



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 01:47 PM EDT

PDB ID : 5S53  
Title : Tubulin-Z1349163663-complex  
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.  
Deposited on : 2020-11-08  
Resolution : 2.75 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

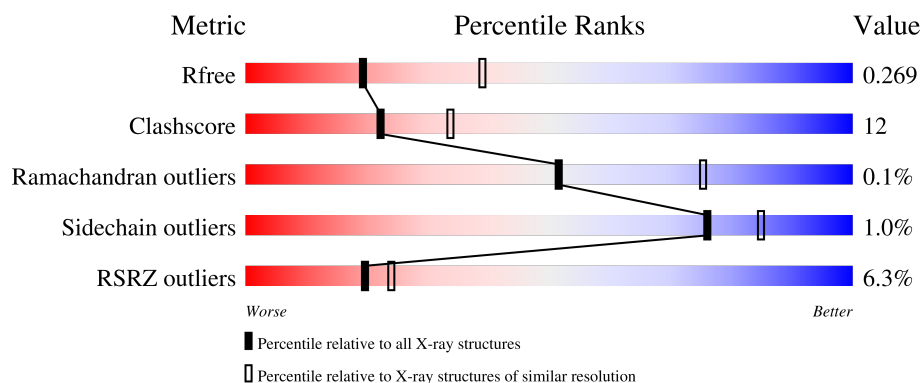
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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>73%</div> <div>24%</div> <div>.</div> </div>
1	C	451	<div> <div>5%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
2	B	445	<div> <div>7%</div> <div>70%</div> <div>24%</div> <div>..</div> </div>
2	D	445	<div> <div>7%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>
3	E	143	<div> <div>13%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>5%</div><div>65%</div><div>26%</div><div>8%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17802 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	425	Total	C	N	O	S	2	1	0
			3359	2109	577	646	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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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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		

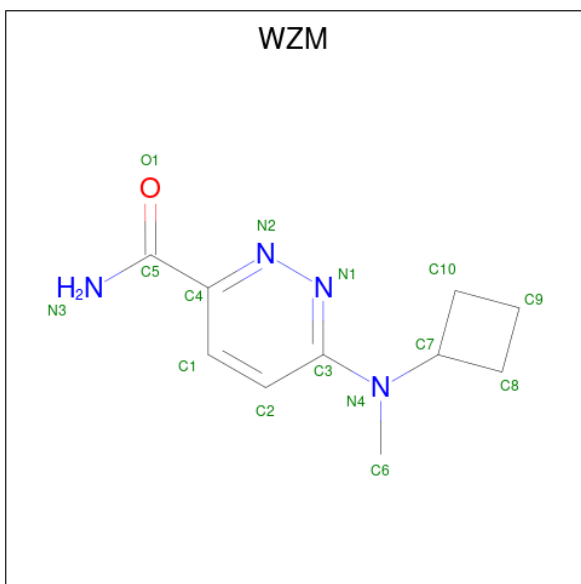
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).





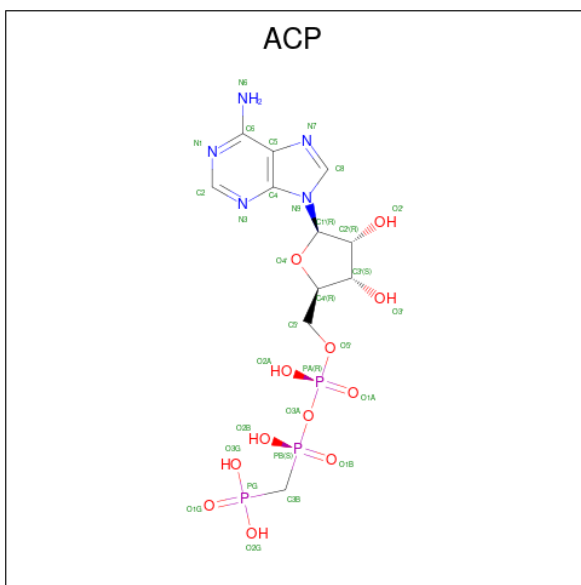
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 6-[cyclobutyl(methyl)amino]pyridazine-3-carboxamide (three-letter code: WZM) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			29	10	14	4	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



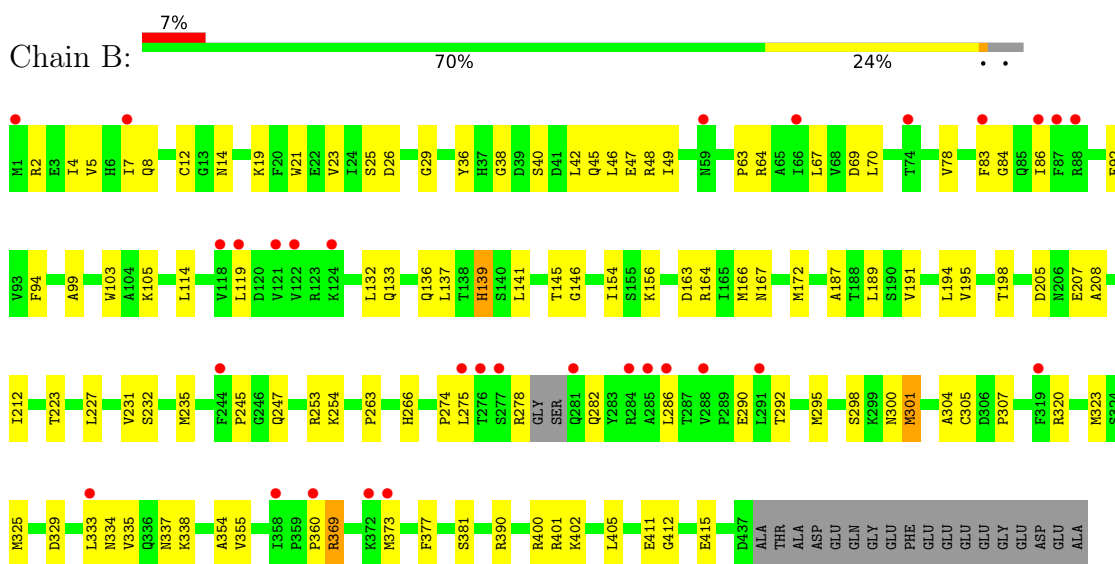
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 12 is water.

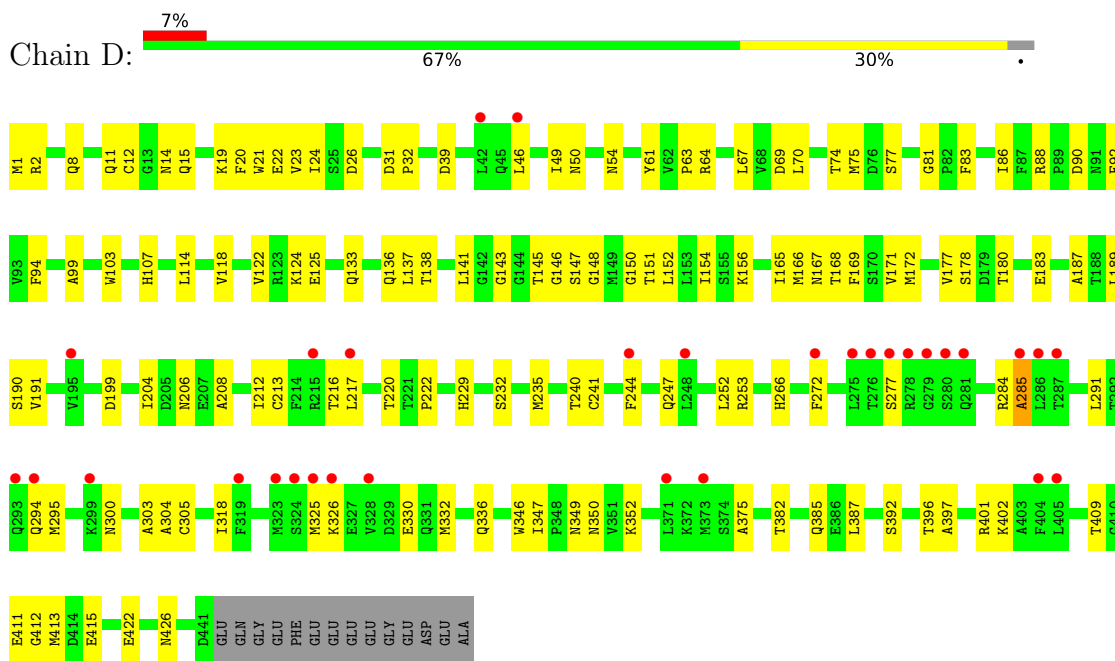
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	14	Total O 14 14	0	0
12	B	34	Total O 34 34	0	0
12	C	55	Total O 55 55	0	0
12	D	9	Total O 9 9	0	0
12	E	2	Total O 2 2	0	0
12	F	2	Total O 2 2	0	0



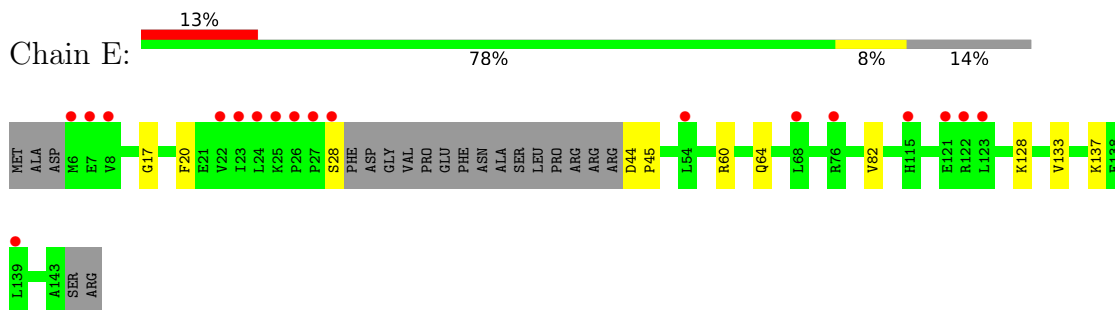




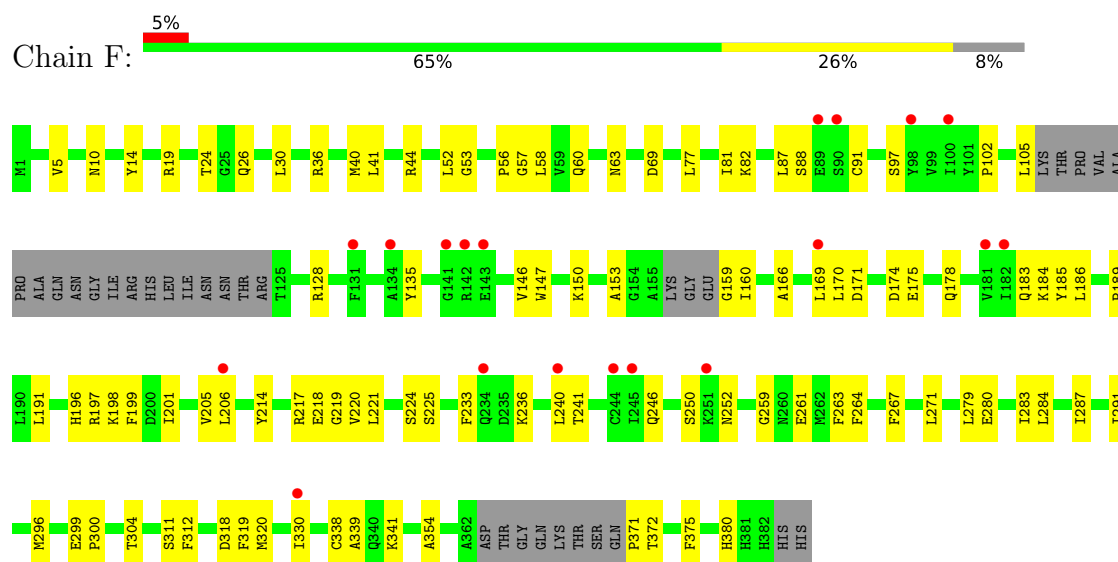
- Molecule 2: Tubulin beta-2B chain



- 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, $\alpha$ , $\beta$ , $\gamma$	105.32Å 159.31Å 178.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.19 – 2.75 118.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (68.19-2.75) 98.5 (118.99-2.75)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.218 , 0.267 0.219 , 0.269	Depositor DCC
$R_{free}$ test set	3795 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.6	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CA, GDP, ACP, MG, WZM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/3502	0.41	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.26	0/3433	0.42	0/4647
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1022	0.34	0/1356
4	F	0.24	0/2944	0.39	0/3978
All	All	0.25	0/17864	0.41	0/24179

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	75	0
1	C	3443	0	3352	85	0
2	B	3359	0	3235	87	0
2	D	3368	0	3236	90	0
3	E	1014	0	1029	10	0
4	F	2877	0	2839	79	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	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	2	0
8	D	28	0	12	3	0
9	B	12	0	12	4	0
10	B	15	14	0	1	0
11	F	31	0	14	4	0
12	A	14	0	0	1	0
12	B	34	0	0	2	0
12	C	55	0	0	3	0
12	D	9	0	0	1	0
12	E	2	0	0	0	0
12	F	2	0	0	1	0
All	All	17788	14	17099	408	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 12.

All (408) 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:209:ILE:HD11	1:C:302:MET:HE3	1.35	1.06
2:D:217:LEU:HA	2:D:277:SER:HB3	1.44	0.97
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.37	0.87
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.93	0.86
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.59	0.84
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.59	0.83
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.13	0.81
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.64	0.80
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.67	0.76
5:C:501:GTP:O1B	12:C:602:HOH:O	2.04	0.76
1:C:47:ASP:OD2	12:C:601:HOH:O	2.02	0.76
1:C:178:SER:OG	2:D:352:LYS:NZ	2.18	0.75
1:C:209:ILE:HD11	1:C:302:MET:CE	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.69	0.74
2:B:145:THR:HB	8:B:501:GDP:O2B	1.88	0.74
4:F:82:LYS:NZ	4:F:97:SER:O	2.20	0.72
2:D:136:GLN:HA	2:D:167:ASN:O	1.91	0.71
2:D:397:ALA:O	2:D:401:ARG:NH1	2.23	0.71
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.74	0.70
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.73	0.69
2:D:141:LEU:HA	2:D:147:SER:HB3	1.73	0.69
2:D:83:PHE:O	2:D:86:ILE:HG22	1.93	0.68
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.28	0.68
1:A:141:PHE:HB3	1:A:187:SER:OG	1.94	0.68
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.24	0.68
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.30	0.67
1:C:76:ASP:O	1:C:80:THR:HG22	1.94	0.67
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.28	0.67
2:B:4:ILE:O	2:B:64:ARG:HD2	1.95	0.67
4:F:91:CYS:HA	12:F:502:HOH:O	1.93	0.67
1:C:271:THR:HG21	1:C:295:CYS:O	1.94	0.66
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.78	0.66
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.30	0.66
2:D:332:MET:O	2:D:336:GLN:HG3	1.96	0.65
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.79	0.65
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.96	0.65
1:A:287:SER:O	1:A:291:ILE:HG23	1.97	0.65
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.31	0.65
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.13	0.64
1:A:320:ARG:HD2	12:A:609:HOH:O	1.96	0.64
1:C:178:SER:HB2	1:C:183:GLU:OE2	1.98	0.64
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.80	0.64
1:A:99:ALA:HA	1:A:105:ARG:HD3	1.80	0.64
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.33	0.64
2:D:143:GLY:O	2:D:147:SER:OG	2.15	0.64
1:C:142:GLY:HA3	1:C:183:GLU:OE1	1.99	0.63
1:C:186:ASN:O	1:C:190:THR:HG22	1.98	0.63
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.80	0.63
4:F:63:ASN:HA	4:F:312:PHE:O	1.99	0.63
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.81	0.63
2:B:390:ARG:NH1	12:B:601:HOH:O	2.27	0.62
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.28	0.62
1:A:166:LYS:HE2	1:A:197:HIS:O	1.98	0.62
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.80	0.62
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.82	0.62
2:D:145:THR:HB	8:D:501:GDP:O2B	2.00	0.62
2:B:415:GLU:HG3	12:B:622:HOH:O	1.99	0.62
2:D:220:THR:O	2:D:222:PRO:HD3	1.99	0.61
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.11	0.61
2:B:19:LYS:O	2:B:23:VAL:HG23	2.01	0.61
2:D:180:THR:O	2:D:183:GLU:HG3	2.00	0.61
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.82	0.61
2:D:141:LEU:HD12	2:D:172:MET:SD	2.40	0.61
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.10	0.61
1:C:165:SER:HA	1:C:199:ASP:OD2	2.01	0.60
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.82	0.60
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.83	0.60
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.84	0.60
4:F:371:PRO:HA	4:F:372:THR:C	2.21	0.60
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.82	0.60
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.17	0.60
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.83	0.59
1:C:114:ILE:O	1:C:118:VAL:HG23	2.01	0.59
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.02	0.59
2:B:223:THR:O	2:B:227:LEU:HD13	2.02	0.59
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.84	0.59
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.33	0.59
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.85	0.59
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.32	0.59
1:A:431:ASP:O	1:A:435:VAL:HG23	2.03	0.58
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.67	0.58
4:F:40:MET:HE3	4:F:52:LEU:HD21	1.84	0.58
2:B:231:VAL:O	2:B:235:MET:HG3	2.04	0.58
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.03	0.58
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.39	0.58
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.86	0.57
4:F:320:MET:CG	4:F:330:ILE:HD11	2.34	0.57
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.85	0.57
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.37	0.57
2:D:69:ASP:O	2:D:94:PHE:HA	2.05	0.57
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.86	0.57
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.86	0.56
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.87	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:O	2:B:86:ILE:HG22	2.05	0.56
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.56
4:F:159:GLY:C	4:F:160:ILE:HD12	2.26	0.56
1:A:3:GLU:OE1	1:A:129:CYS:HB3	2.06	0.56
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.41	0.56
4:F:371:PRO:CA	4:F:372:THR:HB	2.35	0.56
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.20	0.56
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.41	0.56
2:B:278:ARG:HG2	2:B:282:GLN:NE2	2.21	0.56
4:F:225:SER:O	4:F:252:ASN:HB2	2.06	0.56
1:C:216:ASN:HB3	1:C:275:VAL:O	2.06	0.55
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.87	0.55
3:E:60:ARG:O	3:E:64:GLN:HG3	2.06	0.55
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.72	0.55
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.36	0.55
2:D:303:ALA:O	2:D:305:CYS:N	2.40	0.55
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.06	0.55
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.46	0.55
2:D:392:SER:O	2:D:396:THR:HG22	2.07	0.55
4:F:371:PRO:HA	4:F:372:THR:HB	1.87	0.55
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.88	0.54
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.89	0.54
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.90	0.54
4:F:150:LYS:HD2	11:F:401:ACP:O2A	2.08	0.54
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.41	0.54
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.90	0.54
1:A:289:ALA:HA	1:A:331:ALA:HB2	1.89	0.53
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.89	0.53
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.73	0.53
2:B:47:GLU:HG2	2:B:245:PRO:HB3	1.89	0.53
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.90	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.44	0.53
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.41	0.53
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.91	0.53
2:D:2:ARG:CB	2:D:133:GLN:HE21	2.20	0.53
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.38	0.53
2:B:23:VAL:CG2	2:B:232:SER:HB3	2.38	0.53
2:B:205:ASP:OD1	2:B:207:GLU:N	2.39	0.53
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.43	0.53
1:C:100:ALA:HB2	2:D:253:ARG:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.90	0.53
4:F:296:MET:SD	4:F:380:HIS:HB2	2.49	0.53
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.42	0.52
2:B:114:LEU:O	2:B:114:LEU:HG	2.09	0.52
2:B:29:GLY:O	2:B:36:TYR:HA	2.10	0.52
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.91	0.52
1:A:100:ALA:CB	2:B:253[B]:ARG:HG2	2.40	0.52
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.45	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.45	0.52
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.45	0.52
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.92	0.52
1:C:99:ALA:O	1:C:105:ARG:HD3	2.08	0.52
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.45	0.52
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.92	0.51
1:A:231:ILE:O	1:A:235:VAL:HG23	2.10	0.51
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.91	0.51
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.91	0.51
1:A:227:LEU:O	1:A:231:ILE:HG13	2.11	0.51
1:C:141:PHE:HB3	1:C:187:SER:OG	2.09	0.51
2:D:11:GLN:HA	2:D:74:THR:HG21	1.93	0.51
1:A:88:HIS:HD2	1:A:90:GLU:HB2	1.75	0.51
2:B:198:THR:OG1	2:B:266:HIS:NE2	2.40	0.51
1:C:288:VAL:HG23	12:C:649:HOH:O	2.09	0.51
2:D:147:SER:O	2:D:151:THR:HG23	2.11	0.51
2:B:329:ASP:O	2:B:333:LEU:HG	2.11	0.50
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.46	0.50
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.92	0.50
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.46	0.50
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.52	0.50
2:B:136:GLN:HA	2:B:167:ASN:O	2.11	0.50
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.46	0.50
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.47	0.50
2:D:67:LEU:N	2:D:67:LEU:HD12	2.26	0.50
2:B:325:MET:HE1	2:B:355:VAL:HB	1.93	0.50
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.42	0.50
1:A:223:THR:HB	2:B:247:GLN:HE22	1.77	0.50
1:C:267:PHE:O	1:C:384:ILE:HD13	2.11	0.50
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.45	0.50
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.11	0.50
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.93	0.50
1:C:139:HIS:ND1	1:C:146:GLY:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.27	0.50
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.94	0.49
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.93	0.49
2:D:178:SER:HB3	2:D:183:GLU:OE2	2.12	0.49
4:F:150:LYS:NZ	4:F:183:GLN:OE1	2.27	0.49
4:F:267:PHE:O	4:F:271:LEU:HG	2.12	0.49
2:D:411:GLU:OE1	3:E:137:LYS:NZ	2.34	0.49
1:A:270:ALA:HB3	1:A:302:MET:CG	2.42	0.49
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.95	0.49
1:A:12:ALA:CB	1:A:140:SER:HB3	2.42	0.49
2:B:208:ALA:O	2:B:212:ILE:HG13	2.12	0.49
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.12	0.49
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.21	0.49
1:A:289:ALA:HA	1:A:331:ALA:CB	2.42	0.49
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.13	0.49
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.95	0.49
2:B:305:CYS:O	2:B:307:PRO:HD3	2.12	0.48
2:D:118:VAL:O	2:D:122:VAL:HG23	2.12	0.48
2:B:105:LYS:HE2	2:B:411:GLU:OE2	2.12	0.48
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.14	0.48
2:B:402:LYS:CB	2:B:405:LEU:HD12	2.43	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.48
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.28	0.48
2:B:298:SER:HA	2:B:301:MET:HG3	1.95	0.48
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.49	0.48
4:F:19:ARG:HD2	4:F:19:ARG:O	2.14	0.48
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.48	0.48
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.49	0.48
1:A:99:ALA:CA	1:A:105:ARG:HD3	2.44	0.48
4:F:338:CYS:SG	4:F:339:ALA:N	2.87	0.48
2:B:320:ARG:NH1	2:B:360:PRO:HG3	2.29	0.48
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.96	0.48
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.38	0.48
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.48	0.48
1:A:2:ARG:HB3	1:A:131:GLY:O	2.13	0.48
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.94	0.48
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.95	0.48
4:F:198:LYS:HG2	4:F:199:PHE:H	1.79	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.47
2:D:294:GLN:HG2	2:D:300:ASN:ND2	2.29	0.47
1:A:114:ILE:HG12	1:A:114:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:CA	2:D:147:SER:HB3	2.43	0.47
2:D:326:LYS:O	2:D:330:GLU:HG3	2.14	0.47
4:F:69:ASP:OD1	4:F:69:ASP:N	2.47	0.47
2:B:67:LEU:N	2:B:67:LEU:HD12	2.30	0.47
2:D:77:SER:O	2:D:81:GLY:N	2.47	0.47
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.49	0.47
4:F:197:ARG:HB2	4:F:224:SER:O	2.15	0.47
1:C:174:ALA:HB2	1:C:207:GLU:H	1.79	0.47
4:F:246:GLN:O	4:F:250:SER:HB3	2.14	0.47
2:B:334:ASN:O	2:B:338:LYS:HG3	2.15	0.47
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.96	0.47
2:D:19:LYS:O	2:D:23:VAL:HG23	2.13	0.47
1:C:234:ILE:HD12	1:C:234:ILE:H	1.80	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.50	0.47
4:F:128:ARG:HH12	4:F:170:LEU:HB3	1.80	0.47
1:C:241:SER:HA	1:C:249:ASN:OD1	2.14	0.47
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.50	0.47
2:D:103:TRP:CD1	2:D:148:GLY:HA2	2.50	0.47
2:B:253[A]:ARG:NH1	9:B:504:MES:S	2.75	0.47
1:C:234:ILE:HG12	1:C:302:MET:CE	2.44	0.46
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.14	0.46
1:A:188:ILE:HD12	1:A:395:PHE:CB	2.45	0.46
2:B:78:VAL:O	2:B:84:GLY:HA3	2.15	0.46
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.30	0.46
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.78	0.46
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.97	0.46
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.98	0.46
1:C:80:THR:O	1:C:80:THR:OG1	2.32	0.46
2:D:187:ALA:O	2:D:191:VAL:HG23	2.15	0.46
2:B:323:MET:HE2	2:B:373:MET:HB2	1.96	0.46
1:C:25:CYS:HB3	1:C:30:ILE:O	2.16	0.46
4:F:171:ASP:O	4:F:175:GLU:HG3	2.16	0.46
2:B:46:LEU:HA	2:B:49:ILE:HB	1.96	0.46
2:B:69:ASP:OD1	2:B:70:LEU:N	2.48	0.46
2:D:107:HIS:O	2:D:152:LEU:HD22	2.16	0.45
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.81	0.45
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.98	0.45
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.46	0.45
4:F:371:PRO:HA	4:F:372:THR:O	2.17	0.45
2:B:412:GLY:O	3:E:82:VAL:HG13	2.17	0.45
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:CYS:HA	1:C:266:HIS:HB2	1.97	0.45
2:B:42:LEU:H	2:B:42:LEU:HD12	1.82	0.45
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.85	0.45
2:D:70:LEU:HD23	2:D:114:LEU:HD22	1.98	0.45
1:C:108:TYR:O	1:C:112:LYS:HG2	2.17	0.45
1:C:75:ILE:HB	1:C:94:THR:HG21	1.99	0.45
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.52	0.45
4:F:146:VAL:HG11	4:F:233:PHE:CZ	2.52	0.45
1:A:248:LEU:HD23	1:A:354:GLY:HA3	1.99	0.45
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.52	0.45
2:D:284:ARG:O	2:D:285:ALA:HB3	2.17	0.45
2:D:409:THR:HA	2:D:413:MET:O	2.17	0.45
4:F:53:GLY:N	4:F:60:GLN:OE1	2.33	0.45
4:F:304:THR:HG21	4:F:311:SER:OG	2.16	0.45
1:C:236:SER:O	1:C:240:ALA:HB2	2.17	0.45
3:E:128:LYS:O	3:E:128:LYS:HD3	2.17	0.45
4:F:372:THR:O	4:F:372:THR:HG22	2.17	0.45
1:C:192:HIS:CG	1:C:421:ALA:HA	2.52	0.44
2:D:382:THR:O	2:D:385:GLN:HG2	2.16	0.44
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.17	0.44
1:A:355:ILE:O	3:E:17:GLY:HA3	2.17	0.44
2:B:2:ARG:CB	2:B:133:GLN:HE21	2.31	0.44
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.47	0.44
1:C:234:ILE:HD12	1:C:234:ILE:N	2.33	0.44
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.98	0.44
4:F:186:LEU:O	4:F:189:PRO:HD3	2.18	0.44
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.83	0.44
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.44
1:A:176:GLN:HG3	4:F:56:PRO:HB3	2.00	0.44
1:C:75:ILE:HB	1:C:94:THR:CG2	2.47	0.44
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.47	0.44
2:D:152:LEU:O	2:D:156:LYS:HG2	2.17	0.44
1:A:99:ALA:C	1:A:105:ARG:HD3	2.37	0.44
2:B:412:GLY:C	3:E:82:VAL:HG13	2.38	0.44
2:D:8:GLN:HB3	2:D:138:THR:OG1	2.17	0.44
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.52	0.44
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.53	0.44
1:A:100:ALA:HA	2:B:254:LYS:HB2	2.00	0.44
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.44
2:B:70:LEU:HD12	2:B:99:ALA:HB2	2.00	0.44
2:D:295:MET:HE2	2:D:295:MET:HB2	1.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.98	0.43
1:A:201:ALA:HB3	1:A:267:PHE:CD2	2.54	0.43
2:B:163:ASP:O	2:B:164:ARG:NE	2.51	0.43
2:D:212:ILE:O	2:D:216:THR:HB	2.18	0.43
4:F:184:LYS:O	11:F:401:ACP:N6	2.45	0.43
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.48	0.43
2:B:5:VAL:HG23	2:B:132:LEU:HD11	1.99	0.43
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.53	0.43
1:C:419:SER:O	1:C:423:GLU:HG3	2.18	0.43
2:B:194:LEU:HA	2:B:198:THR:HG23	1.99	0.43
1:C:270:ALA:O	1:C:302:MET:HG2	2.18	0.43
2:B:286:LEU:HD12	2:B:286:LEU:HA	1.86	0.43
2:B:369:ARG:HA	2:B:369:ARG:HD3	1.90	0.43
2:B:139:HIS:ND1	2:B:146:GLY:O	2.47	0.43
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.54	0.43
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.00	0.43
1:A:70:LEU:HD12	1:A:145:THR:OG1	2.17	0.43
2:B:354:ALA:HB2	10:B:505:WZM:C8	2.49	0.43
1:C:100:ALA:CB	2:D:253:ARG:HD2	2.49	0.43
1:C:250:VAL:HG11	1:C:352:LYS:HE3	2.00	0.43
4:F:259:GLY:O	4:F:261:GLU:HG3	2.19	0.43
2:D:99:ALA:HB2	2:D:145:THR:OG1	2.19	0.43
4:F:267:PHE:HE2	4:F:279:LEU:HD13	1.83	0.43
2:B:333:LEU:O	2:B:337:ASN:ND2	2.51	0.42
4:F:240:LEU:O	4:F:246:GLN:NE2	2.51	0.42
1:A:11:GLN:HG3	1:A:74:VAL:HG21	2.00	0.42
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.52	0.42
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.18	0.42
2:B:275:LEU:HD12	2:B:300:ASN:ND2	2.34	0.42
2:D:75:MET:CE	2:D:92:PHE:HD2	2.32	0.42
1:A:437:VAL:HG12	1:A:438:ASP:N	2.34	0.42
2:B:119:LEU:HD11	2:B:156:LYS:CB	2.49	0.42
2:D:294:GLN:HG2	2:D:300:ASN:HD21	1.84	0.42
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.54	0.42
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.54	0.42
2:B:191:VAL:O	2:B:195:VAL:HG23	2.19	0.42
2:B:295:MET:HG3	2:B:377:PHE:HB2	2.02	0.42
1:C:168:GLU:OE2	1:C:194:THR:HG21	2.20	0.42
1:C:231:ILE:O	1:C:235:VAL:HG23	2.20	0.42
1:C:271:THR:HG21	1:C:295:CYS:HA	2.01	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:HA	1:A:105:ARG:CD	2.49	0.42
2:D:54:ASN:O	2:D:61:TYR:HA	2.19	0.42
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.54	0.42
4:F:153:ALA:HB3	4:F:178:GLN:HG3	2.01	0.42
1:C:46:ASP:OD1	1:C:46:ASP:N	2.53	0.42
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.55	0.42
1:A:320:ARG:HA	1:A:356:ASN:O	2.20	0.42
2:B:21:TRP:O	2:B:25:SER:OG	2.15	0.42
2:B:40:SER:OG	2:B:42:LEU:HD13	2.20	0.42
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.20	0.42
2:D:124:LYS:C	2:D:124:LYS:HD3	2.39	0.42
2:D:208:ALA:O	2:D:212:ILE:HG13	2.19	0.42
2:D:272:PHE:HE2	12:D:609:HOH:O	2.02	0.42
4:F:146:VAL:O	4:F:185:TYR:HB3	2.20	0.42
4:F:240:LEU:HD12	4:F:240:LEU:N	2.35	0.42
1:A:275:VAL:HG13	1:A:368:LEU:HD22	2.01	0.42
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.55	0.42
2:B:8:GLN:NE2	2:B:14:ASN:HA	2.35	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.41
2:B:141:LEU:HD12	2:B:172:MET:SD	2.60	0.41
1:C:345:ASP:OD1	1:C:346:TRP:N	2.53	0.41
1:C:361:THR:HG22	1:C:362:VAL:N	2.34	0.41
1:C:433:GLU:O	1:C:437:VAL:HG23	2.19	0.41
4:F:87:LEU:O	4:F:88:SER:OG	2.27	0.41
4:F:19:ARG:HD2	4:F:19:ARG:C	2.41	0.41
1:A:54:SER:O	1:A:61:HIS:HA	2.21	0.41
1:C:271:THR:CG2	1:C:295:CYS:HA	2.51	0.41
2:D:11:GLN:O	2:D:15:GLN:HG2	2.20	0.41
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.02	0.41
1:A:115:ILE:HG23	1:A:116:ASP:N	2.36	0.41
2:B:164:ARG:O	9:B:504:MES:H31	2.19	0.41
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.56	0.41
2:D:240:THR:HG23	2:D:244:PHE:HD2	1.86	0.41
2:B:187:ALA:O	2:B:191:VAL:HG23	2.21	0.41
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.50	0.41
2:D:412:GLY:C	3:E:133:VAL:HG13	2.41	0.41
9:B:504:MES:H81	9:B:504:MES:H51	1.83	0.41
4:F:128:ARG:NH1	4:F:170:LEU:HD22	2.35	0.41
4:F:287:ILE:O	4:F:291:ILE:HG13	2.21	0.41
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.56	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:335:ILE:HG13	2.21	0.41
1:A:435:VAL:HG12	1:A:435:VAL:O	2.21	0.41
1:C:175:PRO:HB3	2:D:349:ASN:ND2	2.35	0.41
4:F:77:LEU:HD11	4:F:81:ILE:HD11	2.02	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.41
4:F:225:SER:HB2	4:F:252:ASN:O	2.21	0.41
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.36	0.41
2:D:272:PHE:O	2:D:300:ASN:HB3	2.21	0.41
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.92	0.41
1:A:174:ALA:HB2	1:A:207:GLU:H	1.86	0.40
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.03	0.40
2:D:291:LEU:HG	2:D:375:ALA:HB2	2.03	0.40
4:F:24:THR:O	4:F:26:GLN:HG3	2.21	0.40
1:C:79:ARG:HG2	1:C:92:LEU:HD12	2.04	0.40
1:C:115:ILE:HG23	1:C:116:ASP:N	2.36	0.40
2:D:46:LEU:HA	2:D:49:ILE:HB	2.03	0.40
4:F:283:ILE:O	4:F:287:ILE:HG13	2.21	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.03	0.40
1:A:271:THR:HG21	1:A:295:CYS:O	2.21	0.40
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.03	0.40
2:D:146:GLY:O	2:D:150:GLY:HA3	2.22	0.40
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.36	0.40
1:A:188:ILE:HD11	1:A:392:ASP:HA	2.03	0.40
1:C:9:VAL:CG1	1:C:145:THR:HG22	2.51	0.40
1:C:229:ARG:O	1:C:232:SER:OG	2.36	0.40
2:D:199:ASP:O	2:D:266:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	416 (95%)	20 (5%)	0	100	100
1	C	439/451 (97%)	421 (96%)	18 (4%)	0	100	100
2	B	422/445 (95%)	404 (96%)	18 (4%)	0	100	100
2	D	429/445 (96%)	406 (95%)	21 (5%)	2 (0%)	29	47
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	321 (93%)	23 (7%)	0	100	100
All	All	2189/2319 (94%)	2085 (95%)	102 (5%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	304	ALA
2	D	285	ALA

### 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%)	364 (99%)	5 (1%)	67	79
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	B	368/383 (96%)	363 (99%)	5 (1%)	67	79
2	D	368/383 (96%)	363 (99%)	5 (1%)	67	79
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1902/1993 (95%)	1883 (99%)	19 (1%)	76	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	282	TYR

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Mol	Chain	Res	Type
1	A	300	ASN
1	A	381	THR
2	B	48	ARG
2	B	139	HIS
2	B	301	MET
2	B	369	ARG
2	B	381	SER
1	C	71	GLU
1	C	80	THR
1	C	251	ASP
1	C	381	THR
2	D	26	ASP
2	D	39	ASP
2	D	229	HIS
2	D	241	CYS
2	D	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
2	B	15	GLN
2	B	247	GLN
2	B	282	GLN
2	B	294	GLN
2	B	300	ASN
1	C	15	GLN
1	C	31	GLN
1	C	342	GLN
2	D	133	GLN
2	D	167	ASN
2	D	294	GLN
2	D	349	ASN
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

### 5.3.3 RNA ⓘ

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	$\# Z  > 2$
11	ACP	F	401	6	27,33,33	1.38	5 (18%)	32,52,52	1.49	4 (12%)
5	GTP	C	501	6	26,34,34	1.03	1 (3%)	33,54,54	1.78	8 (24%)
8	GDP	D	501	6	24,30,30	1.16	2 (8%)	31,47,47	1.92	8 (25%)
9	MES	B	504	-	12,12,12	2.22	1 (8%)	14,16,16	1.97	6 (42%)
10	WZM	B	505	-	16,16,16	0.79	1 (6%)	19,22,22	1.24	1 (5%)
8	GDP	B	501	6	24,30,30	1.22	2 (8%)	31,47,47	1.91	7 (22%)
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.74	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
11	ACP	F	401	6	-	8/15/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	WZM	B	505	-	-	4/8/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	501	6	-	2/12/32/32	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.43	1.67	1.77
8	B	501	GDP	C6-C5	4.25	1.48	1.41
8	D	501	GDP	C6-C5	4.10	1.48	1.41
5	C	501	GTP	C6-N1	3.12	1.38	1.33
5	A	501	GTP	C6-N1	3.09	1.38	1.33
11	F	401	ACP	PG-O3G	2.92	1.61	1.54
11	F	401	ACP	PG-O2G	2.89	1.61	1.54
10	B	505	WZM	C7-N4	-2.76	1.44	1.48
11	F	401	ACP	PB-O3A	2.71	1.61	1.58
11	F	401	ACP	C5-C4	2.53	1.47	1.40
8	B	501	GDP	C5-C4	2.44	1.47	1.40
8	D	501	GDP	C5-C4	2.41	1.47	1.40
11	F	401	ACP	PB-O2B	2.26	1.61	1.56

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.28	120.18	127.22
5	A	501	GTP	N3-C2-N1	-5.25	120.21	127.22
8	B	501	GDP	C2-N3-C4	4.82	120.86	115.36
8	D	501	GDP	C2-N3-C4	4.82	120.86	115.36
5	A	501	GTP	C2-N3-C4	4.34	120.32	115.36
11	F	401	ACP	PA-O3A-PB	-4.25	119.09	132.56
5	C	501	GTP	C2-N3-C4	4.23	120.19	115.36
8	D	501	GDP	C5-C6-N1	-4.08	117.84	123.43
8	D	501	GDP	C6-N1-C2	4.06	122.39	115.93
8	B	501	GDP	C6-N1-C2	4.01	122.29	115.93
8	B	501	GDP	C6-C5-C4	-4.00	116.98	120.80
9	B	504	MES	C5-N4-C3	3.94	117.70	108.83
8	B	501	GDP	C5-C6-N1	-3.85	118.16	123.43
11	F	401	ACP	C3'-C2'-C1'	3.60	106.40	100.98
8	D	501	GDP	C6-C5-C4	-3.59	117.37	120.80
8	B	501	GDP	N3-C2-N1	-3.32	122.80	127.22
8	D	501	GDP	N3-C2-N1	-3.31	122.81	127.22
8	D	501	GDP	PA-O3A-PB	-3.27	121.60	132.83
10	B	505	WZM	C6-N4-C7	-3.19	115.17	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	PA-O3A-PB	-3.11	122.15	132.83
11	F	401	ACP	N3-C2-N1	-3.09	123.85	128.68
5	C	501	GTP	PA-O3A-PB	-2.97	122.64	132.83
5	C	501	GTP	C5-C6-N1	-2.93	119.42	123.43
8	B	501	GDP	C4-C5-N7	-2.89	106.39	109.40
9	B	504	MES	C6-C5-N4	-2.88	105.74	110.10
9	B	504	MES	O1S-S-C8	2.87	110.37	106.92
5	A	501	GTP	C5-C6-N1	-2.82	119.58	123.43
8	B	501	GDP	PA-O3A-PB	-2.74	123.41	132.83
8	D	501	GDP	C4-C5-N7	-2.70	106.59	109.40
5	C	501	GTP	PB-O3B-PG	-2.67	123.68	132.83
11	F	401	ACP	C4-C5-N7	-2.59	106.70	109.40
5	C	501	GTP	C6-N1-C2	2.49	119.89	115.93
5	A	501	GTP	C6-N1-C2	2.44	119.80	115.93
5	A	501	GTP	PB-O3B-PG	-2.35	124.76	132.83
5	C	501	GTP	O3G-PG-O3B	2.31	112.39	104.64
9	B	504	MES	C7-N4-C5	2.22	116.92	111.23
9	B	504	MES	O3S-S-C8	2.21	109.34	105.77
5	C	501	GTP	C3'-C2'-C1'	2.05	104.07	100.98
8	D	501	GDP	C3'-C2'-C1'	2.05	104.07	100.98
9	B	504	MES	O2S-S-C8	2.04	109.37	106.92

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
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
10	B	505	WZM	N1-C3-N4-C6
10	B	505	WZM	N1-C3-N4-C7
10	B	505	WZM	C2-C3-N4-C6
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
10	B	505	WZM	C2-C3-N4-C7
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
5	C	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A

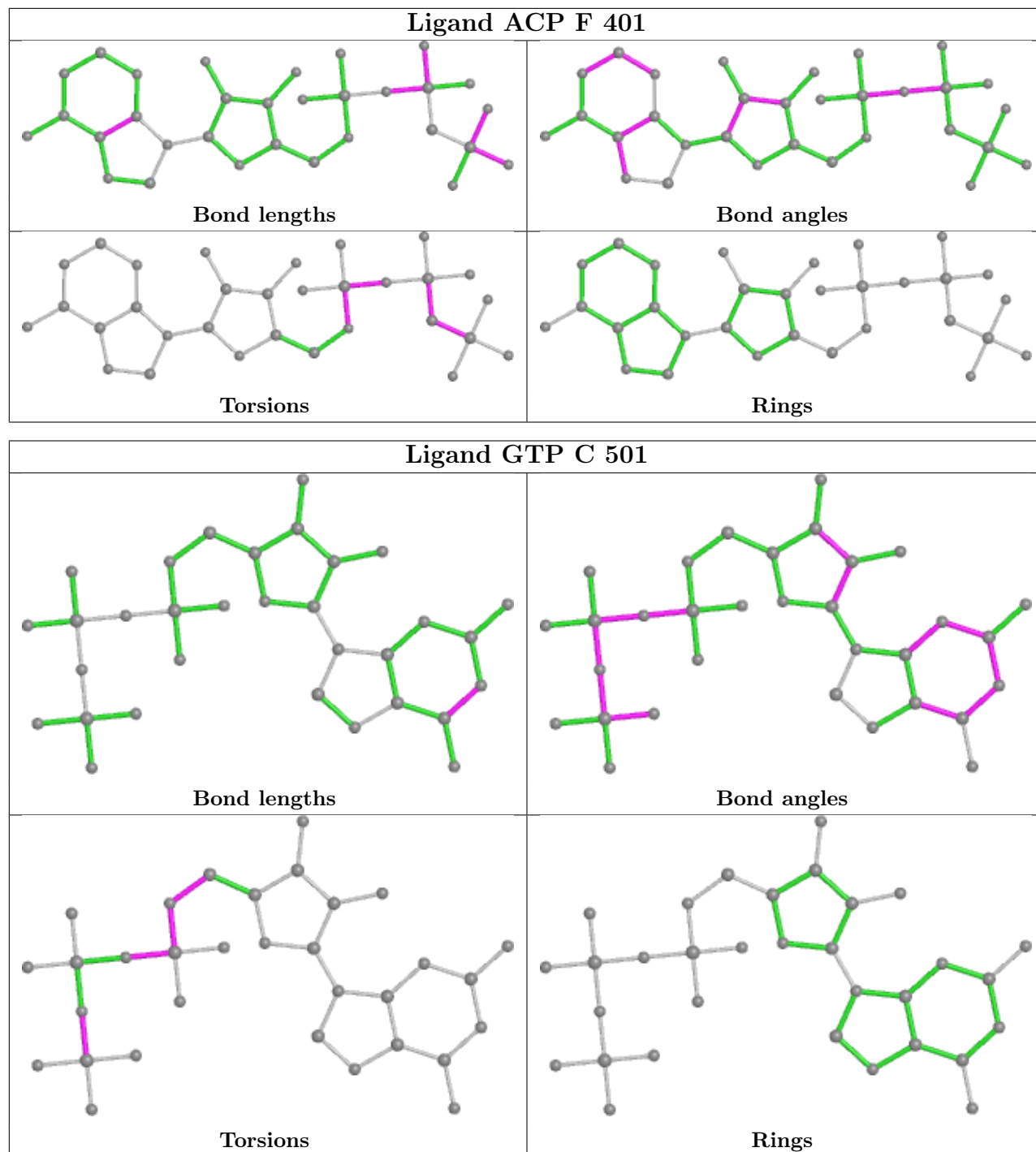
There are no ring outliers.

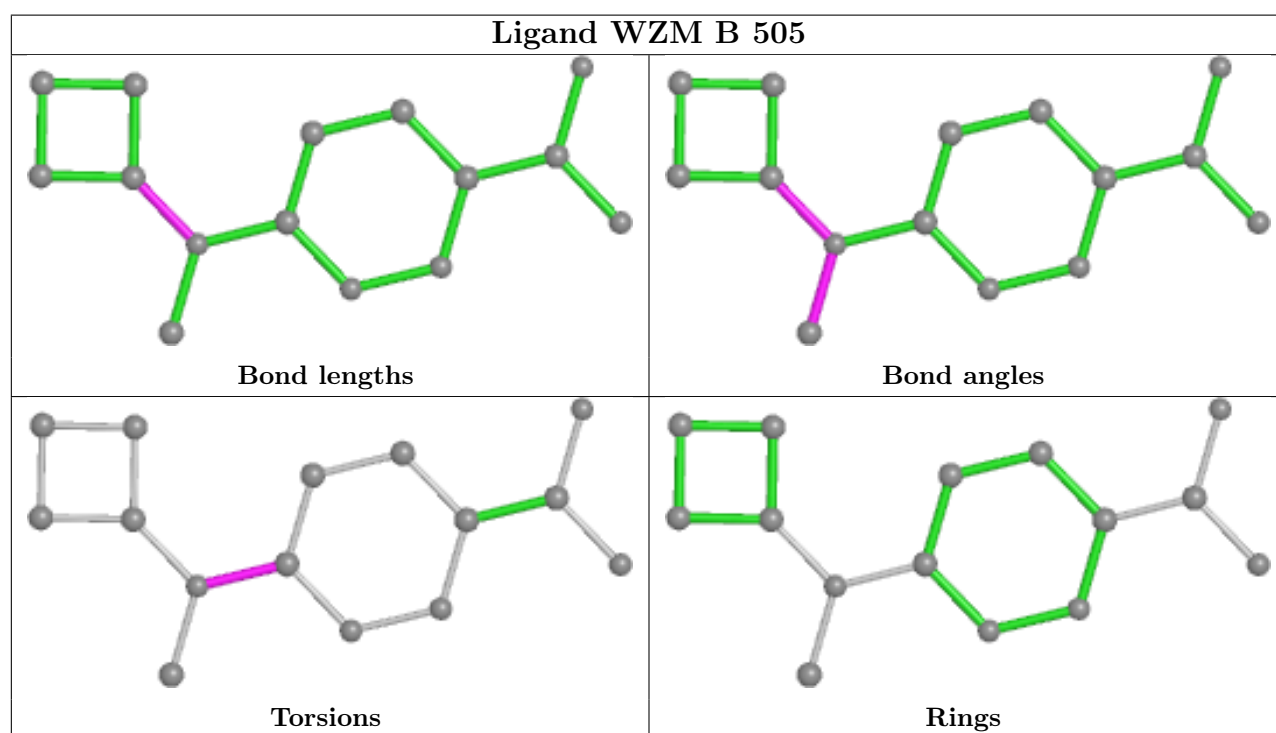
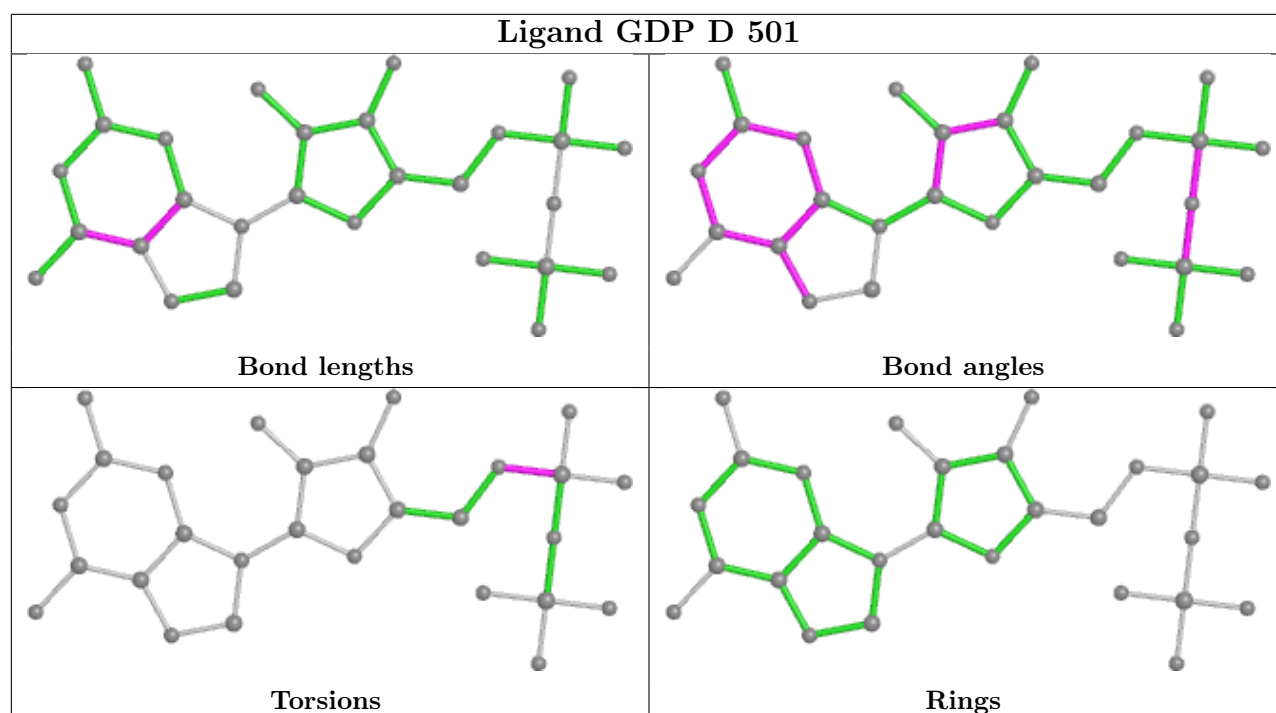
7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	4	0
5	C	501	GTP	1	0
8	D	501	GDP	3	0
9	B	504	MES	4	0
10	B	505	WZM	1	0
8	B	501	GDP	2	0
5	A	501	GTP	2	0

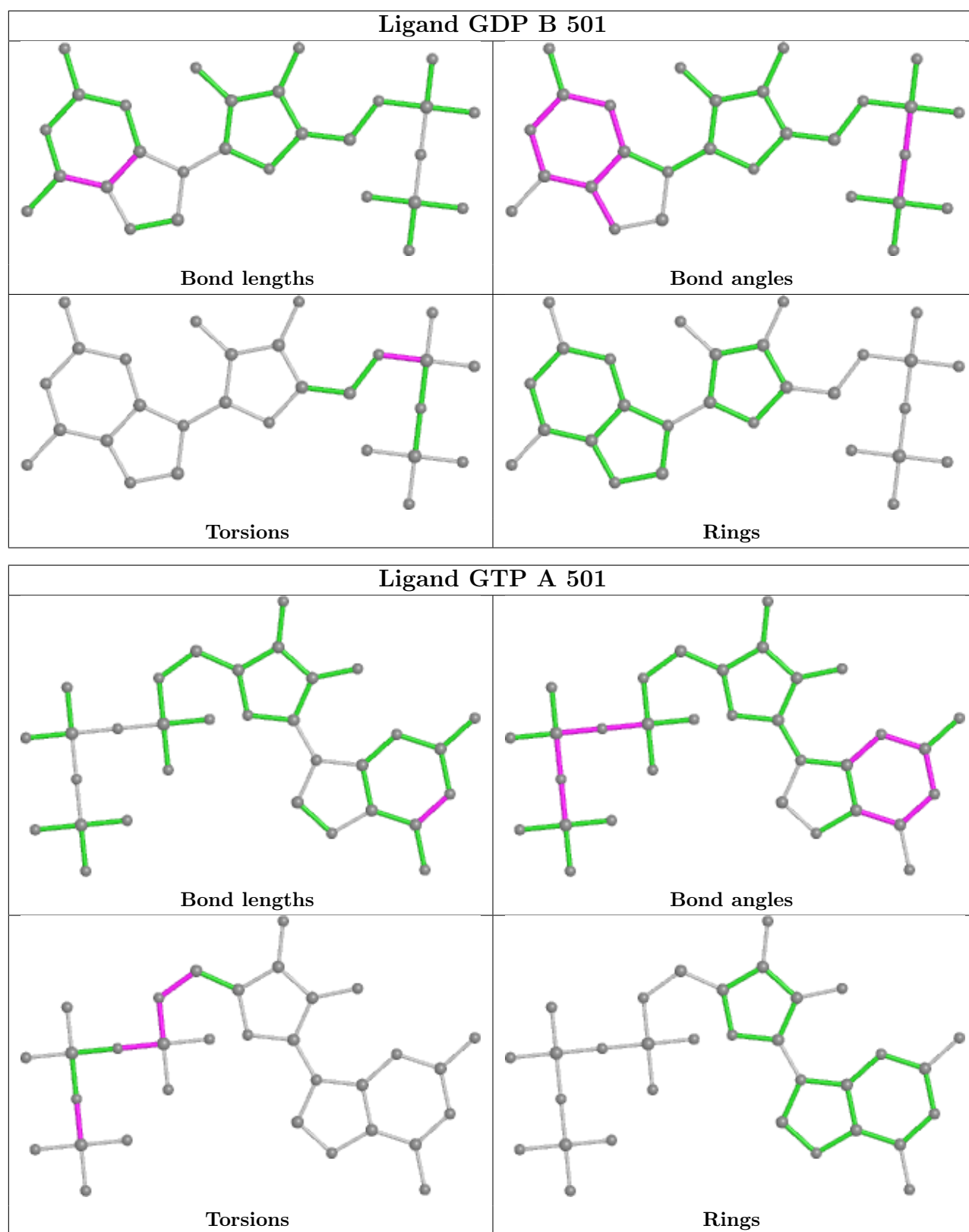
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	438/451 (97%)	0.43	19 (4%)	35	42	65, 88, 131, 206	0
1	C	440/451 (97%)	0.50	22 (5%)	28	35	59, 76, 105, 144	0
2	B	425/445 (95%)	0.65	30 (7%)	16	19	58, 85, 134, 197	2 (0%)
2	D	431/445 (96%)	0.51	31 (7%)	15	18	76, 101, 144, 197	4 (0%)
3	E	123/143 (86%)	0.98	18 (14%)	2	2	81, 112, 179, 231	0
4	F	352/384 (91%)	0.33	19 (5%)	25	31	89, 130, 206, 243	0
All	All	2209/2319 (95%)	0.52	139 (6%)	20	24	58, 93, 162, 243	6 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	7.8
2	B	281	GLN	7.3
4	F	89	GLU	6.6
3	E	6	MET	6.4
3	E	26	PRO	6.3
3	E	24	LEU	6.2
4	F	240	LEU	6.0
2	B	276	THR	5.6
3	E	25	LYS	5.6
3	E	27	PRO	5.5
2	D	277	SER	5.3
3	E	28	SER	5.2
2	B	284	ARG	5.1
1	C	286	LEU	4.9
2	D	276	THR	4.7
4	F	90	SER	4.7
1	A	348	PRO	4.6
2	D	280	SER	4.6
4	F	234	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	349	THR	4.5
4	F	142	ARG	4.4
2	B	59	ASN	4.3
1	C	368	LEU	4.2
2	D	279	GLY	4.1
2	D	248	LEU	4.0
2	B	360	PRO	3.8
1	A	326	LYS	3.7
1	C	221	ARG	3.7
3	E	7	GLU	3.6
2	D	278	ARG	3.5
2	B	372	LYS	3.5
2	D	272	PHE	3.5
1	A	351	PHE	3.4
2	D	275	LEU	3.4
2	D	325	MET	3.4
2	D	286	LEU	3.4
2	D	285	ALA	3.3
4	F	98	TYR	3.2
2	B	122	VAL	3.2
4	F	251	LYS	3.2
1	C	275	VAL	3.2
2	B	373	MET	3.1
4	F	244	CYS	3.1
3	E	22	VAL	3.1
2	D	324	SER	3.0
2	B	87	PHE	3.0
2	D	323	MET	3.0
2	D	281	GLN	3.0
2	D	215	ARG	3.0
2	D	293	GLN	3.0
4	F	181	VAL	3.0
3	E	23	ILE	3.0
2	B	1	MET	3.0
1	C	5	ILE	2.9
2	B	86	ILE	2.9
1	C	179	THR	2.9
1	C	220	GLU	2.8
4	F	134	ALA	2.8
1	A	312	TYR	2.8
1	A	342	GLN	2.8
3	E	8	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	299	LYS	2.8
3	E	54	LEU	2.8
1	C	339	ARG	2.8
2	D	46	LEU	2.8
4	F	141	GLY	2.8
2	B	319	PHE	2.8
2	D	217	LEU	2.7
2	D	319	PHE	2.7
1	A	86	LEU	2.7
4	F	100	ILE	2.7
1	A	296	PHE	2.7
1	A	346	TRP	2.6
2	B	66	ILE	2.6
1	A	329	ASN	2.6
2	B	119	LEU	2.6
1	A	221	ARG	2.6
1	C	341	ILE	2.6
2	B	288	VAL	2.6
4	F	245	ILE	2.5
1	A	318	LEU	2.5
2	B	358	ILE	2.5
2	B	286	LEU	2.5
4	F	182	ILE	2.5
4	F	131	PHE	2.5
3	E	76	ARG	2.5
1	A	378	LEU	2.5
2	D	294	GLN	2.5
1	C	87	PHE	2.5
2	B	285	ALA	2.4
3	E	139	LEU	2.4
2	B	88	ARG	2.4
2	B	7	ILE	2.4
2	D	373	MET	2.4
1	C	230	LEU	2.4
2	B	275	LEU	2.4
2	D	42	LEU	2.4
1	C	218	ASP	2.4
1	C	276	ILE	2.4
2	D	404	PHE	2.3
4	F	330	ILE	2.3
3	E	68	LEU	2.3
3	E	123	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	128	GLN	2.3
1	C	135	PHE	2.3
1	C	357	TYR	2.3
1	C	335	ILE	2.3
1	A	350	GLY	2.2
2	D	328	VAL	2.2
2	B	118	VAL	2.2
2	D	287	THR	2.2
2	D	371	LEU	2.2
2	B	244	PHE	2.2
2	B	291	LEU	2.2
2	B	333	LEU	2.2
2	B	277	SER	2.2
4	F	206	LEU	2.2
1	C	4[A]	CYS	2.2
2	B	124	LYS	2.1
3	E	122	ARG	2.1
1	C	296	PHE	2.1
2	D	405	LEU	2.1
1	C	285	GLN	2.1
2	B	74	THR	2.1
3	E	121	GLU	2.1
1	A	83	TYR	2.1
1	C	219	ILE	2.1
3	E	115	HIS	2.1
2	D	326	LYS	2.1
2	B	83	PHE	2.1
2	D	195	VAL	2.1
2	B	121	VAL	2.0
1	C	308	ARG	2.0
1	A	313	MET	2.0
1	A	77	GLU	2.0
1	A	112	LYS	2.0
2	D	244	PHE	2.0
4	F	143	GLU	2.0
1	A	288	VAL	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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

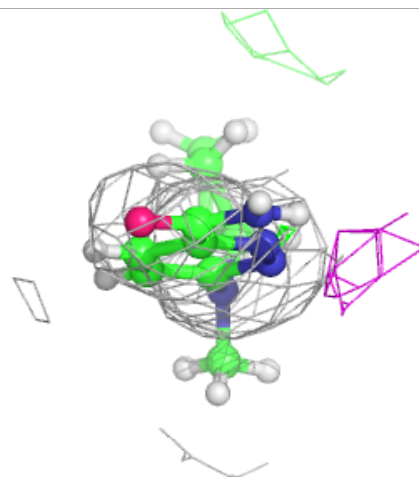
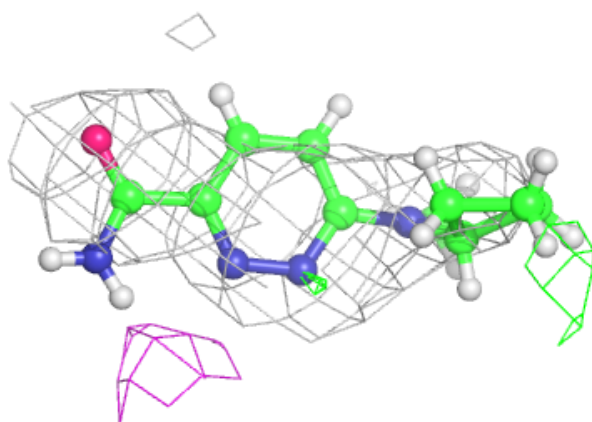
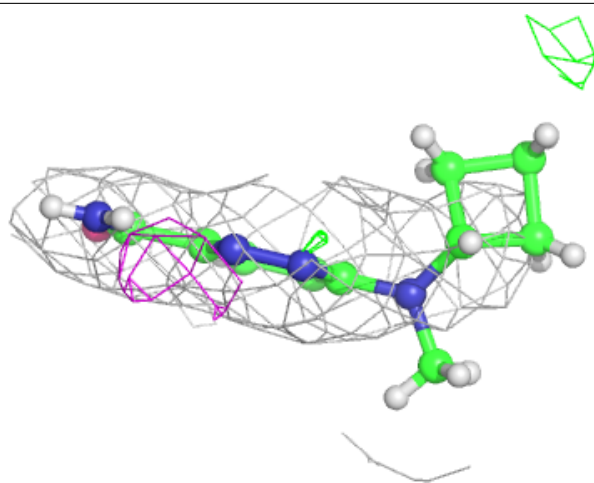
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	CA	A	504	1/1	0.85	0.10	107,107,107,107	0
7	CA	B	503	1/1	0.86	0.08	115,115,115,115	0
10	WZM	B	505	15/15	0.86	0.45	105,122,147,151	0
11	ACP	F	401	31/31	0.87	0.15	123,147,157,164	0
6	MG	D	502	1/1	0.89	0.11	88,88,88,88	0
6	MG	F	402	1/1	0.90	0.12	140,140,140,140	0
9	MES	B	504	12/12	0.94	0.21	92,97,104,105	0
8	GDP	D	501	28/28	0.95	0.17	88,95,102,107	0
6	MG	B	502	1/1	0.96	0.15	70,70,70,70	0
5	GTP	A	501	32/32	0.97	0.17	63,69,77,82	0
5	GTP	C	501	32/32	0.97	0.19	57,67,76,78	0
6	MG	A	502	1/1	0.97	0.21	71,71,71,71	0
7	CA	C	503	1/1	0.98	0.14	91,91,91,91	0
8	GDP	B	501	28/28	0.98	0.16	59,68,74,75	0
7	CA	A	503	1/1	0.98	0.13	114,114,114,114	0
6	MG	C	502	1/1	0.99	0.17	71,71,71,71	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 WZM B 505:**

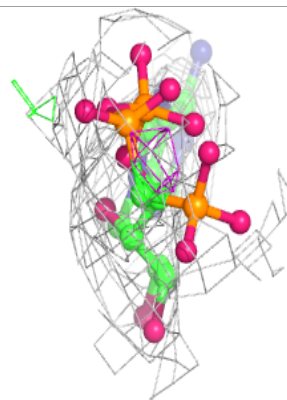
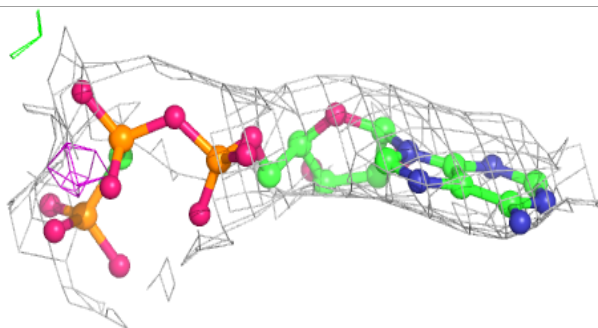
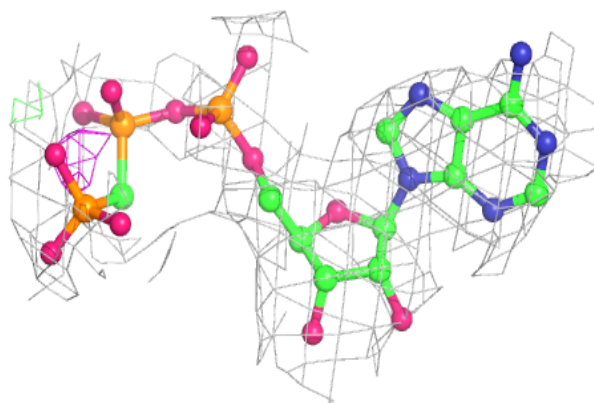
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





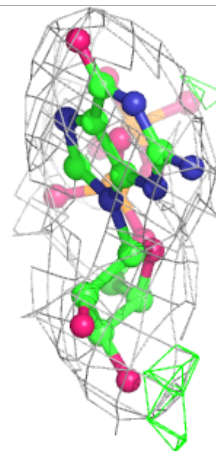
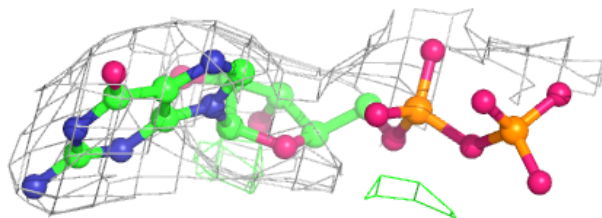
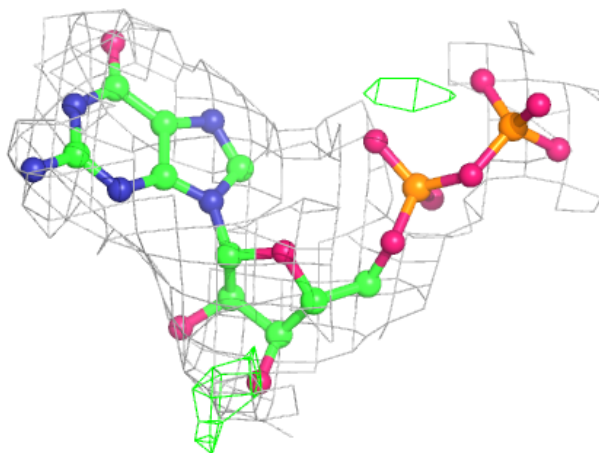
**Electron density around ACP F 401:**

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



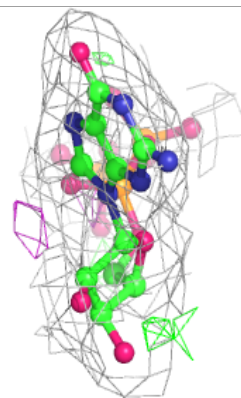
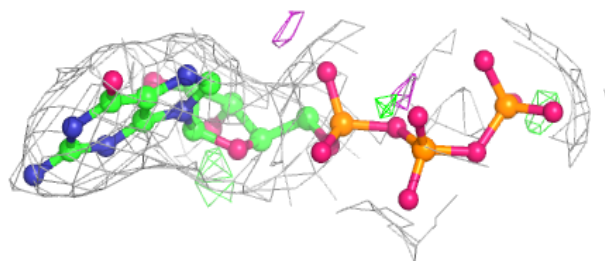
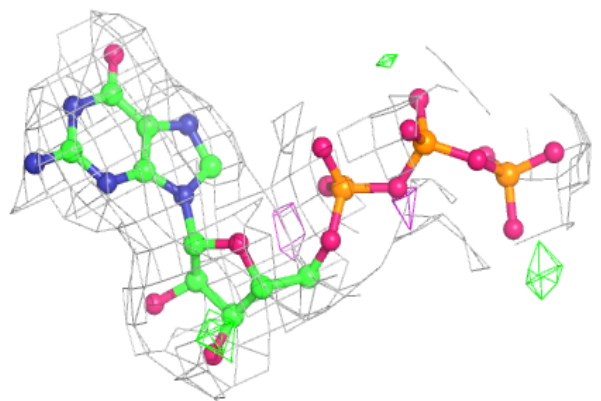
**Electron density around GDP D 501:**

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

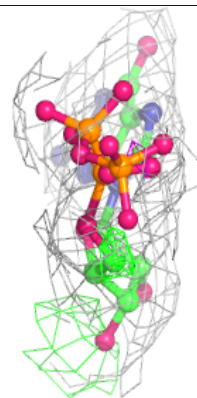
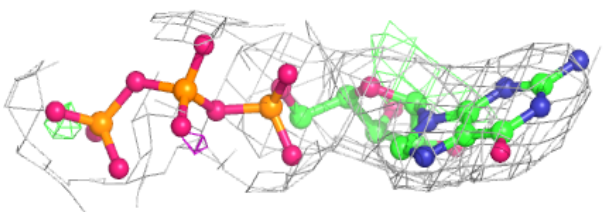
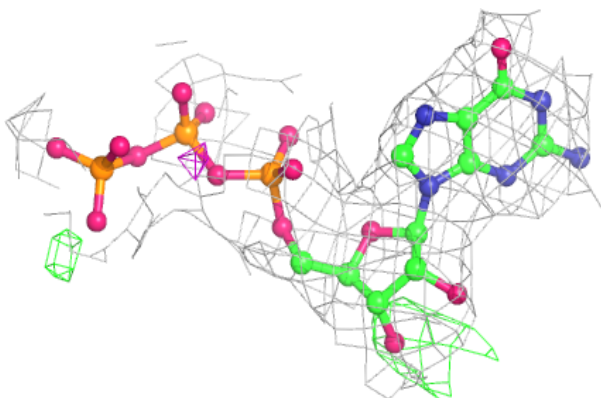


**Electron density around GTP A 501:**

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

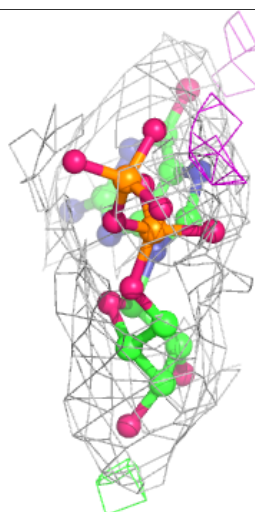
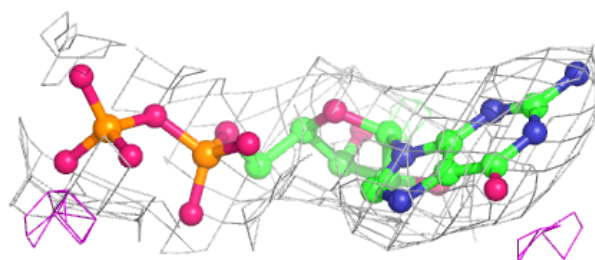
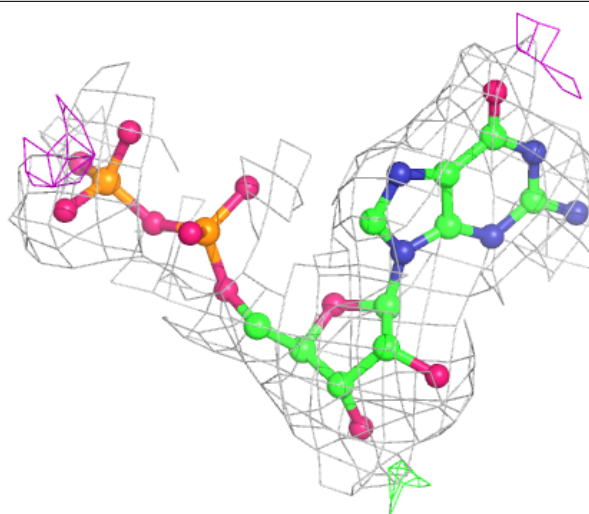
**Electron density around GTP C 501:**

$2mF_o-DF_c$  (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.