Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 06:44 pm GMT

PDB ID	:	5OV7
Title	:	tubulin - rigosertib complex
Authors	:	Menchon, G.; Prota, A.E.; Steinmetz, M.; Jost, M.
Deposited on	:	2017-08-28
Resolution	:	2.40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

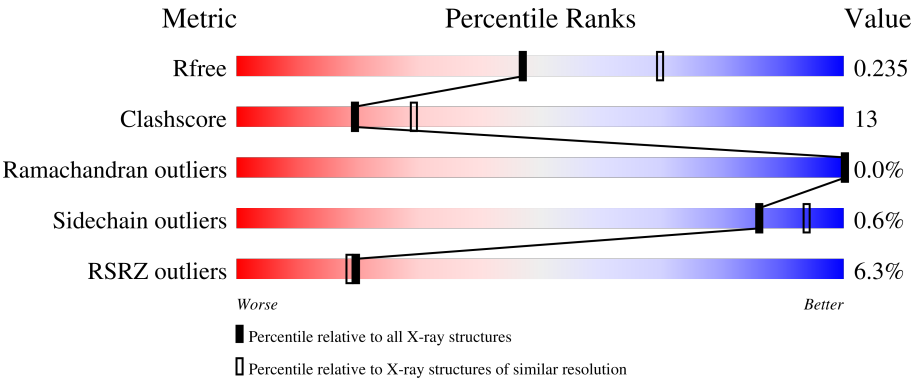
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	2% 75% 22% ·
1	C	451	78% 20% ·
2	B	445	3% 71% 24% 6%
2	D	445	5% 68% 26% 5%
3	E	143	8% 66% 19% · 14%

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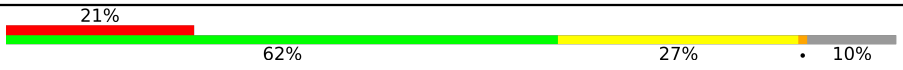
Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	C	501	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18026 atoms, of which 48 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	2	0
			3428	2171	584	651	22			
1	C	440	Total	C	N	O	S	0	2	0
			3449	2183	585	659	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	4	0
			3325	2092	565	640	28			
2	D	422	Total	C	N	O	S	0	0	0
			3314	2083	563	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	1	0
			1021	630	185	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

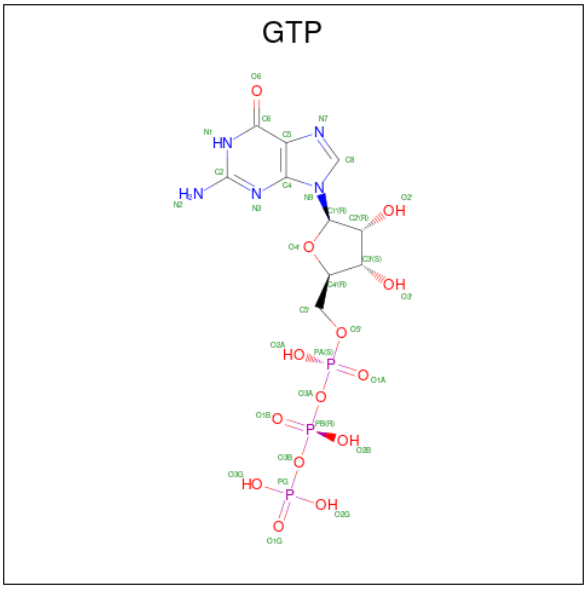
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	347	Total	C	N	O	S	0	0	0
			2830	1811	486	519	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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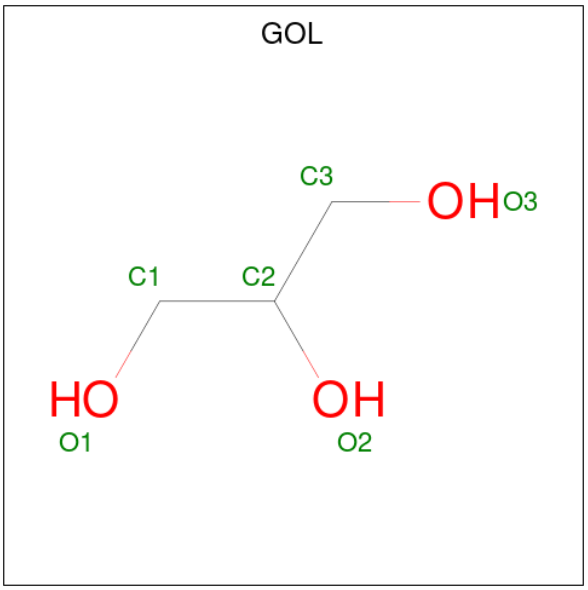
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

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

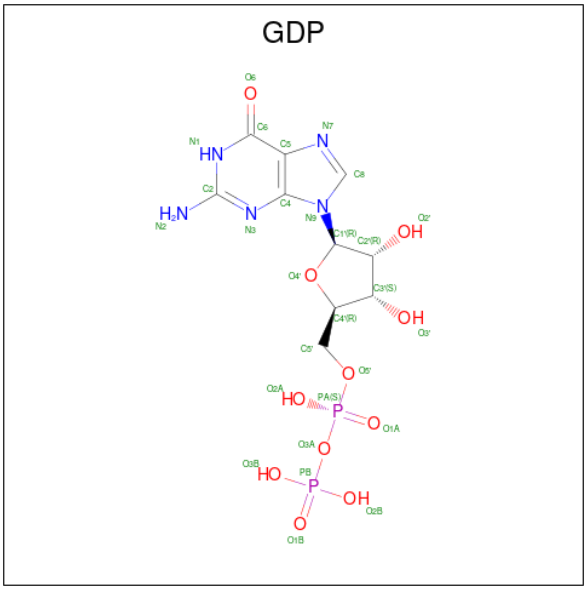
- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

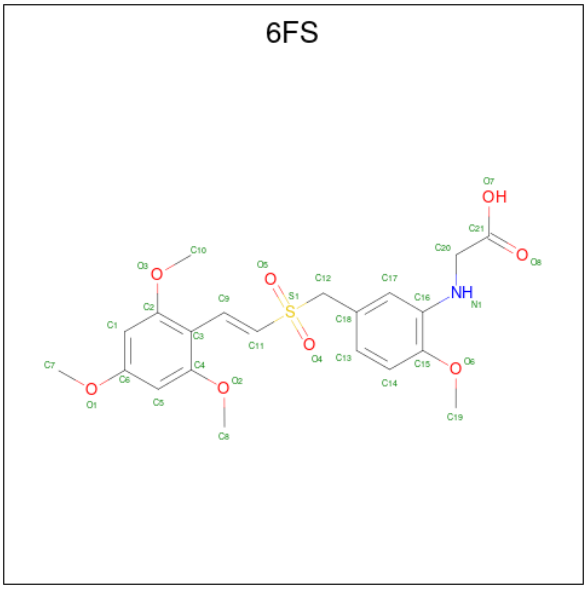
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

$C_{10}H_{15}N_5O_{11}P_2$).



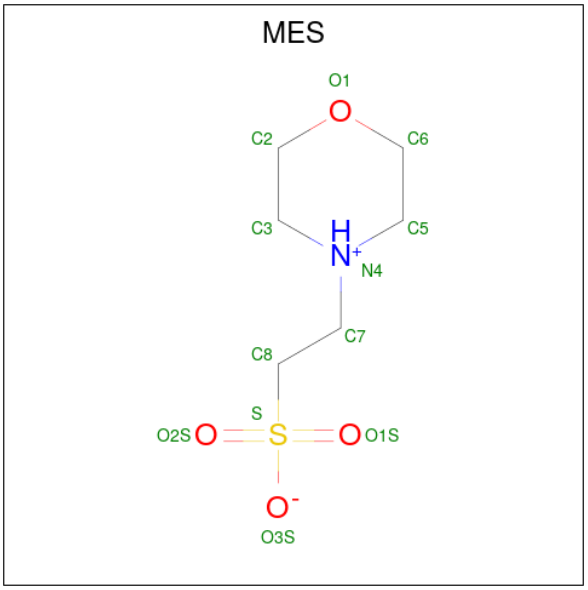
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is N-[2-methoxy-5-({[(E)-2-(2,4,6-trimethoxyphenyl)ethenyl]sulfonyl}methyl)phenyl]glycine (three-letter code: 6FS) (formula: $C_{21}H_{25}NO_8S$).



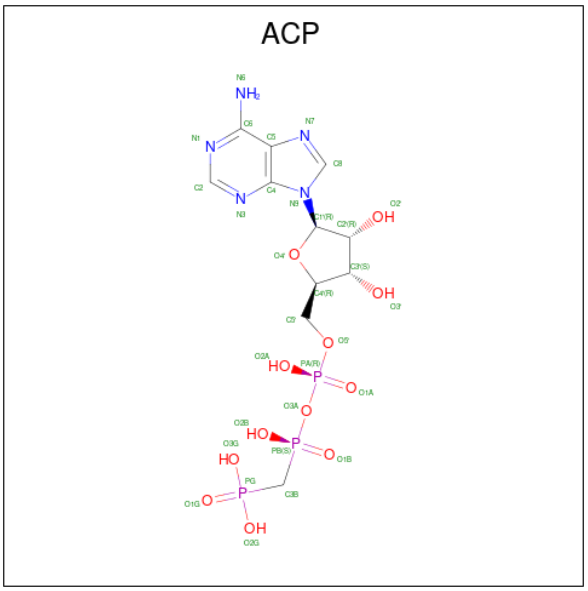
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			55	21	24	1	8	1		
10	D	1	Total	C	H	N	O	S	0	0
			55	21	24	1	8	1		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 12 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
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 13 is water.

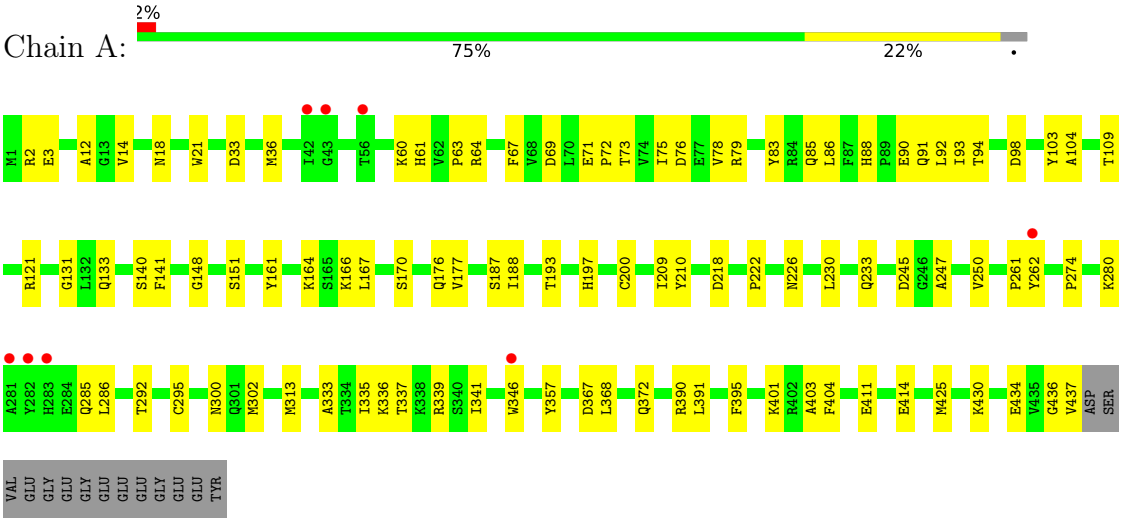
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	50	Total	O	0	0
			50	50		
13	B	88	Total	O	0	0
			88	88		
13	C	133	Total	O	0	0
			133	133		
13	D	43	Total	O	0	0
			43	43		
13	E	9	Total	O	0	0
			9	9		
13	F	21	Total	O	0	0
			21	21		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

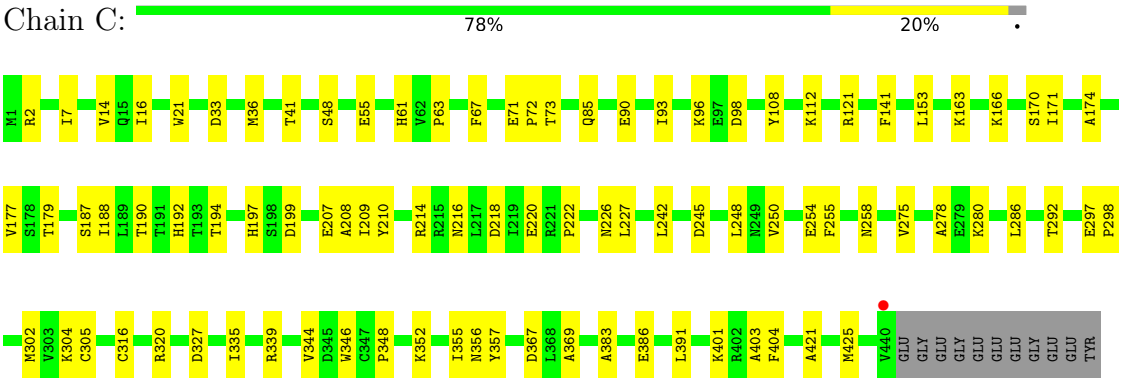
• Molecule 1: Tubulin alpha-1B chain

Chain A:



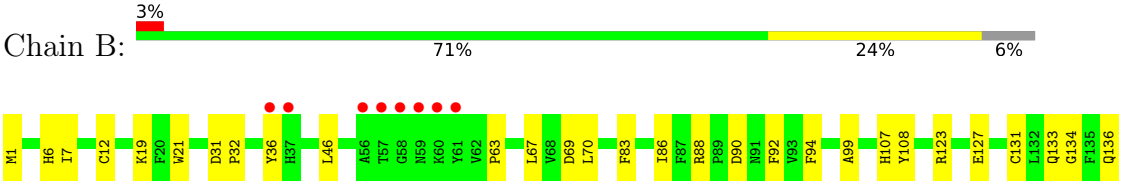
• Molecule 1: Tubulin alpha-1B chain

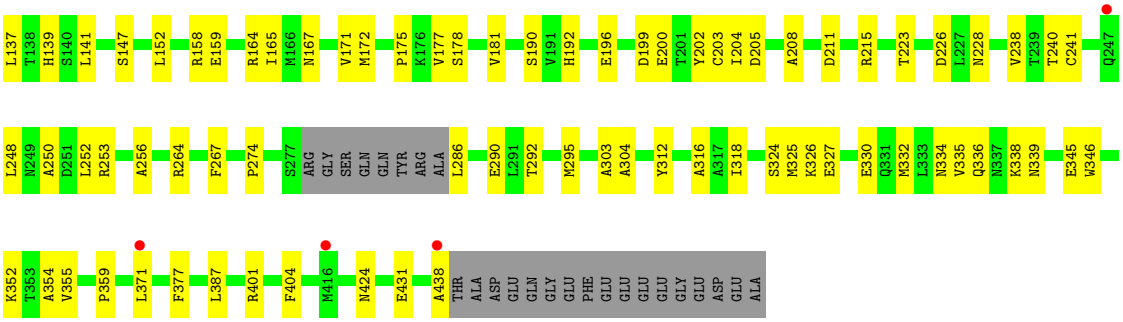
Chain C:



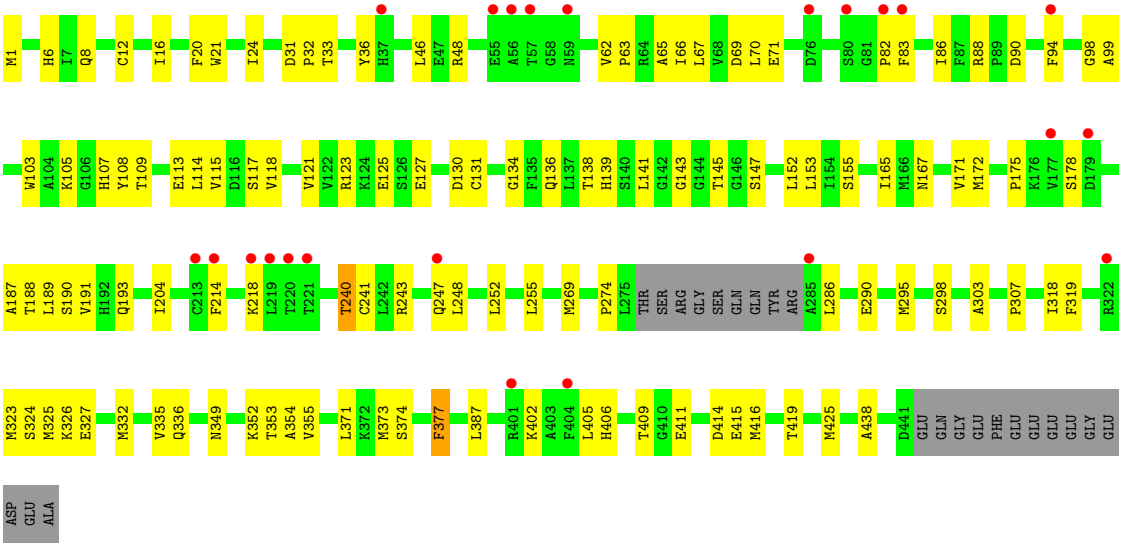
• Molecule 2: Tubulin beta-2B chain

Chain B:

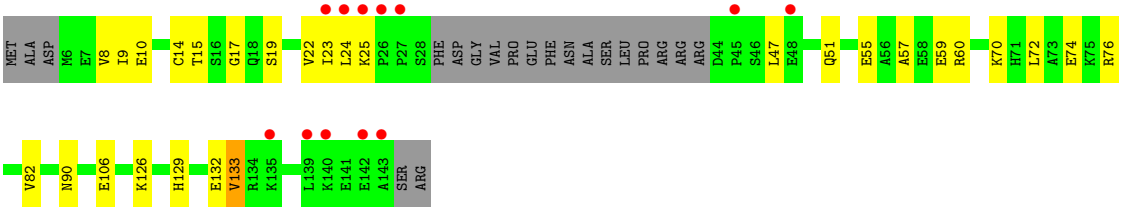




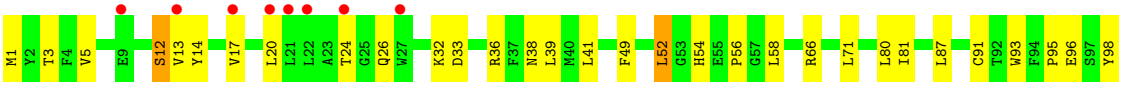
• Molecule 2: Tubulin beta-2B chain

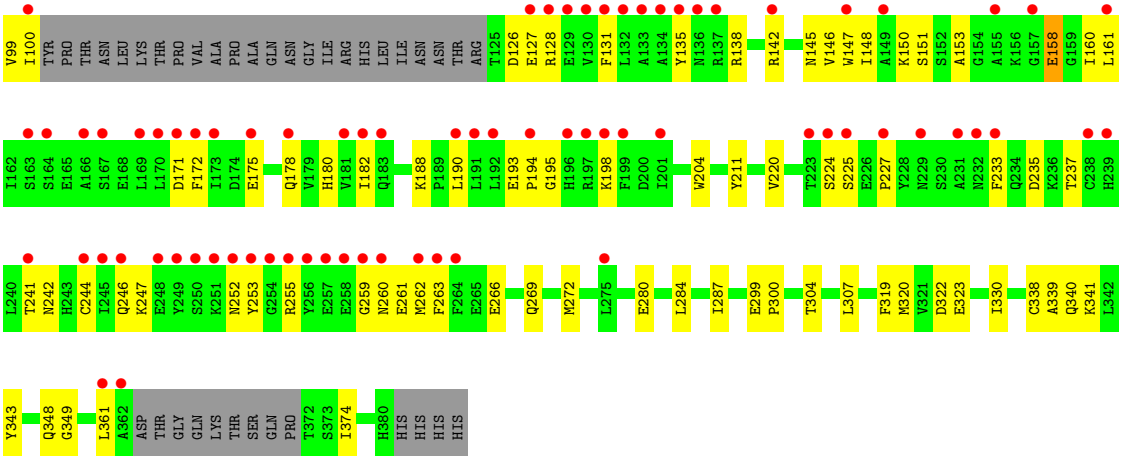


• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein




V99 I100 TYR PRO THR ASN LEU LYS THR PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG T125 D126 E127 R128 E129 V130 F131 L132 A133 A134 Y135 N136 R137 R138 R142 N145 V146 W147 I148 A149 K150 S151 S152 A153 G154 A155 K156 G157 E158 G159 I160 L161
I162 S163 S164 E165 A166 S167 E168 L169 L170 D171 F172 I173 D174 E175 Q178 V179 H180 V181 I182 Q183 K188 P189 L190 L191 L192 E193 P194 G195 H196 R197 K198 F199 D200 I201 W204 Y211 V220 T223 S224 S225 E226 P227 Y228 N229 S230 A231 N232 F233 Q234 D235 K236 T237 C238 H239
L240 T241 N242 H243 C244 Y245 Q246 K247 E248 Y249 S250 K251 N252 Y253 G254 R255 Y256 E257 E258 G259 N260 E261 M262 F263 F264 E265 E266 Q269 M272 L275 E280 L284 I287 E299 P300 T304 L307 F319 M320 V321 D322 E323 I330 C338 A339 Q340 K341 L342
Y343 Q348 G349 L361 A362 ASP THR GLY GLN LYS THR SER GLN PRO T372 S373 I374 H380 HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.73Å 156.76Å 182.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 2.40 48.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.08-2.40) 99.0 (48.08-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, R_{free}	0.190 , 0.235 0.190 , 0.235	Depositor DCC
R_{free} test set	5844 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18026	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, 6FS, GTP, GDP, CA, GOL, MG, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/3512	0.48	0/4767
1	C	0.33	0/3533	0.49	0/4797
2	B	0.32	0/3410	0.48	0/4616
2	D	0.29	0/3387	0.46	0/4588
3	E	0.27	0/1033	0.41	0/1371
4	F	0.24	0/2893	0.42	0/3906
All	All	0.30	0/17768	0.47	0/24045

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

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	3428	0	3350	80	0
1	C	3449	0	3363	64	0
2	B	3325	0	3222	91	0
2	D	3314	0	3194	103	0
3	E	1021	0	1036	28	0
4	F	2830	0	2800	99	0
5	A	32	0	12	0	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	1	0	0	0	0
8	A	12	0	16	1	0
8	B	12	0	16	1	0
8	C	12	0	16	1	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	B	31	24	0	8	0
10	D	31	24	0	4	0
11	B	12	0	12	1	0
12	F	31	0	14	2	0
13	A	50	0	0	5	0
13	B	88	0	0	5	0
13	C	133	0	0	8	0
13	D	43	0	0	2	1
13	E	9	0	0	0	0
13	F	21	0	0	2	1
All	All	17978	48	17087	444	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 13.

All (444) 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)
2:D:248:LEU:HD21	2:D:352:LYS:CE	1.74	1.16
4:F:87:LEU:O	4:F:87:LEU:HD12	1.45	1.16
2:B:352:LYS:HE2	10:B:504:6FS:C20	1.77	1.14
4:F:81:ILE:HA	4:F:87:LEU:HD11	1.27	1.12
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.35	1.02
2:D:248:LEU:HD13	10:D:503:6FS:O4	1.61	1.00
2:D:248:LEU:HD21	2:D:352:LYS:HE3	1.42	0.98
1:A:336:LYS:HD2	3:E:24:LEU:HD23	1.42	0.98
4:F:81:ILE:HA	4:F:87:LEU:CD1	1.92	0.98
1:A:2:ARG:O	1:A:133:GLN:NE2	1.99	0.95
2:D:318:ILE:HD13	2:D:354:ALA:HB3	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:VAL:HG11	2:D:153:LEU:HD21	1.50	0.93
1:C:254:GLU:O	13:C:601:HOH:O	1.87	0.92
1:A:71:GLU:OE1	1:A:73:THR:OG1	1.89	0.91
1:A:109:THR:HG21	1:A:411:GLU:OE2	1.77	0.85
2:D:406:HIS:HA	2:D:409:THR:HG22	1.58	0.84
4:F:91:CYS:SG	4:F:93:TRP:NE1	2.50	0.84
4:F:81:ILE:HG23	4:F:87:LEU:HD13	1.60	0.83
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.44	0.82
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.59	0.82
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.58	0.82
1:A:218:ASP:OD2	1:A:280:LYS:NZ	2.14	0.81
1:A:3:GLU:OE1	1:A:131:GLY:O	1.98	0.81
2:D:248:LEU:HD21	2:D:352:LYS:HE2	1.62	0.81
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.64	0.79
4:F:13:VAL:O	4:F:17:VAL:HG23	1.83	0.79
4:F:225:SER:HB2	4:F:260:ASN:HD21	1.49	0.78
1:A:430:LYS:HE2	1:A:434:GLU:OE1	1.84	0.77
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.65	0.77
1:A:414:GLU:OE2	3:E:60:ARG:NH2	2.17	0.77
4:F:182:ILE:HD12	4:F:182:ILE:O	1.85	0.77
4:F:91:CYS:SG	4:F:93:TRP:CE2	2.77	0.76
2:B:1:MET:N	2:B:131:CYS:SG	2.54	0.76
4:F:151:SER:HB2	4:F:180:HIS:CD2	2.21	0.76
4:F:95:PRO:HB2	13:F:501:HOH:O	1.86	0.75
2:D:352:LYS:HB2	10:D:503:6FS:C20	2.16	0.75
1:C:163:LYS:HG2	3:E:90:ASN:OD1	1.85	0.75
2:D:83:PHE:O	2:D:86:ILE:HG22	1.87	0.74
1:C:327:ASP:OD1	13:C:603:HOH:O	2.05	0.74
4:F:98:TYR:HB2	4:F:182:ILE:HD11	1.70	0.74
2:D:175:PRO:HA	2:D:178:SER:HB2	1.70	0.73
2:D:1:MET:N	2:D:131:CYS:SG	2.57	0.72
1:C:71:GLU:OE2	1:C:73:THR:HB	1.88	0.72
1:A:245:ASP:OD2	13:A:601:HOH:O	2.07	0.72
4:F:81:ILE:CA	4:F:87:LEU:HD11	2.15	0.72
4:F:26:GLN:OE1	4:F:361:LEU:HB2	1.90	0.72
4:F:81:ILE:HG23	4:F:87:LEU:CD1	2.19	0.72
1:A:167:LEU:CD1	1:A:200:CYS:HB3	2.20	0.71
13:C:705:HOH:O	2:D:349:ASN:HB2	1.89	0.71
1:C:199:ASP:OD1	8:C:504:GOL:H12	1.90	0.71
2:B:253[A]:ARG:NH1	11:B:505:MES:O1S	2.23	0.71
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:THR:HG21	2:D:318:ILE:HG21	1.72	0.70
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.70
1:A:177:VAL:O	13:A:602:HOH:O	2.10	0.70
4:F:87:LEU:O	4:F:87:LEU:CD1	2.33	0.69
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.74	0.69
4:F:150:LYS:HD3	4:F:160:ILE:HD11	1.75	0.69
2:D:416:MET:O	2:D:419:THR:HG22	1.92	0.69
2:D:136:GLN:HA	2:D:167:ASN:O	1.92	0.69
4:F:224:SER:HB2	4:F:241:THR:HG22	1.73	0.69
4:F:158:GLU:OE1	4:F:158:GLU:HA	1.93	0.68
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.74	0.68
2:D:31:ASP:OD1	2:D:33:THR:HG22	1.92	0.68
2:D:318:ILE:CD1	2:D:354:ALA:HB3	2.22	0.68
1:C:383:ALA:O	1:C:386[A]:GLU:HG2	1.94	0.68
2:D:175:PRO:HD2	13:D:602:HOH:O	1.93	0.68
1:C:112:LYS:NZ	13:C:604:HOH:O	2.10	0.68
1:A:285:GLN:HG2	1:A:372:GLN:OE1	1.94	0.68
4:F:98:TYR:CD1	4:F:182:ILE:HD11	2.29	0.67
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.28	0.67
2:B:339:ASN:ND2	13:B:602:HOH:O	2.26	0.67
4:F:1:MET:HB2	4:F:26:GLN:O	1.93	0.67
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.21	0.67
4:F:49:PHE:HA	4:F:52:LEU:CD1	2.23	0.67
2:D:123:ARG:O	2:D:127:GLU:HG2	1.95	0.66
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.24	0.66
1:A:436:GLY:O	1:A:437:VAL:HG22	1.95	0.66
1:C:320:ARG:HA	1:C:356:ASN:O	1.95	0.66
1:C:41:THR:OG1	13:C:602:HOH:O	1.89	0.65
1:A:167:LEU:HD13	1:A:200:CYS:HB3	1.78	0.65
1:A:2:ARG:C	1:A:133:GLN:HE21	1.98	0.65
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.78	0.65
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.27	0.65
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.79	0.65
2:B:136:GLN:HA	2:B:167:ASN:O	1.98	0.64
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.27	0.64
2:B:208:ALA:HB2	2:B:304:ALA:N	2.11	0.64
1:C:209:ILE:HD11	1:C:302:MET:SD	2.37	0.64
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.78	0.64
3:E:9:ILE:HG12	3:E:10:GLU:HG3	1.80	0.64
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.80	0.64
2:D:295:MET:HE2	2:D:377:PHE:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HE3	3:E:25:LYS:HE3	1.80	0.64
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.16	0.64
4:F:100:ILE:HG23	4:F:128:ARG:HG2	1.80	0.64
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.12	0.63
2:D:406:HIS:HA	2:D:409:THR:CG2	2.28	0.63
4:F:81:ILE:CA	4:F:87:LEU:CD1	2.74	0.63
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.34	0.62
4:F:5:VAL:CG1	4:F:32:LYS:HA	2.29	0.62
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.33	0.62
3:E:55:GLU:O	3:E:59:GLU:HG2	1.99	0.62
1:A:166:LYS:HE2	1:A:197:HIS:O	1.99	0.62
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.80	0.62
2:B:438:ALA:HA	13:B:651:HOH:O	2.00	0.61
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.35	0.61
2:D:247:GLN:NE2	13:D:601:HOH:O	2.32	0.61
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.35	0.61
1:C:71:GLU:HG2	1:C:72:PRO:N	2.15	0.61
1:A:247:ALA:HB3	3:E:19:SER:OG	2.00	0.61
1:C:166:LYS:HE2	1:C:197:HIS:O	2.00	0.61
1:A:88:HIS:N	1:A:91:GLN:OE1	2.22	0.60
4:F:20:LEU:O	4:F:24:THR:HG23	2.01	0.60
4:F:32:LYS:HG3	4:F:33:ASP:OD1	2.00	0.60
2:D:147:SER:HB3	2:D:190:SER:OG	2.02	0.60
1:A:33:ASP:HA	1:A:85:GLN:HG3	1.84	0.60
2:B:274:PRO:CD	2:B:371:LEU:HD21	2.32	0.59
2:B:326:LYS:HE2	2:B:330:GLU:OE2	2.02	0.59
2:B:248:LEU:HD11	2:B:354:ALA:HB2	1.83	0.59
2:B:431:GLU:OE1	13:B:601:HOH:O	2.17	0.59
3:E:70:LYS:O	3:E:74:GLU:HG2	2.03	0.59
3:E:72:LEU:O	3:E:76:ARG:HG2	2.03	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.85	0.59
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.59
1:C:297:GLU:OE2	1:C:298:PRO:HD2	2.01	0.59
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.38	0.58
4:F:252:ASN:ND2	4:F:255:ARG:HD2	2.19	0.58
1:C:242:LEU:N	1:C:242:LEU:HD12	2.19	0.58
2:D:31:ASP:CG	2:D:33:THR:HG22	2.24	0.58
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.38	0.58
1:C:55:GLU:OE2	13:C:602:HOH:O	2.16	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.58
4:F:171:ASP:O	4:F:175:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.86	0.58
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.39	0.58
3:E:8:VAL:HG22	3:E:22:VAL:HG12	1.85	0.58
1:C:71:GLU:HG2	1:C:73:THR:H	1.68	0.57
2:D:188:THR:HA	2:D:191:VAL:HG12	1.87	0.57
1:A:333:ALA:O	1:A:337:THR:HG23	2.05	0.57
3:E:57:ALA:HA	3:E:60:ARG:NH1	2.18	0.57
4:F:150:LYS:HD3	4:F:160:ILE:CD1	2.34	0.57
2:B:192:HIS:CG	2:B:424:ASN:HD22	2.23	0.57
4:F:36:ARG:NH1	13:F:502:HOH:O	2.37	0.57
4:F:98:TYR:HD1	4:F:182:ILE:HD11	1.69	0.57
4:F:142:ARG:O	4:F:142:ARG:HG2	2.04	0.57
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.04	0.56
4:F:151:SER:HB2	4:F:180:HIS:NE2	2.21	0.56
1:C:187:SER:O	1:C:190:THR:HG22	2.05	0.56
2:D:248:LEU:CD2	2:D:352:LYS:HE3	2.27	0.56
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.86	0.56
2:D:191:VAL:HG11	2:D:425:MET:SD	2.46	0.56
4:F:146:VAL:HG11	4:F:233:PHE:CE1	2.40	0.56
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.41	0.56
2:D:71:GLU:HG3	2:D:98:GLY:HA2	1.87	0.55
2:D:109:THR:O	2:D:113:GLU:HG3	2.06	0.55
2:B:248:LEU:CD1	2:B:354:ALA:HB2	2.36	0.55
4:F:99:VAL:O	4:F:127:GLU:HB2	2.07	0.55
1:A:209:ILE:HD11	1:A:302:MET:SD	2.46	0.55
2:D:171:VAL:HA	2:D:204:ILE:O	2.07	0.55
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.37	0.55
2:B:352:LYS:CE	10:B:504:6FS:C20	2.70	0.55
2:D:6:HIS:NE2	2:D:8:GLN:HG3	2.21	0.55
2:B:141:LEU:HA	2:B:147:SER:HB3	1.88	0.55
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.89	0.55
1:C:96:LYS:HE3	2:D:130:ASP:OD1	2.07	0.55
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.89	0.55
4:F:320:MET:HG2	4:F:330:ILE:CD1	2.22	0.55
1:C:48:SER:OG	1:C:245:ASP:HB2	2.05	0.55
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.88	0.55
2:D:332:MET:O	2:D:335:VAL:HG12	2.07	0.54
2:B:211:ASP:O	2:B:215:ARG:HG2	2.07	0.54
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.54
4:F:188:LYS:HD2	4:F:323:GLU:OE1	2.07	0.54
2:D:16:ILE:HD11	2:D:138:THR:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.88	0.54
2:D:141:LEU:HD12	2:D:172:MET:SD	2.47	0.54
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.90	0.54
2:B:67:LEU:N	2:B:67:LEU:HD12	2.23	0.54
2:B:202:TYR:CZ	2:B:238:VAL:HG11	2.43	0.54
2:B:177:VAL:HG13	8:B:503:GOL:H11	1.90	0.53
2:D:88:ARG:NH2	2:D:90:ASP:OD2	2.41	0.53
3:E:23:ILE:HD12	3:E:23:ILE:N	2.23	0.53
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.91	0.53
2:D:109:THR:HG21	2:D:411:GLU:OE1	2.08	0.53
2:D:65:ALA:O	2:D:66:ILE:HD13	2.08	0.53
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.43	0.53
1:C:305:CYS:HA	1:C:386[A]:GLU:OE2	2.09	0.53
2:D:69:ASP:O	2:D:94:PHE:HA	2.09	0.53
2:D:371:LEU:HD23	2:D:374:SER:HB3	1.89	0.53
1:C:85:GLN:HG2	13:C:615:HOH:O	2.08	0.53
3:E:47:LEU:HD12	3:E:47:LEU:O	2.08	0.53
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.90	0.52
2:D:145:THR:N	9:D:501:GDP:O2B	2.35	0.52
2:D:274:PRO:HD2	2:D:371:LEU:HD21	1.90	0.52
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.92	0.52
2:B:123:ARG:O	2:B:127:GLU:HG3	2.10	0.52
2:D:115:VAL:HG23	2:D:153:LEU:HD13	1.91	0.52
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.92	0.52
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.91	0.52
2:D:62:VAL:HG11	2:D:88:ARG:HG3	1.91	0.52
2:D:66:ILE:HD12	2:D:121:VAL:CG1	2.40	0.51
4:F:150:LYS:NZ	12:F:401:ACP:O2A	2.34	0.51
2:B:181:VAL:HG21	2:B:404:PHE:CZ	2.44	0.51
2:B:264:ARG:HD3	13:B:669:HOH:O	2.10	0.51
2:D:352:LYS:HD2	2:D:353:THR:H	1.76	0.51
4:F:161:LEU:HD12	4:F:172:PHE:HB2	1.92	0.51
2:B:332:MET:O	2:B:336:GLN:HG3	2.09	0.51
2:D:66:ILE:HD11	2:D:125:GLU:HG3	1.93	0.51
2:B:274:PRO:HD2	2:B:371:LEU:CD2	2.41	0.51
2:D:248:LEU:HD11	2:D:352:LYS:HE3	1.91	0.51
4:F:81:ILE:HG12	4:F:87:LEU:CD1	2.41	0.51
1:C:177:VAL:HG13	1:C:177:VAL:O	2.11	0.51
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.93	0.51
2:B:248:LEU:HD11	10:B:504:6FS:C8	2.41	0.51
2:B:274:PRO:HD2	2:B:371:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:20:LEU:O	4:F:20:LEU:HD12	2.11	0.51
4:F:100:ILE:HA	4:F:126:ASP:OD1	2.09	0.51
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.51	0.50
1:A:233:GLN:HG3	1:A:368:LEU:HD13	1.92	0.50
1:A:390:ARG:HD3	4:F:54:HIS:CD2	2.46	0.50
1:C:108:TYR:O	1:C:112:LYS:HE3	2.12	0.50
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.12	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.50
2:B:274:PRO:CG	2:B:371:LEU:HD21	2.42	0.50
2:D:377:PHE:C	2:D:377:PHE:CD2	2.85	0.50
4:F:20:LEU:HD21	4:F:348:GLN:OE1	2.10	0.50
4:F:247:LYS:HA	4:F:253:TYR:CD1	2.47	0.50
2:B:223:THR:HG23	2:B:226:ASP:H	1.77	0.50
4:F:225:SER:HB2	4:F:260:ASN:ND2	2.21	0.50
2:B:19:LYS:HD2	2:B:228:ASN:HB3	1.93	0.49
2:B:316:ALA:HB1	10:B:504:6FS:C4	2.42	0.49
1:A:83:TYR:CD2	1:A:86:LEU:HD22	2.47	0.49
2:B:1:MET:SD	2:B:133:GLN:HA	2.53	0.49
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.77	0.49
1:C:33:ASP:HA	1:C:85:GLN:HG3	1.93	0.49
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.95	0.49
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.42	0.49
1:C:98:ASP:HB2	5:C:502:GTP:O2G	2.12	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.49
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.40	0.49
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.47	0.49
2:D:324:SER:HB3	2:D:327:GLU:HG2	1.94	0.49
4:F:190:LEU:HB2	4:F:322:ASP:O	2.12	0.49
1:A:60:LYS:NZ	1:A:85:GLN:O	2.44	0.49
1:A:188:ILE:HG12	1:A:425:MET:HG3	1.95	0.49
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.48	0.49
2:B:334:ASN:OD1	2:B:338:LYS:HE2	2.12	0.49
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.48	0.49
2:B:295:MET:HE2	2:B:377:PHE:CB	2.42	0.49
4:F:135:TYR:O	4:F:138:ARG:HB2	2.12	0.49
1:A:73:THR:O	1:A:76:ASP:HB2	2.13	0.48
1:A:79:ARG:HG3	1:A:92:LEU:HD12	1.94	0.48
1:A:261:PRO:HG3	1:A:313:MET:HB3	1.95	0.48
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.48	0.48
1:C:90:GLU:O	1:C:121:ARG:HD2	2.12	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.95	0.48
4:F:153:ALA:HB2	4:F:178:GLN:HG2	1.95	0.48
1:A:71:GLU:HG3	13:A:649:HOH:O	2.13	0.48
2:B:318:ILE:O	2:B:318:ILE:HG13	2.13	0.48
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.94	0.48
2:D:248:LEU:CD2	2:D:352:LYS:HE2	2.40	0.48
2:B:205:ASP:CB	2:B:303:ALA:HA	2.43	0.48
2:B:248:LEU:HD22	10:B:504:6FS:O4	2.13	0.48
4:F:39:LEU:HD11	4:F:41:LEU:CD2	2.44	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.44	0.48
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.49	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.47
4:F:12:SER:HB2	4:F:343:TYR:CE1	2.49	0.47
2:B:147:SER:HB2	2:B:190:SER:OG	2.14	0.47
2:D:66:ILE:HD12	2:D:121:VAL:HG11	1.97	0.47
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.23	0.47
1:C:286:LEU:H	1:C:286:LEU:HD12	1.79	0.47
4:F:146:VAL:HG21	4:F:233:PHE:CZ	2.49	0.47
1:A:250:VAL:O	1:A:250:VAL:HG22	2.14	0.47
13:A:601:HOH:O	3:E:14:CYS:HB2	2.14	0.47
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.49	0.47
2:D:108:TYR:CG	3:E:133:VAL:HG11	2.50	0.47
2:D:319:PHE:HB3	2:D:323:MET:SD	2.55	0.47
2:D:248:LEU:CD1	10:D:503:6FS:O4	2.50	0.47
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.97	0.47
1:C:401:LYS:HE3	2:D:438:ALA:HB1	1.97	0.47
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.50	0.47
2:D:63:PRO:HD3	2:D:86:ILE:HG13	1.97	0.47
2:D:332:MET:O	2:D:336:GLN:HG3	2.15	0.47
1:A:336:LYS:HE3	3:E:25:LYS:CE	2.45	0.47
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.50	0.46
4:F:98:TYR:HD1	4:F:182:ILE:CD1	2.28	0.46
4:F:195:GLY:O	4:F:227:PRO:HB3	2.16	0.46
3:E:51:GLN:O	3:E:55:GLU:HG3	2.15	0.46
1:A:71:GLU:HG2	1:A:72:PRO:N	2.29	0.46
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.96	0.46
1:A:90:GLU:O	1:A:121:ARG:HD2	2.16	0.46
2:B:192:HIS:CD2	2:B:424:ASN:HD22	2.34	0.46
2:B:199:ASP:C	2:B:200:GLU:HG3	2.35	0.46
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.38	0.46
4:F:193:GLU:HA	4:F:194:PRO:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:GLU:HG3	2:D:98:GLY:CA	2.44	0.46
1:A:104:ALA:HB1	1:A:411:GLU:HB2	1.96	0.46
1:A:151:SER:HB2	1:A:193:THR:CG2	2.46	0.46
4:F:3:THR:H	4:F:38:ASN:HD22	1.63	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.46
1:C:220:GLU:HG2	2:D:326:LYS:HD2	1.98	0.46
1:C:286:LEU:HD12	1:C:286:LEU:N	2.31	0.46
2:D:155:SER:HB2	3:E:126:LYS:HZ3	1.81	0.46
2:D:402:LYS:CB	2:D:405:LEU:HD12	2.46	0.46
3:E:106:GLU:HA	3:E:106:GLU:OE1	2.16	0.46
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.77	0.46
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.51	0.46
1:A:69:ASP:O	1:A:94:THR:HA	2.16	0.45
2:B:7:ILE:O	2:B:137:LEU:HA	2.16	0.45
4:F:98:TYR:CB	4:F:182:ILE:HD11	2.44	0.45
2:D:188:THR:HA	2:D:191:VAL:CG1	2.46	0.45
3:E:57:ALA:HA	3:E:60:ARG:HH11	1.80	0.45
4:F:204:TRP:CH2	4:F:220:VAL:HG23	2.51	0.45
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.98	0.45
4:F:96:GLU:HG2	4:F:98:TYR:CE1	2.51	0.45
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.98	0.45
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.98	0.45
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.51	0.45
1:C:403:ALA:O	1:C:404:PHE:HB2	2.17	0.45
4:F:252:ASN:HD22	4:F:255:ARG:HD2	1.81	0.45
2:B:107:HIS:O	2:B:152:LEU:HD22	2.17	0.45
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.99	0.45
2:D:103:TRP:HD1	2:D:147:SER:HB2	1.82	0.45
4:F:131:PHE:CE1	4:F:182:ILE:HD13	2.51	0.45
2:B:345:GLU:OE1	2:B:345:GLU:N	2.41	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.45
4:F:269:GLN:HA	4:F:272:MET:CE	2.47	0.45
1:A:167:LEU:HD11	1:A:200:CYS:HB3	1.99	0.45
2:D:248:LEU:HD21	2:D:352:LYS:NZ	2.30	0.45
2:D:255:LEU:HD22	10:D:503:6FS:C10	2.47	0.45
4:F:242:ASN:ND2	4:F:244:CYS:SG	2.89	0.44
4:F:49:PHE:CB	4:F:66:ARG:HD2	2.48	0.44
1:A:176:GLN:HG3	13:A:625:HOH:O	2.18	0.44
2:D:105:LYS:HA	2:D:109:THR:OG1	2.17	0.44
2:D:134:GLY:HA3	2:D:165:ILE:O	2.17	0.44
2:B:318:ILE:HG23	10:B:504:6FS:C5	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:OD1	8:A:504:GOL:H31	2.18	0.44
2:B:19:LYS:CD	2:B:228:ASN:HB3	2.47	0.44
2:B:241[B]:CYS:SG	2:B:318:ILE:HG21	2.57	0.44
3:E:129:HIS:HA	3:E:132:GLU:OE1	2.18	0.44
2:B:336:GLN:NE2	13:B:611:HOH:O	2.49	0.44
2:B:359:PRO:HB2	2:B:371:LEU:O	2.18	0.44
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.53	0.44
1:C:216:ASN:HB3	1:C:275:VAL:O	2.17	0.44
2:D:414:ASP:OD1	2:D:415:GLU:N	2.51	0.44
4:F:338:CYS:SG	4:F:339:ALA:N	2.91	0.43
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.00	0.43
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.53	0.43
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.18	0.43
1:C:192:HIS:CG	1:C:421:ALA:HA	2.53	0.43
4:F:262:MET:HG2	4:F:266:GLU:HG3	2.00	0.43
1:A:339:ARG:HB2	1:A:341:ILE:CD1	2.49	0.43
2:B:325:MET:HG2	2:B:355:VAL:HG21	2.00	0.43
3:E:59:GLU:HA	3:E:59:GLU:OE2	2.18	0.43
4:F:98:TYR:HB2	4:F:182:ILE:CD1	2.44	0.43
4:F:100:ILE:CG2	4:F:128:ARG:HG2	2.46	0.43
4:F:178:GLN:OE1	4:F:178:GLN:N	2.51	0.43
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.53	0.43
2:D:107:HIS:O	2:D:152:LEU:HD22	2.19	0.43
2:D:298:SER:OG	2:D:307:PRO:HD2	2.18	0.43
4:F:237:THR:O	4:F:246:GLN:NE2	2.49	0.43
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.49	0.43
2:B:316:ALA:HB1	10:B:504:6FS:O2	2.19	0.43
2:B:346:TRP:HE1	2:B:438:ALA:HB2	1.82	0.43
1:C:242:LEU:N	1:C:242:LEU:CD1	2.82	0.43
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.99	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.19	0.43
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.54	0.43
2:D:188:THR:O	2:D:191:VAL:HG12	2.19	0.43
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.00	0.42
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.38	0.42
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.54	0.42
4:F:81:ILE:CG2	4:F:87:LEU:CD1	2.95	0.42
1:C:41:THR:O	13:C:602:HOH:O	2.22	0.42
2:D:325:MET:HG2	2:D:355:VAL:HG21	2.02	0.42
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.83	0.42
4:F:99:VAL:O	4:F:100:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ALA:O	1:A:404:PHE:HB2	2.19	0.42
2:B:326:LYS:O	2:B:330:GLU:HG3	2.19	0.42
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.20	0.42
4:F:259:GLY:O	4:F:261:GLU:HG3	2.20	0.42
4:F:263:PHE:CZ	4:F:341:LYS:HD3	2.55	0.42
2:D:114:LEU:HG	2:D:114:LEU:O	2.20	0.42
2:D:240:THR:CG2	2:D:241:CYS:N	2.82	0.42
4:F:348:GLN:OE1	4:F:348:GLN:HA	2.19	0.42
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.55	0.42
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.55	0.42
2:B:175:PRO:HA	2:B:178:SER:HB2	2.00	0.42
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.20	0.42
2:B:181:VAL:HG12	1:C:348:PRO:CG	2.50	0.42
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.02	0.42
2:D:187:ALA:O	2:D:191:VAL:HG12	2.19	0.42
3:E:22:VAL:O	3:E:22:VAL:HG23	2.20	0.42
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.55	0.42
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.41
4:F:71:LEU:HD12	4:F:80:LEU:HD23	2.02	0.41
4:F:96:GLU:HG2	4:F:98:TYR:HE1	1.86	0.41
4:F:338:CYS:HB3	4:F:343:TYR:CZ	2.55	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.41
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.50	0.41
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.19	0.41
4:F:39:LEU:HD11	4:F:41:LEU:HD21	2.03	0.41
1:A:341:ILE:O	1:A:341:ILE:HG22	2.19	0.41
1:C:194:THR:O	1:C:194:THR:HG22	2.21	0.41
1:C:218:ASP:OD2	1:C:280:LYS:HE2	2.20	0.41
2:D:36:TYR:CE2	2:D:46:LEU:HD11	2.54	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.41
2:B:88:ARG:HG2	2:B:90:ASP:OD1	2.21	0.41
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.03	0.41
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.56	0.41
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.03	0.41
1:A:285:GLN:HG2	1:A:372:GLN:CD	2.41	0.41
2:B:240:THR:HB	2:B:318:ILE:HD13	2.01	0.41
1:A:75:ILE:CG2	1:A:92:LEU:HB3	2.51	0.41
2:B:134:GLY:HA2	2:B:164:ARG:HB3	2.03	0.41
2:B:208:ALA:HB2	2:B:304:ALA:HB2	2.02	0.41
4:F:153:ALA:CB	4:F:178:GLN:HG2	2.51	0.41
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.55	0.41
2:B:158:ARG:NH1	2:B:196:GLU:O	2.54	0.41
2:B:250:ALA:HA	10:B:504:6FS:O5	2.21	0.41
2:B:324:SER:HB3	2:B:327:GLU:HG2	2.03	0.41
2:D:82:PRO:O	2:D:83:PHE:HB2	2.20	0.41
2:D:323:MET:HB3	2:D:373:MET:SD	2.61	0.41
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.57	0.40
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.03	0.40
2:D:214:PHE:O	2:D:218:LYS:HA	2.22	0.40
1:A:93:ILE:HD11	1:A:121:ARG:CG	2.49	0.40
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.56	0.40
4:F:198:LYS:HD2	4:F:320:MET:HE1	2.04	0.40
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	3.09	0.40
1:A:292:THR:O	1:A:295:CYS:HB2	2.21	0.40
2:B:181:VAL:HG22	1:C:258:ASN:OD1	2.21	0.40
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.85	0.40
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.40
2:D:48:ARG:HB2	2:D:243:ARG:O	2.21	0.40
2:D:63:PRO:CD	2:D:86:ILE:HG13	2.51	0.40
4:F:14:TYR:HA	4:F:17:VAL:CG2	2.50	0.40
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.04	0.40
2:B:401:ARG:HA	2:B:401:ARG:HD2	1.92	0.40
12:F:401:ACP:O1B	12:F:401:ACP:O3G	2.40	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)
13:D:634:HOH:O	13:F:520:HOH:O[3_545]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/451 (97%)	427 (98%)	10 (2%)	0	100	100
1	C	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
2	B	420/445 (94%)	411 (98%)	9 (2%)	0	100	100
2	D	418/445 (94%)	408 (98%)	10 (2%)	0	100	100
3	E	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
4	F	341/384 (89%)	328 (96%)	12 (4%)	1 (0%)	41	55
All	All	2176/2319 (94%)	2119 (97%)	56 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	235	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/379 (98%)	370 (100%)	0	100	100
1	C	373/379 (98%)	371 (100%)	2 (0%)	88	95
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	97
2	D	364/383 (95%)	360 (99%)	4 (1%)	73	87
3	E	111/127 (87%)	109 (98%)	2 (2%)	59	76
4	F	309/342 (90%)	306 (99%)	3 (1%)	76	88
All	All	1895/1993 (95%)	1883 (99%)	12 (1%)	86	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
1	C	2	ARG
1	C	179	THR
2	D	117	SER

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Mol	Chain	Res	Type
2	D	139	HIS
2	D	240	THR
2	D	377	PHE
3	E	15	THR
3	E	133	VAL
4	F	12	SER
4	F	52	LEU
4	F	158	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	192	HIS
2	B	424	ASN
4	F	38	ASN
4	F	242	ASN
4	F	333	ASN

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 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.16	2 (7%)	32,54,54	1.42	6 (18%)
11	MES	B	505	-	12,12,12	2.19	1 (8%)	14,16,16	2.39	8 (57%)
9	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.20	4 (13%)
8	GOL	C	501	-	5,5,5	0.89	0	5,5,5	1.01	0
9	GDP	B	501	6	24,30,30	1.57	4 (16%)	30,47,47	1.12	3 (10%)
8	GOL	C	504	-	5,5,5	0.90	0	5,5,5	1.01	0
5	GTP	C	502	6	26,34,34	1.14	2 (7%)	32,54,54	1.44	6 (18%)
10	6FS	B	504	-	31,32,32	1.14	2 (6%)	40,44,44	1.72	8 (20%)
8	GOL	B	506	-	5,5,5	0.88	0	5,5,5	1.01	0
10	6FS	D	503	-	31,32,32	1.03	3 (9%)	40,44,44	1.76	7 (17%)
8	GOL	B	503	-	5,5,5	0.15	0	5,5,5	0.40	0
12	ACP	F	401	6	27,33,33	1.38	3 (11%)	32,52,52	1.43	4 (12%)
8	GOL	A	505	-	5,5,5	0.89	0	5,5,5	1.03	0
8	GOL	A	504	-	5,5,5	0.89	0	5,5,5	1.00	0

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
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
11	MES	B	505	-	-	5/6/14/14	0/1/1/1
9	GDP	D	501	6	-	4/12/32/32	0/3/3/3
8	GOL	C	501	-	-	0/4/4/4	-
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	GOL	C	504	-	-	0/4/4/4	-
5	GTP	C	502	6	-	9/18/38/38	0/3/3/3
10	6FS	B	504	-	-	16/24/24/24	0/2/2/2
8	GOL	B	506	-	-	0/4/4/4	-
10	6FS	D	503	-	-	8/24/24/24	0/2/2/2
8	GOL	B	503	-	-	0/4/4/4	-
12	ACP	F	401	6	-	8/15/38/38	0/3/3/3
8	GOL	A	505	-	-	0/4/4/4	-
8	GOL	A	504	-	-	0/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	MES	C8-S	-7.31	1.67	1.77
9	B	501	GDP	C6-N1	-4.14	1.31	1.37
5	A	501	GTP	C5-C6	-3.96	1.39	1.47
5	C	502	GTP	C5-C6	-3.83	1.39	1.47
12	F	401	ACP	C2'-C1'	-3.33	1.48	1.53
10	B	504	6FS	O4-S1	3.20	1.46	1.44
10	B	504	6FS	O5-S1	3.00	1.46	1.44
9	B	501	GDP	C2'-C1'	-2.89	1.49	1.53
10	D	503	6FS	O4-S1	2.75	1.46	1.44
12	F	401	ACP	PG-O3G	2.56	1.60	1.54
9	B	501	GDP	PB-O3B	-2.36	1.45	1.54
9	D	501	GDP	C6-N1	-2.34	1.34	1.37
12	F	401	ACP	PG-O2G	2.31	1.60	1.54
9	B	501	GDP	PB-O2B	-2.23	1.46	1.54
10	D	503	6FS	O5-S1	2.22	1.45	1.44
5	A	501	GTP	C2-N3	2.17	1.38	1.33
10	D	503	6FS	C20-N1	2.03	1.48	1.45
5	C	502	GTP	C2-N3	2.02	1.38	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	503	6FS	C20-N1-C16	-6.29	114.96	123.98
10	B	504	6FS	O5-S1-O4	-4.86	115.57	118.22
10	B	504	6FS	C20-N1-C16	-4.23	117.92	123.98
11	B	505	MES	C5-N4-C3	4.12	118.10	108.83
10	D	503	6FS	O5-S1-O4	-4.11	115.99	118.22
11	B	505	MES	C7-N4-C3	3.71	120.73	111.23
12	F	401	ACP	N3-C2-N1	-3.64	122.98	128.68
12	F	401	ACP	PB-O3A-PA	-3.60	121.16	132.56
10	D	503	6FS	C8-O2-C4	3.54	122.87	117.53
10	B	504	6FS	C9-C11-S1	3.20	125.05	120.79
5	A	501	GTP	C5-C6-N1	3.18	119.57	113.95
5	C	502	GTP	PB-O3B-PG	-3.15	122.03	132.83
9	D	501	GDP	PA-O3A-PB	-3.14	122.05	132.83
10	D	503	6FS	C21-C20-N1	3.10	116.64	110.96
5	C	502	GTP	C5-C6-N1	3.06	119.35	113.95
9	B	501	GDP	C5-C6-N1	3.05	119.34	113.95
12	F	401	ACP	C3'-C2'-C1'	3.05	105.56	100.98
5	C	502	GTP	C8-N7-C5	2.99	108.69	102.99
10	B	504	6FS	O3-C2-C1	-2.93	119.07	124.12
5	C	502	GTP	PA-O3A-PB	-2.93	122.77	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	505	MES	C2-C3-N4	-2.93	105.67	110.10
11	B	505	MES	C6-C5-N4	-2.90	105.71	110.10
10	D	503	6FS	C10-O3-C2	2.90	121.90	117.53
5	A	501	GTP	C8-N7-C5	2.88	108.47	102.99
11	B	505	MES	O3S-S-C8	2.85	110.37	105.77
5	A	501	GTP	PB-O3B-PG	-2.82	123.15	132.83
5	A	501	GTP	C2-N1-C6	-2.80	119.94	125.10
11	B	505	MES	C7-N4-C5	2.80	118.40	111.23
10	D	503	6FS	C7-O1-C6	2.72	123.42	117.51
5	A	501	GTP	PA-O3A-PB	-2.67	123.67	132.83
10	B	504	6FS	O2-C4-C5	-2.66	119.55	124.12
10	D	503	6FS	O6-C15-C16	2.66	118.06	114.80
5	C	502	GTP	C2-N1-C6	-2.61	120.29	125.10
11	B	505	MES	O1S-S-C8	2.53	109.96	106.92
10	B	504	6FS	C10-O3-C2	2.43	121.19	117.53
10	B	504	6FS	O3-C2-C3	2.40	119.90	115.26
9	D	501	GDP	C5-C6-N1	2.34	118.08	113.95
9	D	501	GDP	C8-N7-C5	2.34	107.44	102.99
9	B	501	GDP	C8-N7-C5	2.31	107.39	102.99
5	A	501	GTP	O6-C6-C5	-2.23	120.02	124.37
9	B	501	GDP	C2-N1-C6	-2.11	121.21	125.10
11	B	505	MES	O2S-S-C8	2.10	109.45	106.92
10	B	504	6FS	C8-O2-C4	2.10	120.70	117.53
12	F	401	ACP	N6-C6-N1	2.09	122.92	118.57
5	C	502	GTP	O6-C6-C5	-2.06	120.35	124.37
9	D	501	GDP	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (61) 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	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A
10	B	504	6FS	C9-C11-S1-C12
10	B	504	6FS	C9-C11-S1-O4
10	B	504	6FS	C9-C11-S1-O5

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Mol	Chain	Res	Type	Atoms
10	B	504	6FS	C15-C16-N1-C20
10	B	504	6FS	N1-C20-C21-O7
10	B	504	6FS	N1-C20-C21-O8
10	B	504	6FS	C21-C20-N1-C16
10	D	503	6FS	C15-C16-N1-C20
10	D	503	6FS	C17-C16-N1-C20
11	B	505	MES	C8-C7-N4-C3
11	B	505	MES	C8-C7-N4-C5
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
10	B	504	6FS	C17-C16-N1-C20
10	D	503	6FS	C16-C15-O6-C19
10	B	504	6FS	C3-C4-O2-C8
12	F	401	ACP	O4'-C4'-C5'-O5'
10	D	503	6FS	N1-C20-C21-O7
10	D	503	6FS	C14-C15-O6-C19
12	F	401	ACP	C3'-C4'-C5'-O5'
10	B	504	6FS	C5-C4-O2-C8
11	B	505	MES	C7-C8-S-O3S
10	D	503	6FS	N1-C20-C21-O8
10	B	504	6FS	C2-C3-C9-C11
10	D	503	6FS	C4-C3-C9-C11
10	B	504	6FS	C16-C15-O6-C19
9	B	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	6FS	C14-C15-O6-C19
10	B	504	6FS	C4-C3-C9-C11
10	D	503	6FS	C2-C3-C9-C11
11	B	505	MES	C7-C8-S-O1S
11	B	505	MES	C7-C8-S-O2S
12	F	401	ACP	PB-C3B-PG-O2G
12	F	401	ACP	PB-C3B-PG-O3G
10	B	504	6FS	C1-C6-O1-C7
5	A	501	GTP	PB-O3A-PA-O2A
10	B	504	6FS	C5-C6-O1-C7
5	C	502	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O1G
5	C	502	GTP	PB-O3B-PG-O2G
5	C	502	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
9	D	501	GDP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O1A
5	C	502	GTP	PB-O3A-PA-O1A
5	C	502	GTP	PB-O3A-PA-O2A
5	C	502	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA

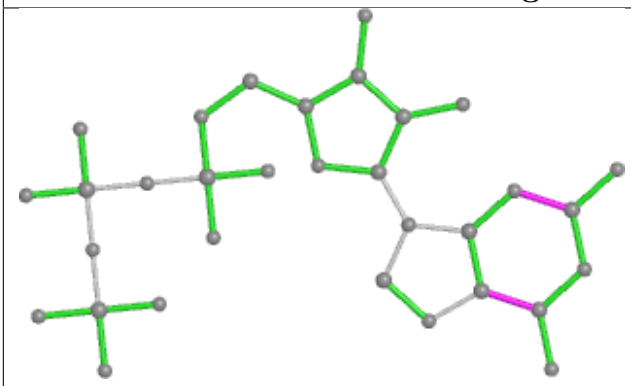
There are no ring outliers.

10 monomers are involved in 23 short contacts:

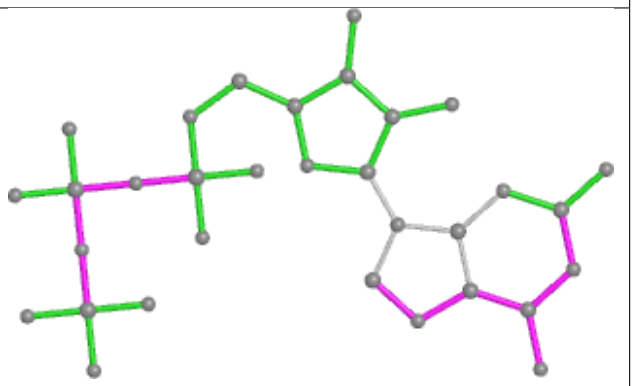
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	505	MES	1	0
9	D	501	GDP	3	0
9	B	501	GDP	1	0
8	C	504	GOL	1	0
5	C	502	GTP	1	0
10	B	504	6FS	8	0
10	D	503	6FS	4	0
8	B	503	GOL	1	0
12	F	401	ACP	2	0
8	A	504	GOL	1	0

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

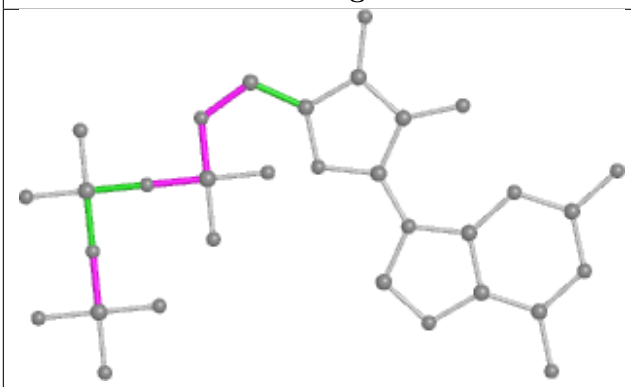
Ligand GTP A 501



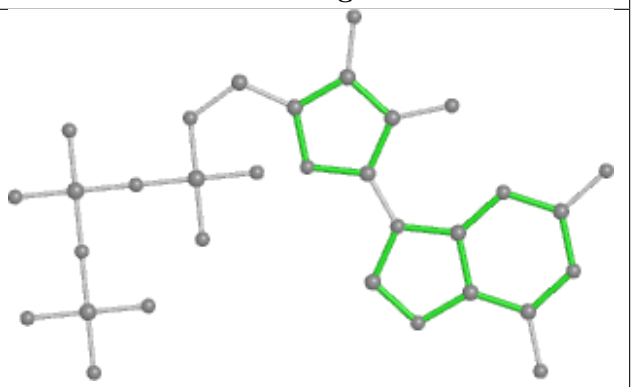
Bond lengths



Bond angles

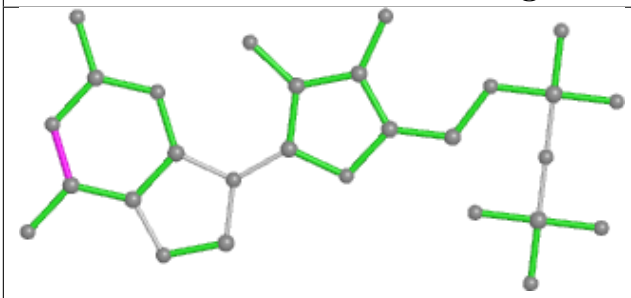


Torsions



Rings

Ligand GDP D 501



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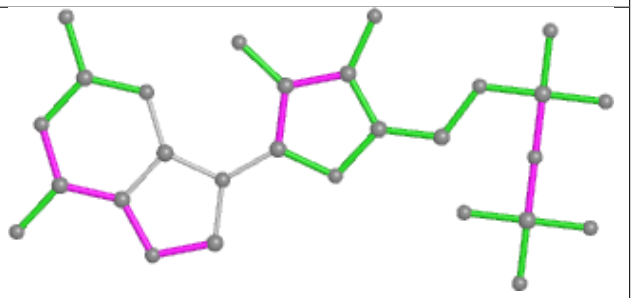

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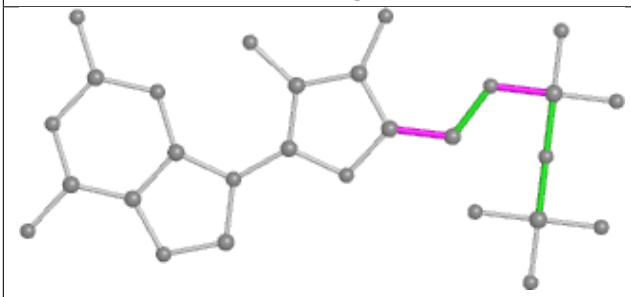

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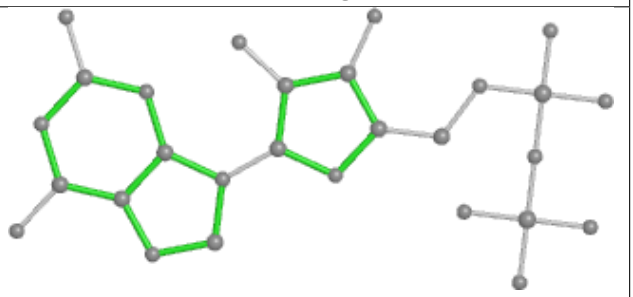
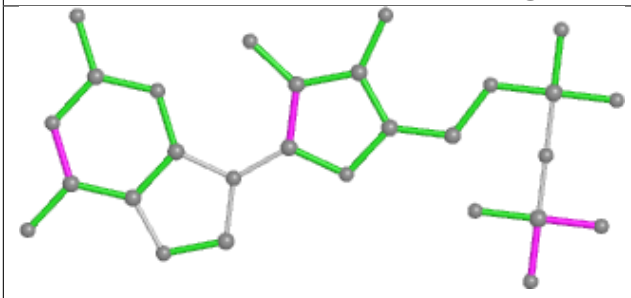
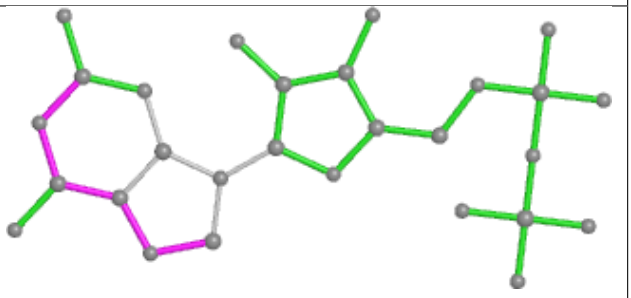


Rings

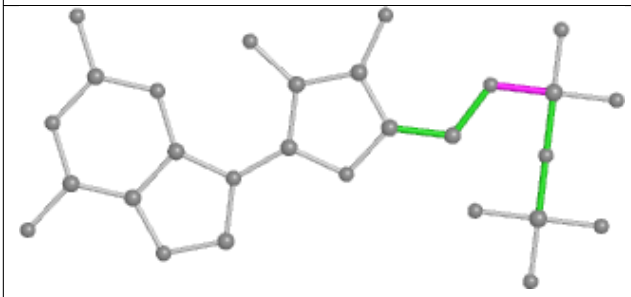
Ligand GDP B 501



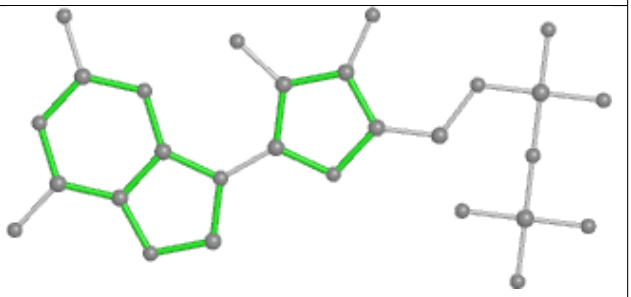
Bond lengths



Bond angles

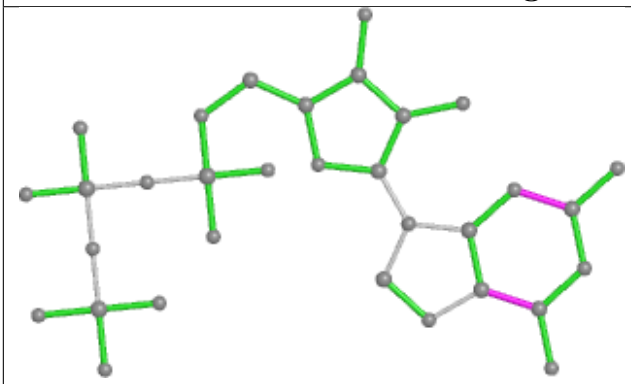


Torsions

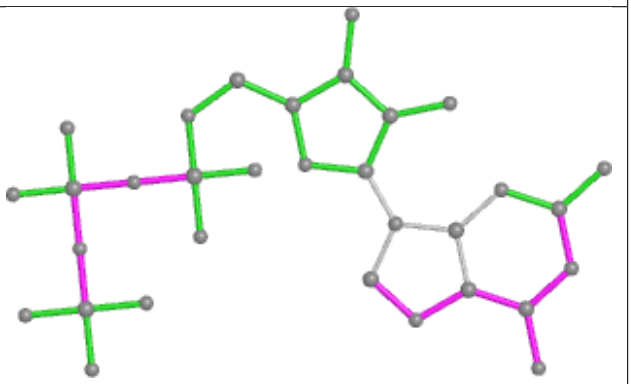


Rings

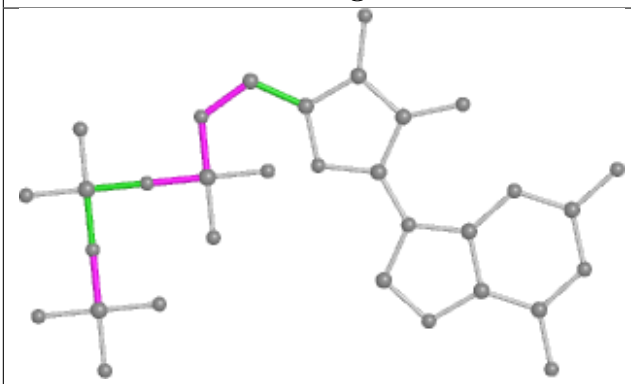
Ligand GTP C 502



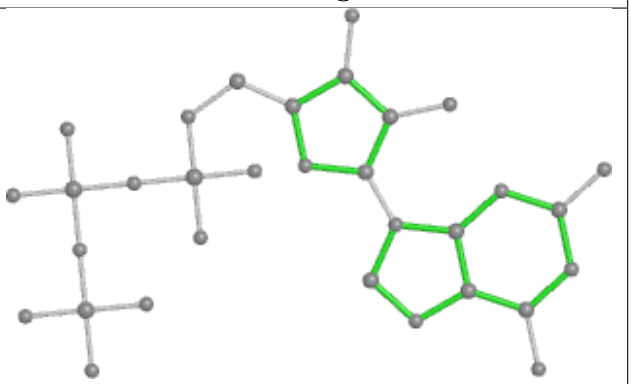
Bond lengths



Bond angles

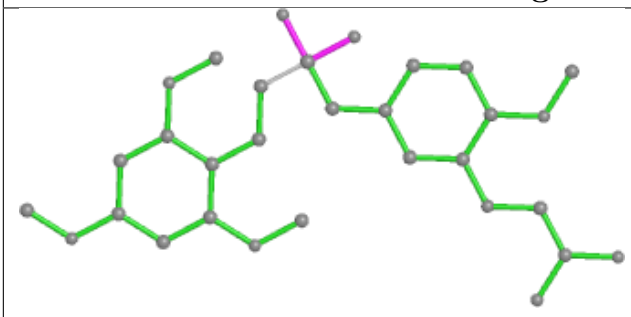


Torsions

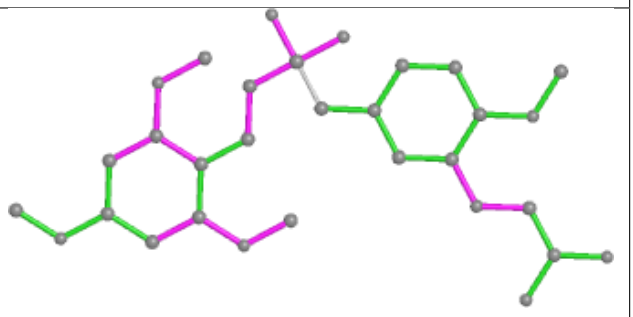


Rings

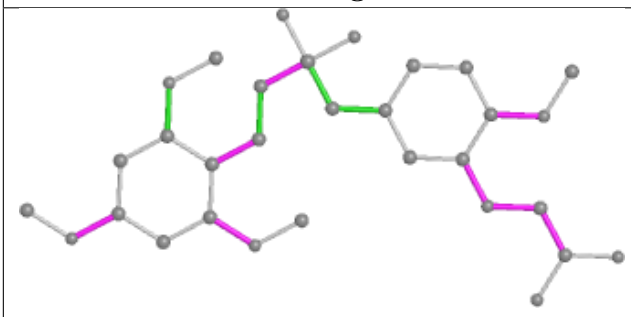
Ligand 6FS B 504



Bond lengths



Bond angles



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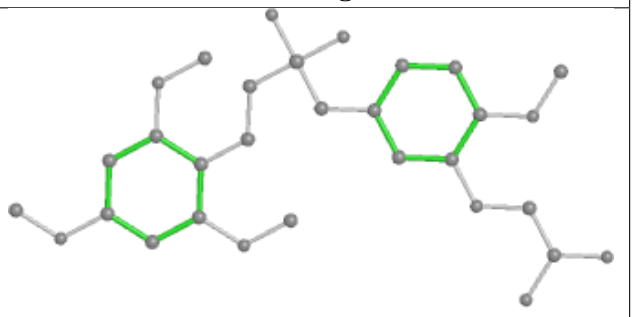
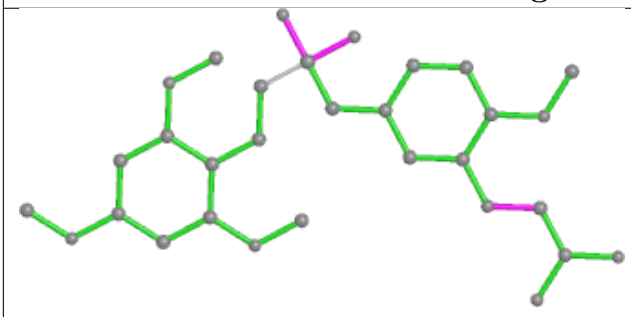
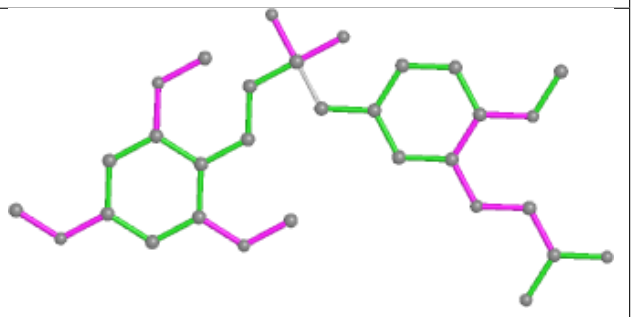


Rings

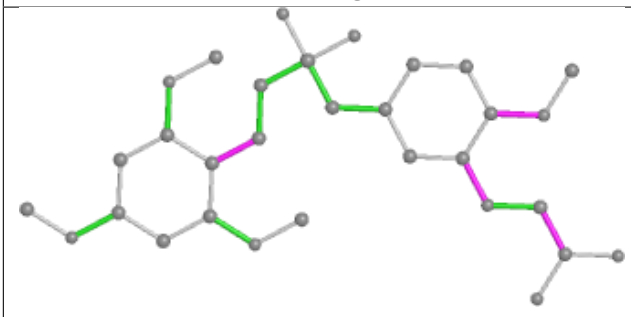
Ligand 6FS D 503



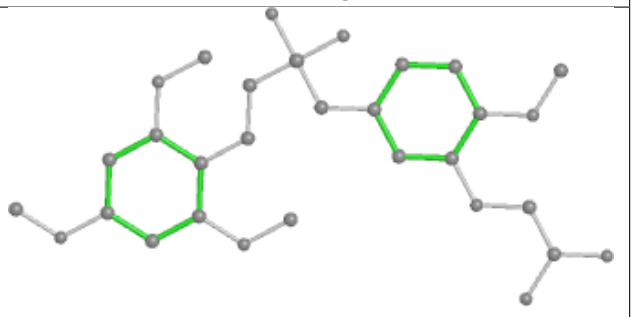
Bond lengths



Bond angles

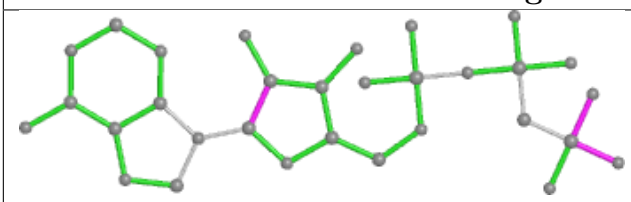


Torsions

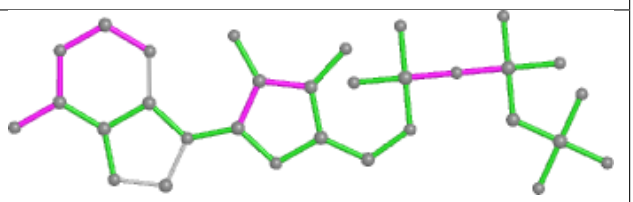


Rings

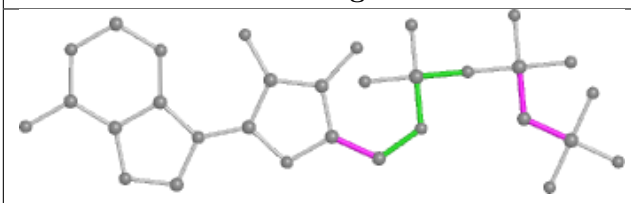
Ligand ACP F 401



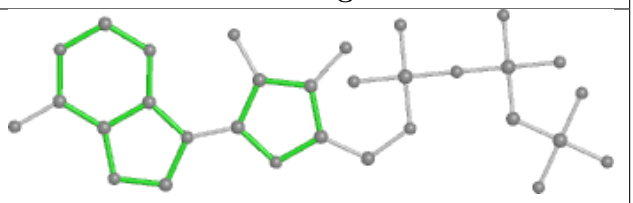
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	437/451 (96%)	0.03	8 (1%) 68 66	44, 68, 110, 171	0
1	C	440/451 (97%)	-0.17	1 (0%) 95 94	34, 50, 86, 121	0
2	B	420/445 (94%)	0.04	12 (2%) 51 50	37, 60, 101, 158	1 (0%)
2	D	422/445 (94%)	0.21	23 (5%) 25 24	44, 87, 129, 168	6 (1%)
3	E	123/143 (86%)	0.26	12 (9%) 7 7	49, 84, 138, 180	0
4	F	347/384 (90%)	0.97	82 (23%) 0 0	54, 103, 173, 225	0
All	All	2189/2319 (94%)	0.19	138 (6%) 20 18	34, 71, 136, 225	7 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	6.7
1	A	282	TYR	6.5
4	F	233	PHE	6.1
2	B	59	ASN	6.0
4	F	134	ALA	5.4
4	F	166	ALA	5.3
4	F	155	ALA	5.3
4	F	169	LEU	5.1
4	F	173	ILE	5.1
2	D	82	PRO	4.9
4	F	132	LEU	4.9
4	F	251	LYS	4.9
4	F	149	ALA	4.8
4	F	225	SER	4.7
4	F	254	GLY	4.6
2	D	57	THR	4.5
2	B	438	ALA	4.4
2	D	247	GLN	4.4
3	E	139	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
4	F	256	TYR	4.3
4	F	238	CYS	4.2
4	F	253	TYR	4.2
4	F	133	ALA	4.2
4	F	252	ASN	4.1
3	E	24	LEU	4.0
4	F	231	ALA	4.0
4	F	362	ALA	4.0
4	F	255	ARG	4.0
4	F	142	ARG	3.9
4	F	164	SER	3.9
2	B	57	THR	3.8
4	F	239	HIS	3.8
4	F	131	PHE	3.8
3	E	142	GLU	3.6
1	A	262	TYR	3.5
4	F	250	SER	3.5
4	F	361	LEU	3.5
4	F	17	VAL	3.5
2	B	61	TYR	3.5
4	F	167	SER	3.4
4	F	157	GLY	3.4
4	F	20	LEU	3.4
4	F	178	GLN	3.3
4	F	100	ILE	3.3
4	F	170	LEU	3.3
4	F	128	ARG	3.3
4	F	197	ARG	3.2
4	F	249	TYR	3.2
2	D	218	LYS	3.1
3	E	25	LYS	3.1
2	B	58	GLY	3.0
4	F	129	GLU	3.0
4	F	130	VAL	3.0
3	E	140	LYS	3.0
4	F	172	PHE	3.0
4	F	258	GLU	3.0
2	B	56	ALA	3.0
1	A	346	TRP	3.0
4	F	22	LEU	2.9
1	A	281	ALA	2.9
2	D	219	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	21	LEU	2.9
4	F	147	TRP	2.9
4	F	9	GLU	2.9
2	B	37	HIS	2.9
4	F	191	LEU	2.9
3	E	135	LYS	2.9
2	D	59	ASN	2.8
2	D	83	PHE	2.8
4	F	259	GLY	2.8
2	D	404	PHE	2.8
4	F	182	ILE	2.8
4	F	244	CYS	2.8
4	F	136	ASN	2.8
2	B	36	TYR	2.8
4	F	190	LEU	2.8
2	D	80	SER	2.8
4	F	181	VAL	2.7
4	F	245	ILE	2.7
2	D	177	VAL	2.7
4	F	24	THR	2.7
4	F	137	ARG	2.7
2	D	221	THR	2.6
4	F	263	PHE	2.6
2	B	371	LEU	2.6
2	D	401	ARG	2.6
2	B	247	GLN	2.6
1	A	42	ILE	2.6
3	E	26	PRO	2.6
2	D	322	ARG	2.6
2	D	214	PHE	2.5
2	D	56	ALA	2.5
4	F	161	LEU	2.5
2	B	60	LYS	2.5
4	F	198	LYS	2.5
4	F	163	SER	2.5
4	F	262	MET	2.5
4	F	248	GLU	2.4
4	F	194	PRO	2.4
4	F	257	GLU	2.4
2	D	37	HIS	2.4
4	F	196	HIS	2.4
4	F	232	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	213	CYS	2.4
2	D	94	PHE	2.3
4	F	135	TYR	2.3
3	E	27	PRO	2.3
4	F	260	ASN	2.3
4	F	192	LEU	2.3
3	E	48	GLU	2.3
4	F	229	ASN	2.3
4	F	201	ILE	2.2
4	F	27	TRP	2.2
3	E	45	PRO	2.2
1	A	43	GLY	2.2
4	F	246	GLN	2.2
1	A	283	HIS	2.2
2	D	220	THR	2.2
3	E	23	ILE	2.2
4	F	171	ASP	2.2
4	F	175	GLU	2.2
2	D	76	ASP	2.1
2	D	285	ALA	2.1
4	F	13	VAL	2.1
1	A	56	THR	2.1
4	F	241	THR	2.1
4	F	264	PHE	2.1
2	B	416	MET	2.1
4	F	183	GLN	2.1
2	D	55	GLU	2.1
4	F	223	THR	2.1
2	D	179	ASP	2.1
4	F	275	LEU	2.1
1	C	440	VAL	2.0
4	F	127	GLU	2.0
4	F	224	SER	2.0
4	F	199	PHE	2.0
4	F	227	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

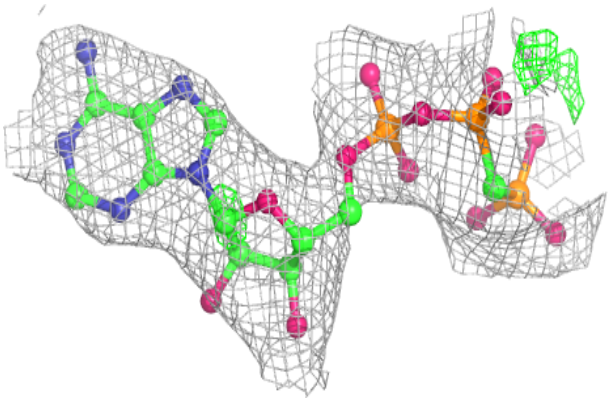
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

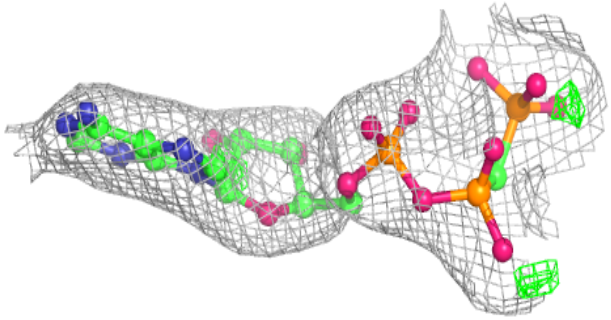
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	C	501	6/6	0.73	0.49	70,80,81,82	0
8	GOL	C	504	6/6	0.75	0.25	94,96,99,103	0
8	GOL	A	505	6/6	0.82	0.14	90,97,105,114	0
12	ACP	F	401	31/31	0.86	0.14	82,104,152,159	0
6	MG	D	502	1/1	0.87	0.06	66,66,66,66	0
6	MG	B	502	1/1	0.87	0.26	49,49,49,49	0
8	GOL	B	506	6/6	0.87	0.12	95,105,107,112	0
10	6FS	D	503	31/31	0.91	0.25	64,106,140,143	0
8	GOL	B	503	6/6	0.91	0.34	81,87,91,92	0
7	CA	A	503	1/1	0.92	0.04	91,91,91,91	0
6	MG	F	402	1/1	0.92	0.26	155,155,155,155	0
9	GDP	D	501	28/28	0.94	0.13	62,77,96,111	0
10	6FS	B	504	31/31	0.95	0.20	54,77,118,134	0
8	GOL	A	504	6/6	0.96	0.16	81,83,85,86	0
11	MES	B	505	12/12	0.96	0.14	49,70,89,102	0
6	MG	A	502	1/1	0.96	0.17	47,47,47,47	0
6	MG	C	503	1/1	0.97	0.14	42,42,42,42	0
9	GDP	B	501	28/28	0.98	0.21	33,47,62,100	0
5	GTP	A	501	32/32	0.98	0.21	34,49,58,65	0
5	GTP	C	502	32/32	0.98	0.17	31,42,48,59	0

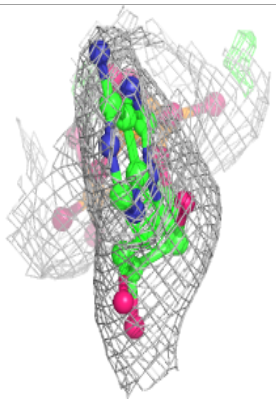
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

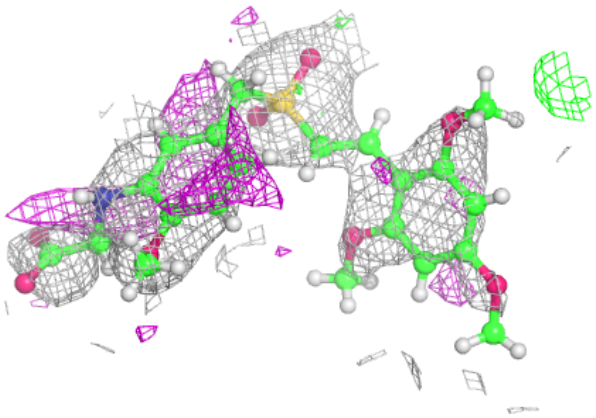


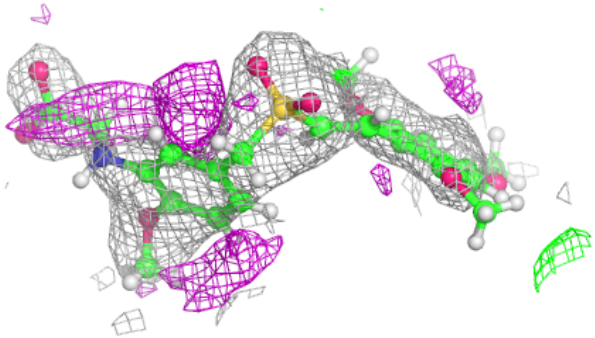


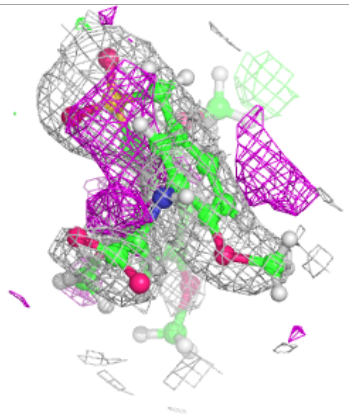


Electron density around 6FS D 503:

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

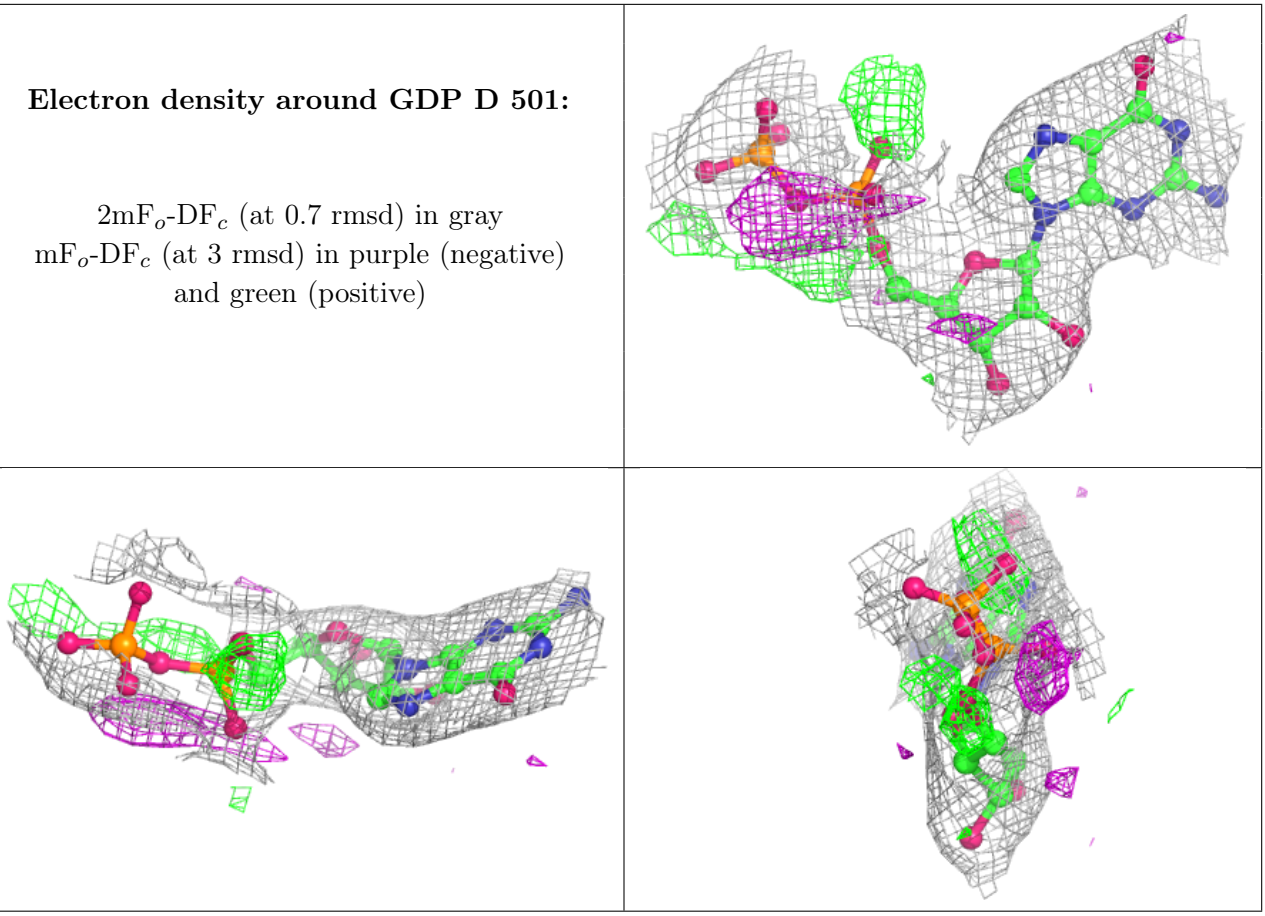






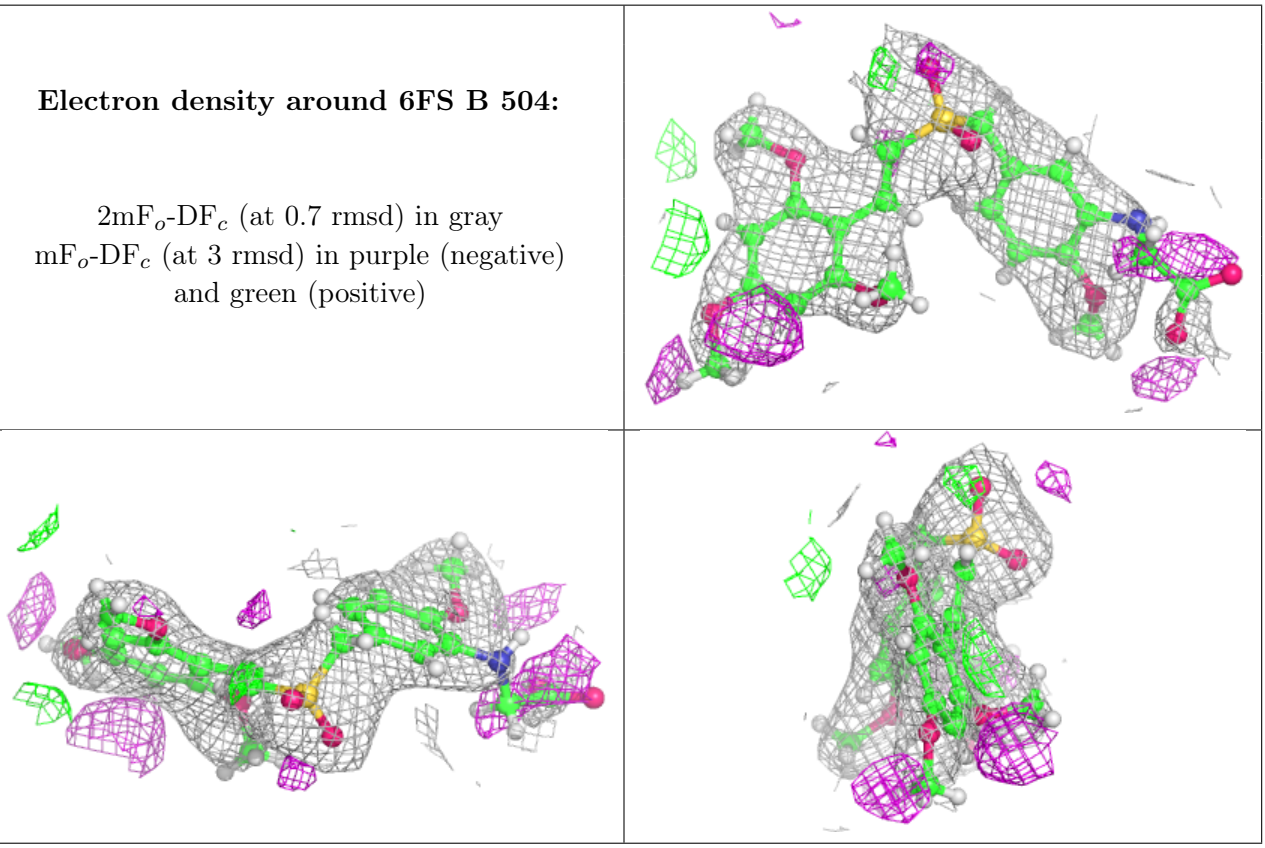
Electron density around GDP D 501:

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



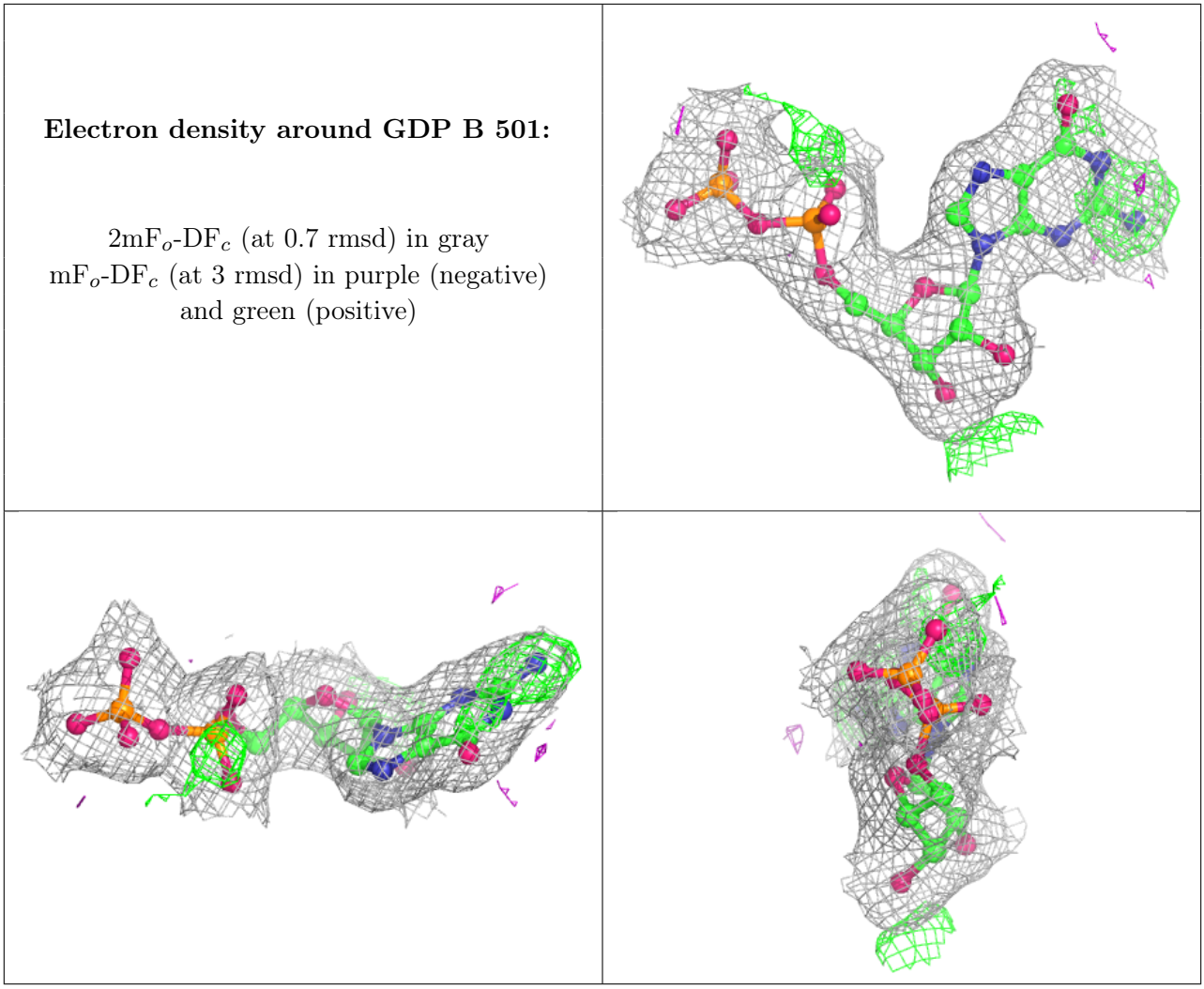
Electron density around 6FS B 504:

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



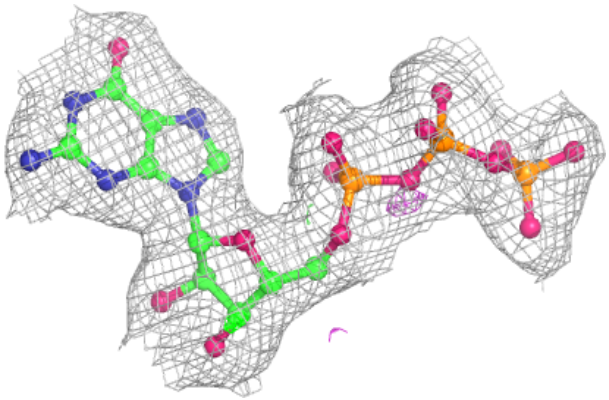
Electron density around GDP B 501:

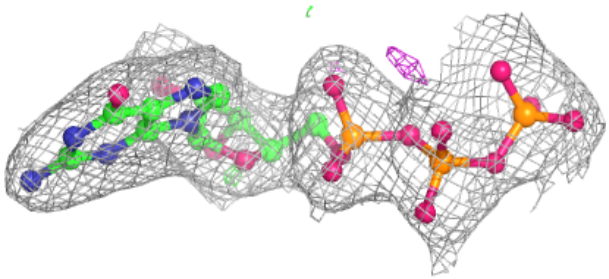
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

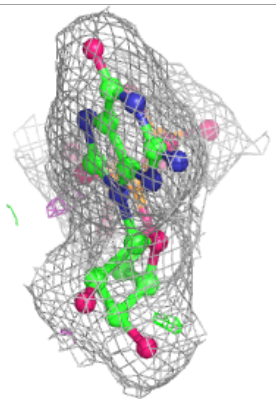


Electron density around GTP A 501:

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

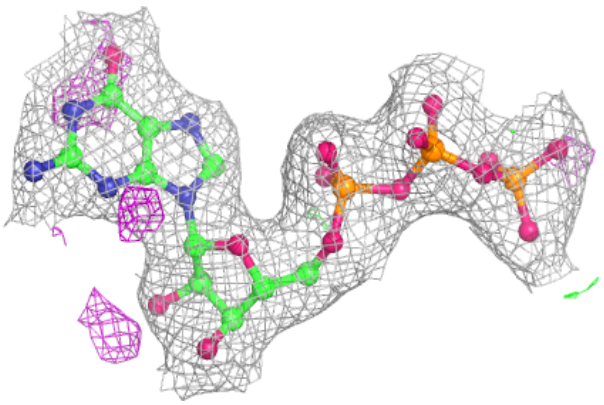


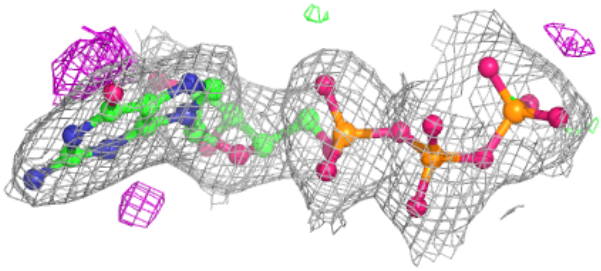


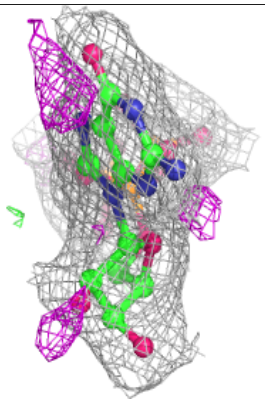


Electron density around GTP C 502:

$2mF_o$-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.