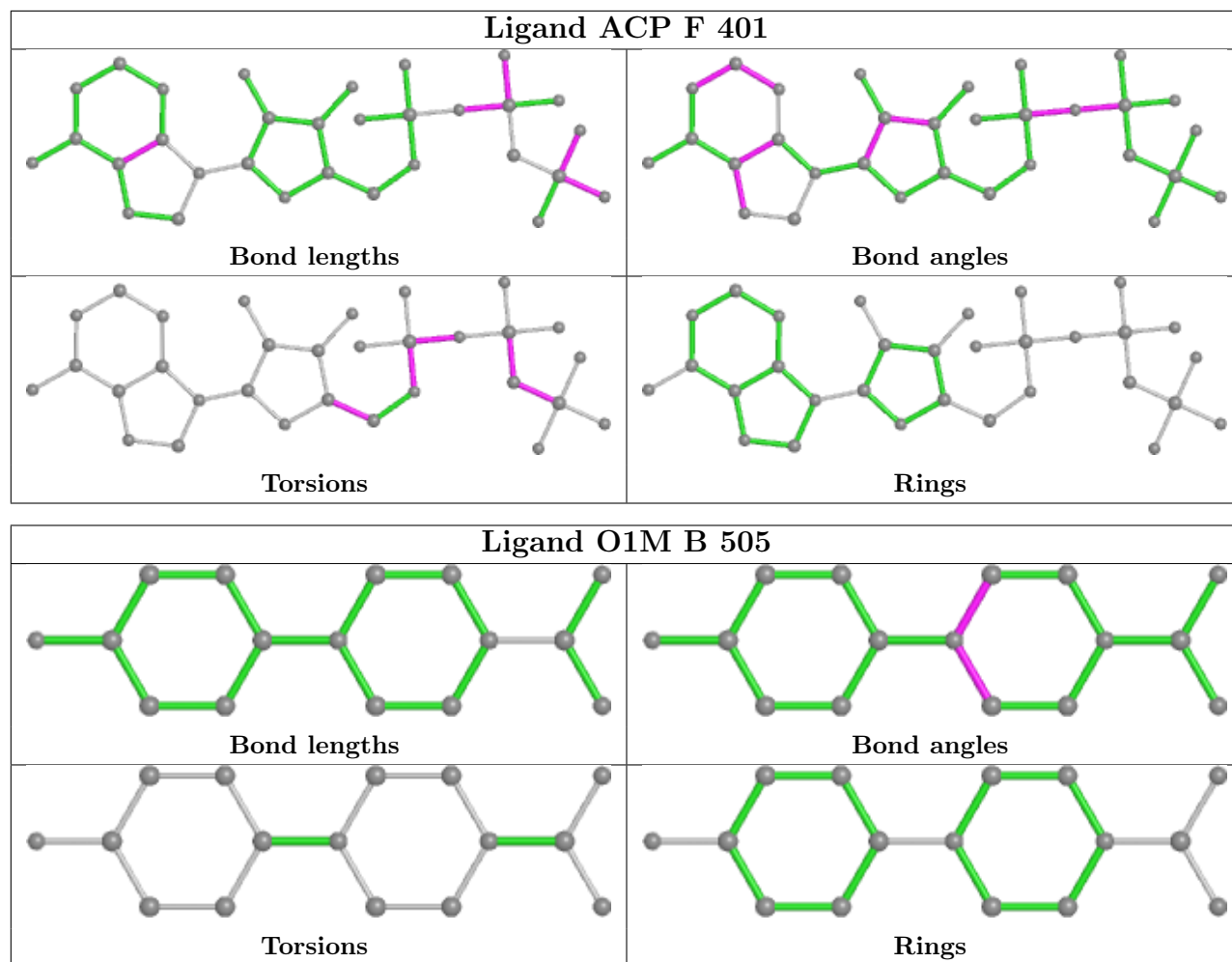


Ligand GTP A 501



Ligand GDP D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	-0.01	10 (2%) 60 64	38, 57, 98, 157	0
1	C	440/451 (97%)	0.03	5 (1%) 80 83	33, 47, 78, 114	0
2	B	421/445 (94%)	0.33	12 (2%) 51 55	35, 58, 105, 160	3 (0%)
2	D	431/445 (96%)	0.18	15 (3%) 44 48	42, 66, 102, 136	4 (0%)
3	E	123/143 (86%)	0.48	11 (8%) 9 10	46, 71, 120, 154	0
4	F	352/384 (91%)	0.83	58 (16%) 1 1	54, 86, 146, 191	0
All	All	2205/2319 (95%)	0.26	111 (5%) 28 31	33, 62, 115, 191	7 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	281	GLN	10.1
3	E	27	PRO	6.6
4	F	173	ILE	6.4
2	D	57	THR	6.3
2	B	284	ARG	6.3
4	F	240	LEU	5.7
4	F	105	LEU	5.4
4	F	249	TYR	5.2
3	E	26	PRO	5.1
2	B	1	MET	5.1
4	F	103	THR	5.0
4	F	253	TYR	4.9
2	B	276	THR	4.6
2	D	279	GLY	4.5
4	F	169	LEU	4.2
4	F	231	ALA	4.2
2	B	283	TYR	4.0
4	F	251	LYS	3.9
4	F	254	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	248	GLU	3.5
4	F	125	THR	3.4
4	F	372	THR	3.4
4	F	232	ASN	3.4
3	E	142	GLU	3.3
4	F	233	PHE	3.3
4	F	234	GLN	3.3
4	F	245	ILE	3.3
4	F	259	GLY	3.2
4	F	90	SER	3.1
4	F	252	ASN	3.1
1	A	284	GLU	3.1
4	F	250	SER	3.0
4	F	371	PRO	3.0
2	B	277	SER	3.0
2	D	278	ARG	3.0
2	B	57	THR	2.9
2	D	415	GLU	2.9
4	F	152	SER	2.9
4	F	236	LYS	2.9
2	B	285	ALA	2.9
4	F	142	ARG	2.9
4	F	20	LEU	2.9
3	E	24	LEU	2.8
2	B	59	ASN	2.8
4	F	135	TYR	2.8
4	F	225	SER	2.8
4	F	131	PHE	2.8
3	E	25	LYS	2.8
4	F	104	ASN	2.7
4	F	244	CYS	2.7
4	F	21	LEU	2.6
1	A	88	HIS	2.6
1	A	262	TYR	2.6
4	F	177	GLY	2.6
4	F	176	GLN	2.6
4	F	241	THR	2.6
4	F	243	HIS	2.6
1	C	335	ILE	2.5
3	E	6	MET	2.5
1	A	281	ALA	2.5
2	D	1	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	337	THR	2.5
2	B	333	LEU	2.4
4	F	149	ALA	2.4
2	D	280	SER	2.4
4	F	143	GLU	2.4
4	F	100	ILE	2.4
4	F	186	LEU	2.4
4	F	24	THR	2.4
2	D	88	ARG	2.4
4	F	256	TYR	2.4
1	C	247	ALA	2.4
2	D	293	GLN	2.3
1	C	339	ARG	2.3
2	D	401	ARG	2.3
4	F	258	GLU	2.3
2	D	276	THR	2.3
1	A	346	TRP	2.3
4	F	381	HIS	2.3
4	F	340	GLN	2.3
4	F	382	HIS	2.3
1	C	248	LEU	2.2
2	B	275	LEU	2.2
4	F	91	CYS	2.2
1	A	163	LYS	2.2
4	F	139	ARG	2.2
3	E	44	ASP	2.2
1	C	218	ASP	2.2
2	B	288	VAL	2.2
3	E	28	SER	2.2
4	F	179	VAL	2.2
4	F	161	LEU	2.2
4	F	178	GLN	2.2
4	F	17	VAL	2.1
1	A	219	ILE	2.1
2	D	87	PHE	2.1
2	D	127	GLU	2.1
1	A	349	THR	2.1
3	E	48	GLU	2.1
2	D	219	LEU	2.1
3	E	7	GLU	2.1
4	F	168	GLU	2.1
4	F	226	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	17	GLY	2.1
1	A	438	ASP	2.1
4	F	164	SER	2.0
2	D	58	GLY	2.0
4	F	27	TRP	2.0
4	F	239	HIS	2.0
4	F	170	LEU	2.0
2	D	94	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.80	0.13	87,87,87,87	0
6	MG	F	402	1/1	0.86	0.08	86,86,86,86	0
11	ACP	F	401	31/31	0.87	0.13	81,95,107,111	0
7	CA	A	503	1/1	0.89	0.04	80,80,80,80	0
9	MES	B	504	12/12	0.91	0.19	72,76,88,92	0
10	O1M	B	505	16/16	0.92	0.23	61,74,89,89	0
7	CA	E	201	1/1	0.92	0.10	80,80,80,80	0
7	CA	C	503	1/1	0.94	0.07	66,66,66,66	0
6	MG	D	502	1/1	0.96	0.06	69,69,69,69	0
6	MG	B	502	1/1	0.96	0.12	46,46,46,46	0
8	GDP	D	501	28/28	0.96	0.15	55,62,71,79	0
6	MG	A	502	1/1	0.97	0.12	39,39,39,39	0
5	GTP	A	501	32/32	0.98	0.14	33,42,45,51	0
6	MG	C	502	1/1	0.98	0.11	38,38,38,38	0
5	GTP	C	501	32/32	0.99	0.17	29,36,41,45	0

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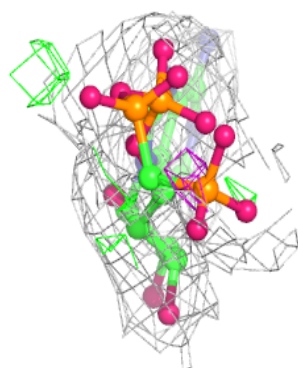
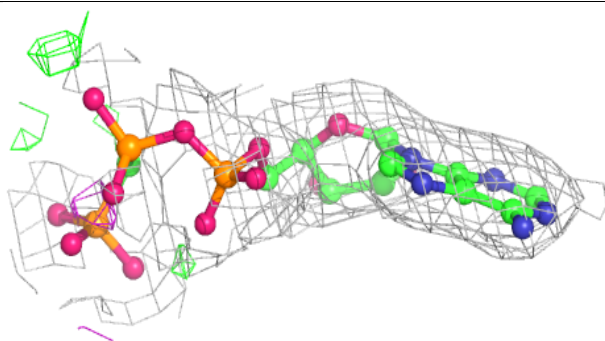
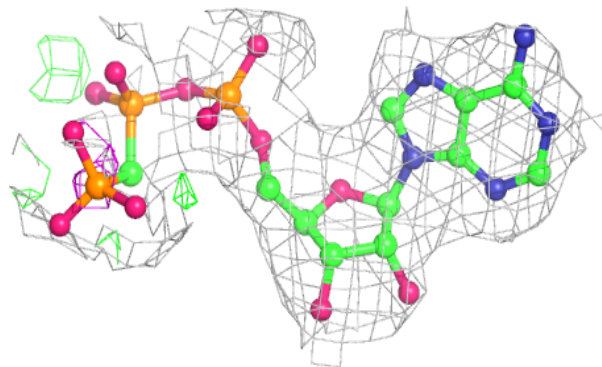
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GDP	B	501	28/28	0.99	0.15	35,42,46,54	0

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.

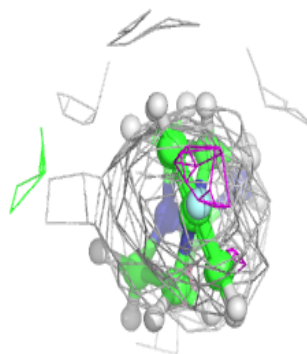
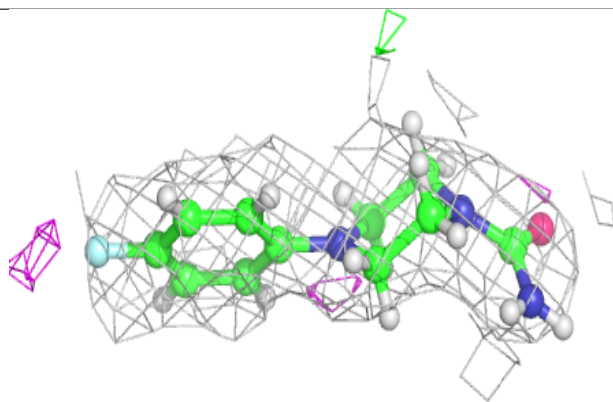
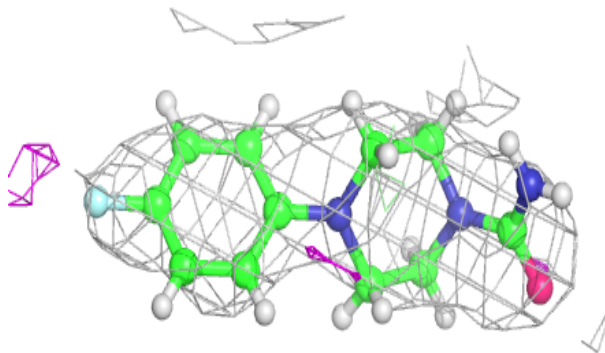
Electron density around ACP F 401:

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



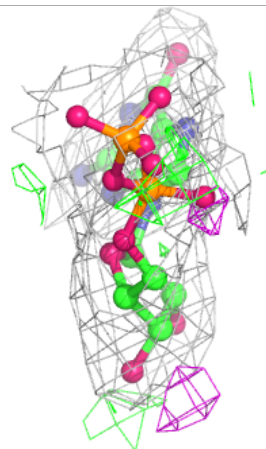
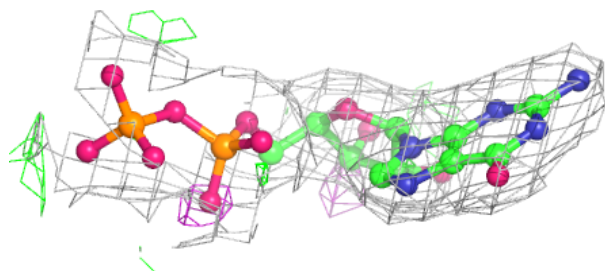
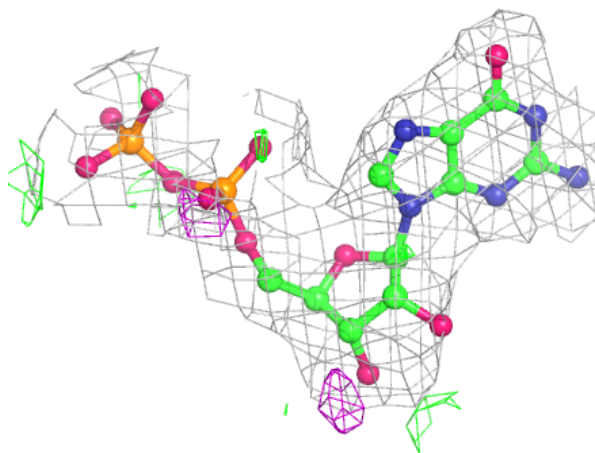
Electron density around O1M B 505:

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



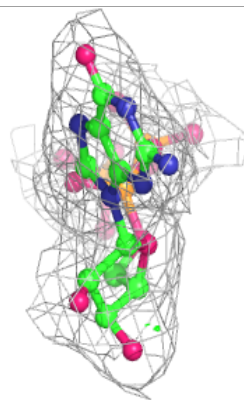
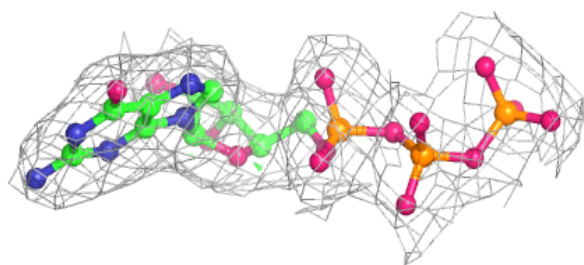
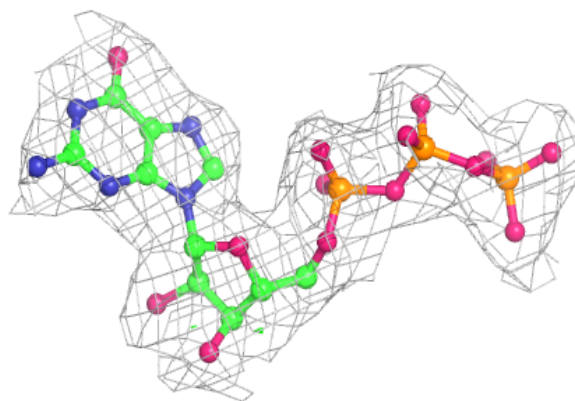
Electron density around GDP D 501:

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

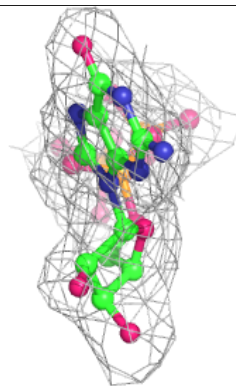
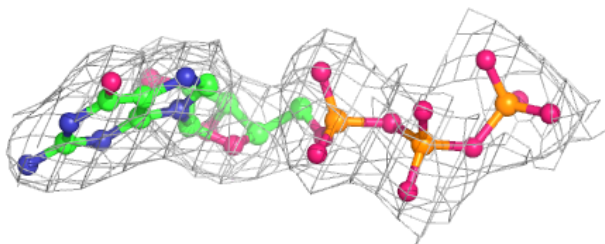
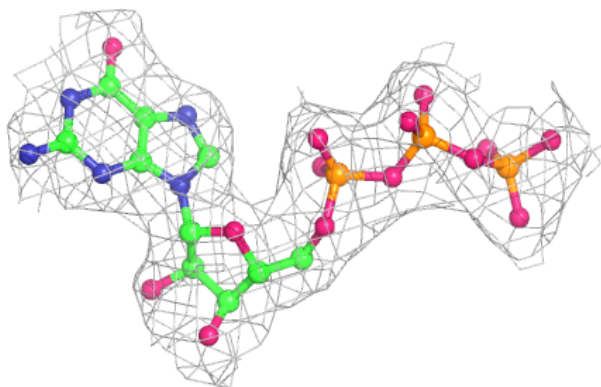


Electron density around GTP A 501:

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

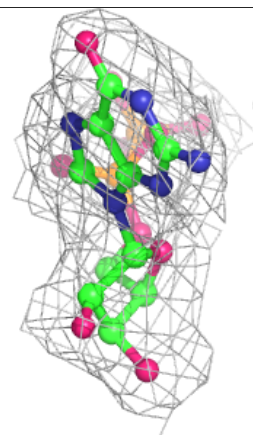
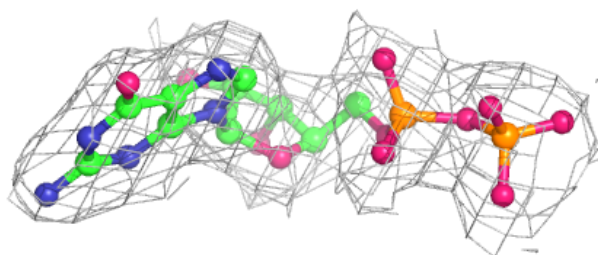
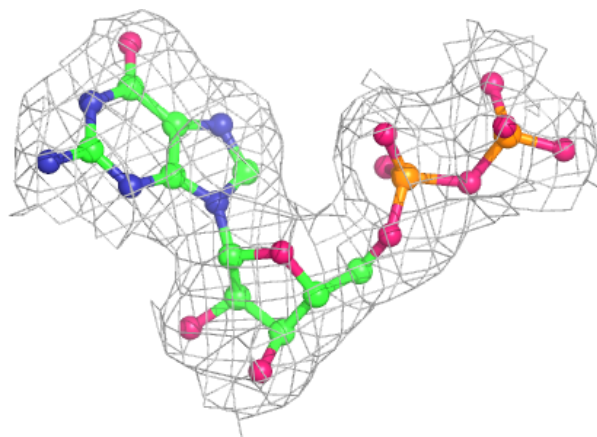
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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.