Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 11:46 am GMT

PDB ID	:	8CLH
Title	:	Drug cocktail (Colchicine, Epothilone A, Peloruside, Ansamitocin P3, Vinblastine) bound to tubulin (T2R-TTL) complex
Authors	:	Wranik, M.; Bertrand, Q.; Kepa, M.W.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on	:	2023-02-16
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

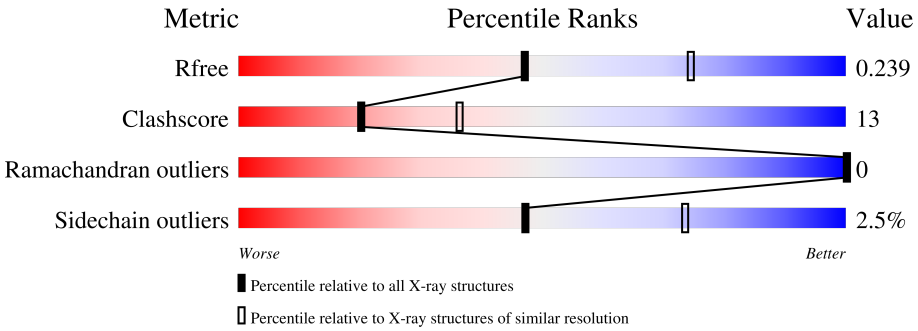
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	440	74% 25% .
1	C	440	83% 16%
2	B	430	79% 21%
2	D	430	76% 23% .
3	E	138	72% 16% . 11%
4	F	381	56% 30% . 13%

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
10	EP	B	504	X	-	-	-
10	EP	D	503	X	-	-	-
11	POU	B	505	X	-	-	-
13	BKF	D	504	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18174 atoms, of which 252 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	439	Total	C	N	O	S	0	2	0
			3441	2175	585	658	23			
1	C	440	Total	C	N	O	S	0	4	0
			3464	2190	590	661	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	2	3	0
			3386	2125	579	655	27			
2	D	430	Total	C	N	O	S	2	1	0
			3376	2117	577	656	26			

- 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
			1020	628	184	202	6			

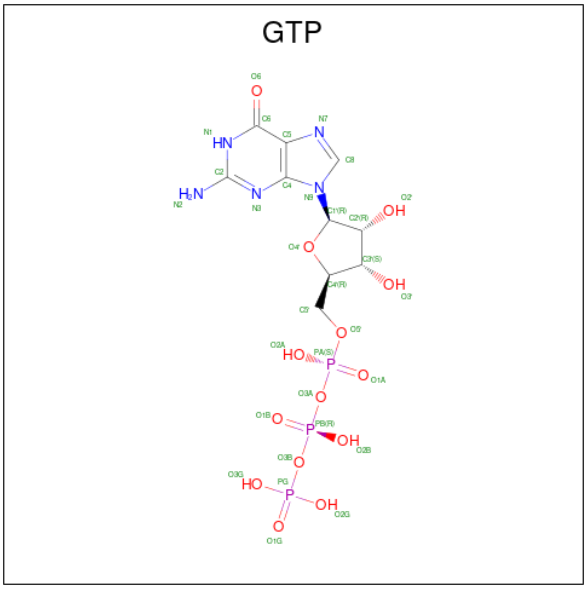
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	1	0
			2714	1740	464	495	15			

There are 3 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

- 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 32 10 5 14 3	0	0
5	C	1	Total C N O P 32 10 5 14 3	0	0

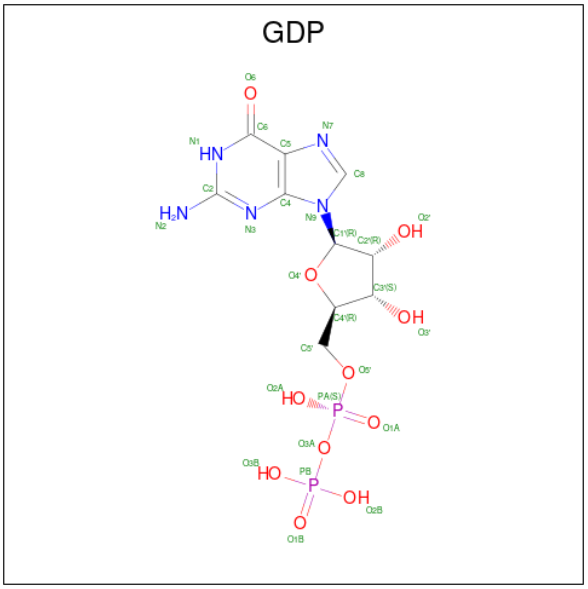
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

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

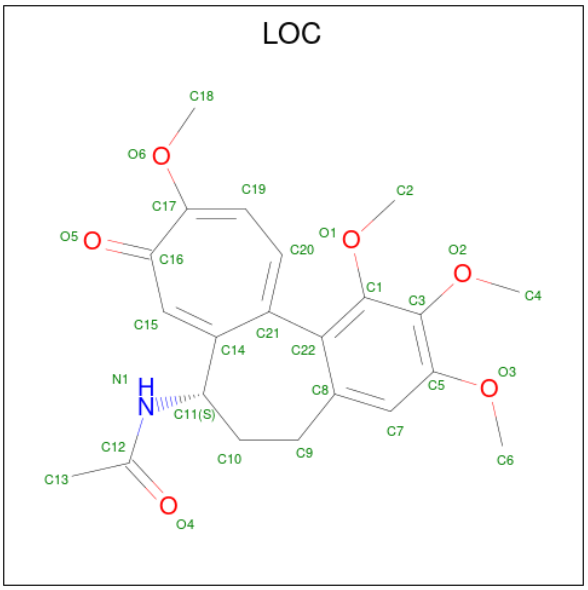
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



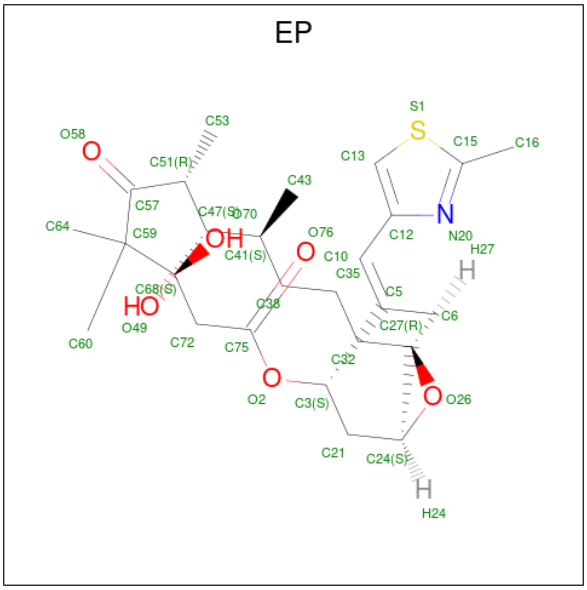
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]et hanamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$) (labeled as "Ligand of Interest" by depositor).



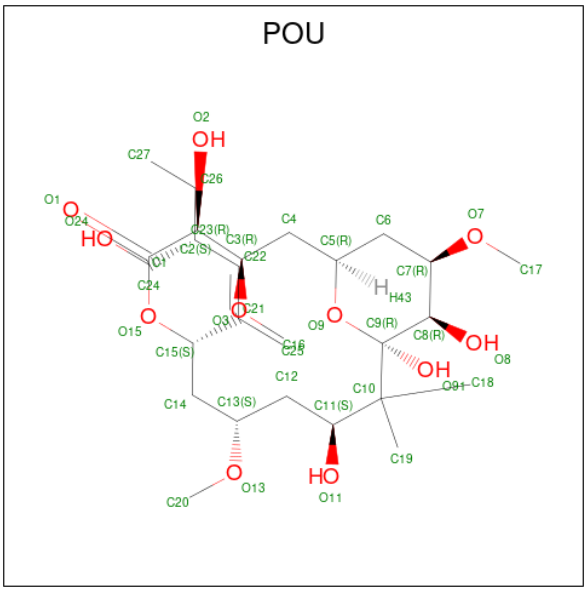
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			54	22	25	1	6		

- Molecule 10 is EPOTHILONE A (three-letter code: EP) (formula: $C_{26}H_{39}NO_6S$) (labeled as "Ligand of Interest" by depositor).



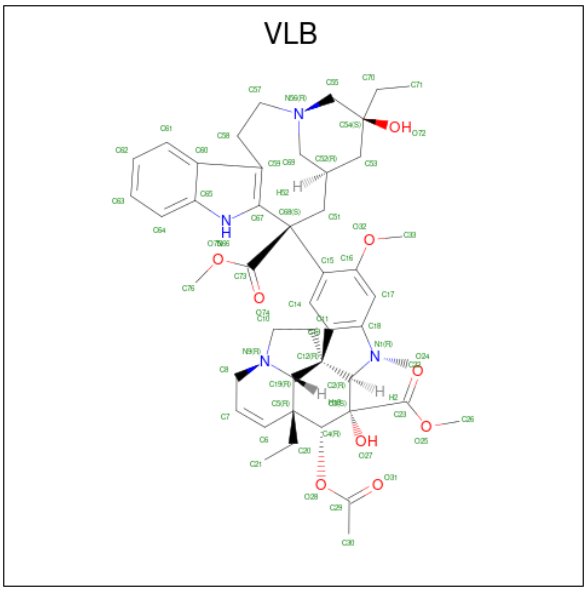
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		
10	D	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		

- Molecule 11 is Peloruside A (three-letter code: POU) (formula: $C_{27}H_{48}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
11	B	1	86	27	48	11	0	0

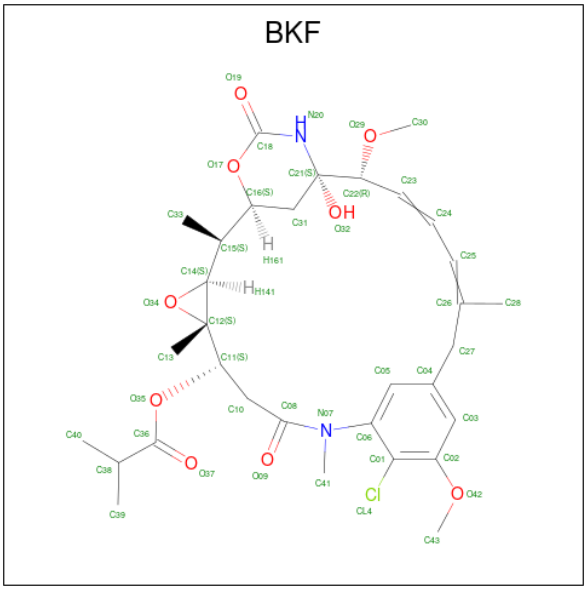
- Molecule 12 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula: $C_{46}H_{58}N_4O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
12	C	1	117	46	58	4	9	0	0

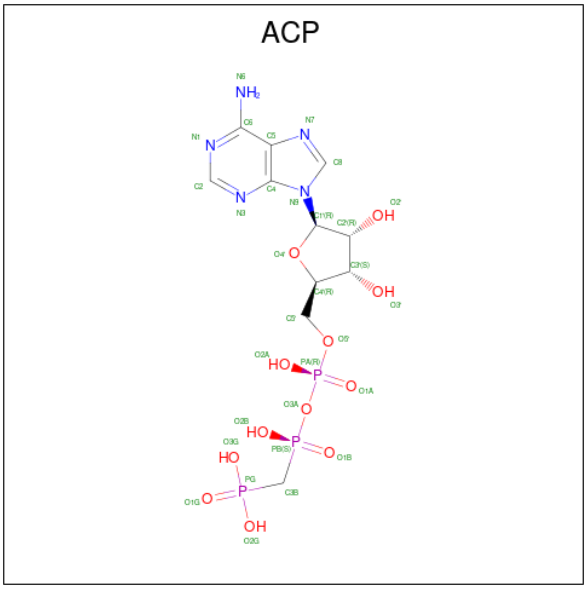
- Molecule 13 is (1S,2S,3S,5S,6S,16Z,18Z,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,

5,9,16-tetramethyl-8,23-dioxo-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16,18-pentaen-6-yl 2-methylpropanoate (three-letter code: BKF) (formula: $C_{32}H_{43}ClN_2O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	D	1	Total	C	Cl	H	N	O	0	0
			87	32	1	43	2	9		

- Molecule 14 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
14	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 15 is water.

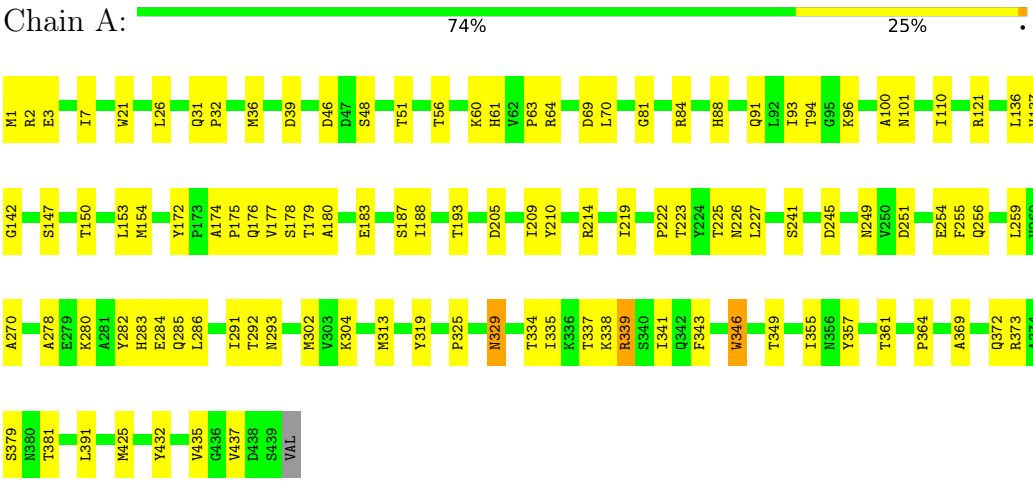
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	28	Total	O	0	0
			28	28		
15	B	25	Total	O	0	0
			25	25		
15	C	54	Total	O	0	0
			54	54		
15	D	10	Total	O	0	0
			10	10		
15	E	3	Total	O	0	0
			3	3		
15	F	6	Total	O	0	0
			6	6		

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. 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. 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.

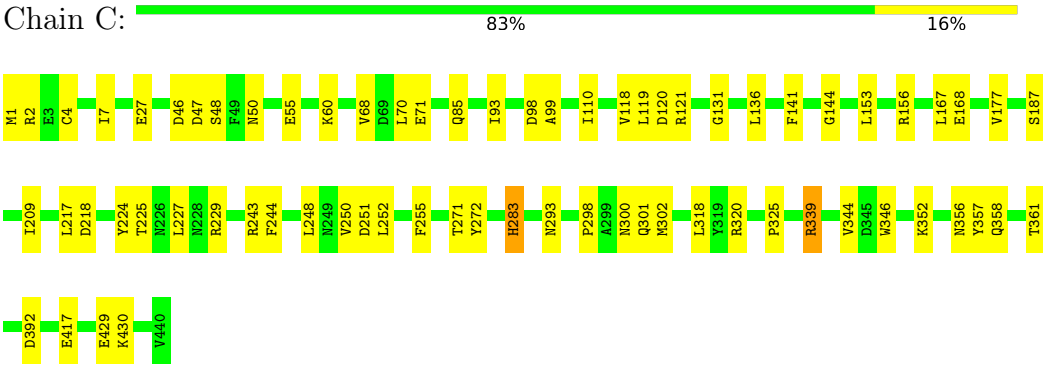
• Molecule 1: Tubulin alpha-1B chain

Chain A:



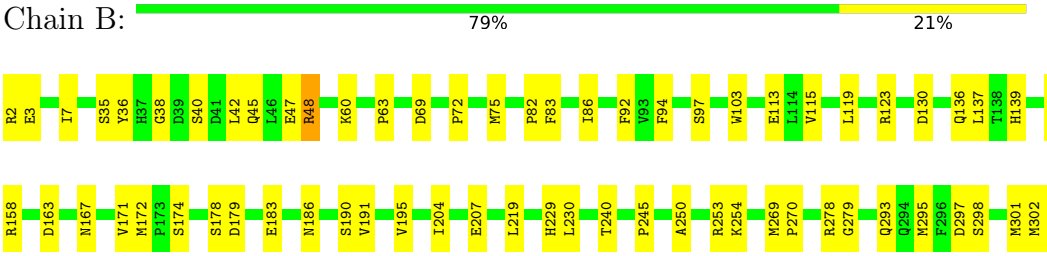
• Molecule 1: Tubulin alpha-1B chain

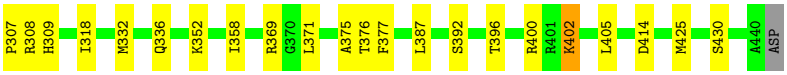
Chain C:



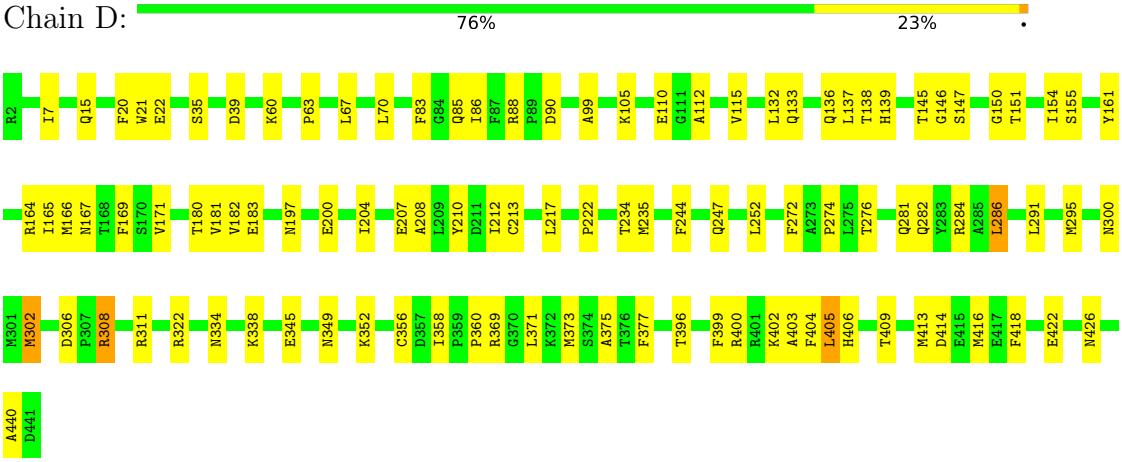
• Molecule 2: Tubulin beta-2B chain

Chain B:

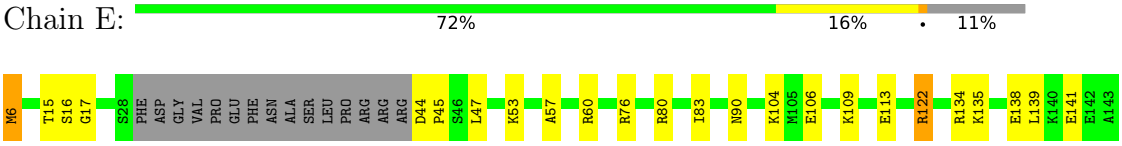




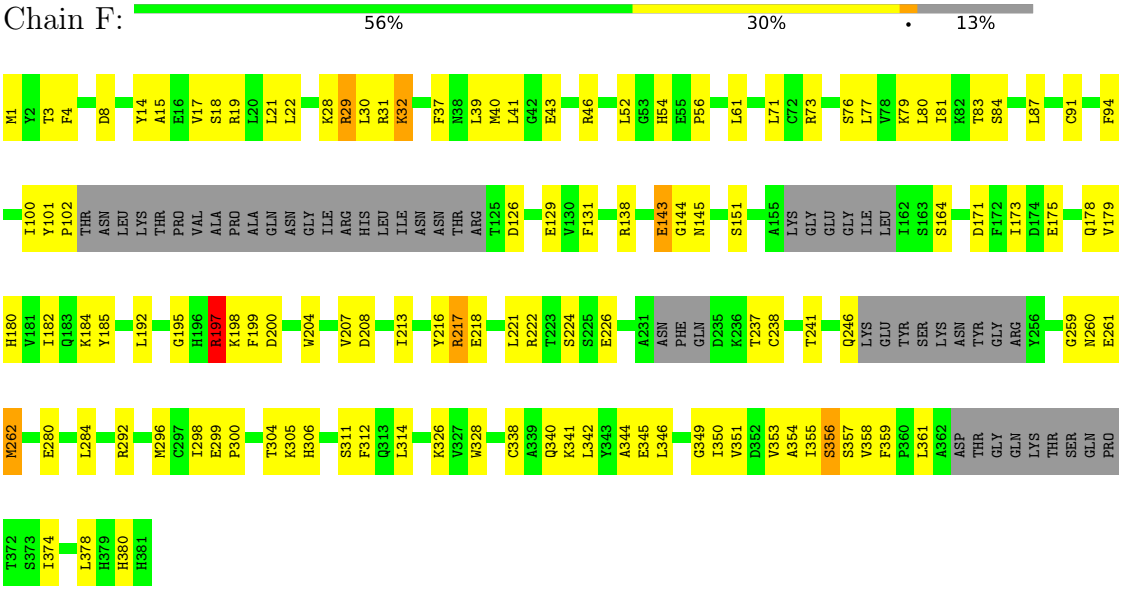
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.00Å 160.34Å 181.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.29 – 2.50 15.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.29-2.50) 74.4 (15.29-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.04 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.185 , 0.239 0.187 , 0.239	Depositor DCC
R_{free} test set	1990 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	-7.5	Xtriage
Anisotropy	-0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.64	EDS
Total number of atoms	18174	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: MG, CA, BKF, LOC, EP, POU, GDP, VLB, ACP, GTP

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	0.31	0/3517	0.52	0/4772
1	C	0.33	0/3550	0.54	0/4817
2	B	0.33	0/3463	0.54	0/4690
2	D	0.31	0/3449	0.52	0/4671
3	E	0.28	0/1028	0.46	0/1364
4	F	0.31	0/2777	0.50	0/3750
All	All	0.31	0/17784	0.52	0/24064

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
3	E	0	1
4	F	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	311	ARG	Sidechain
3	E	122	ARG	Sidechain
4	F	197	ARG	Sidechain
4	F	29	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	F	31	ARG	Sidechain

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	3441	0	3340	101	0
1	C	3464	0	3364	60	1
2	B	3386	0	3254	84	1
2	D	3376	0	3241	87	0
3	E	1020	0	1033	21	0
4	F	2714	0	2682	94	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	29	25	25	6	0
10	B	34	39	37	9	0
10	D	34	39	37	5	0
11	B	38	48	48	6	0
12	C	59	58	58	5	0
13	D	44	43	0	3	0
14	F	31	0	14	0	0
15	A	28	0	0	1	0
15	B	25	0	0	2	0
15	C	54	0	0	5	0
15	D	10	0	0	0	0
15	E	3	0	0	0	0
15	F	6	0	0	1	0
All	All	17922	252	17181	438	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 (438) 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:B:40:SER:OG	2:B:42:LEU:HD13	1.56	1.05
4:F:304:THR:HG21	4:F:311:SER:HB2	1.40	1.03
4:F:100:ILE:HG13	4:F:182:ILE:HD12	1.41	1.01
2:B:396:THR:O	2:B:400:ARG:HG3	1.58	1.01
4:F:14:TYR:HA	4:F:17:VAL:HG12	1.49	0.95
1:A:285:GLN:HE21	1:A:372:GLN:HG2	1.35	0.91
2:D:137:LEU:HD23	2:D:139:HIS:CD2	2.06	0.90
2:B:40:SER:HG	2:B:42:LEU:HD13	1.36	0.88
2:B:75:MET:HG3	2:B:94:PHE:CD2	2.08	0.87
2:B:115:VAL:O	2:B:119:LEU:HD23	1.75	0.86
2:D:137:LEU:CD2	2:D:139:HIS:CD2	2.59	0.86
2:D:137:LEU:CD2	2:D:139:HIS:HD2	1.88	0.84
2:B:83:PHE:O	2:B:86:ILE:HG22	1.78	0.84
4:F:192:LEU:HD11	4:F:262:MET:HE1	1.59	0.83
15:C:635:HOH:O	3:E:104:LYS:HE2	1.78	0.83
1:C:293:ASN:ND2	1:C:339:ARG:HH12	1.78	0.81
2:B:308:ARG:HG2	11:B:505:POU:H22	1.62	0.81
2:B:240:THR:HB	2:B:318:ILE:CD1	2.11	0.80
1:A:285:GLN:NE2	1:A:372:GLN:HG2	1.96	0.80
2:D:137:LEU:HD23	2:D:139:HIS:HD2	1.48	0.77
1:C:271:THR:HG23	1:C:300:ASN:O	1.86	0.75
2:D:83:PHE:O	2:D:86:ILE:HG22	1.86	0.75
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.67	0.74
2:B:229:HIS:CE1	10:B:504:EP:H433	2.24	0.73
2:D:358:ILE:O	2:D:358:ILE:HD12	1.88	0.72
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.70	0.72
2:D:208:ALA:O	2:D:212:ILE:HG12	1.88	0.72
4:F:131:PHE:CE2	4:F:182:ILE:HG21	2.25	0.72
1:A:372:GLN:HA	1:A:372:GLN:NE2	2.05	0.71
4:F:340:GLN:CD	4:F:340:GLN:H	1.93	0.71
4:F:39:LEU:HD23	4:F:40:MET:N	2.06	0.71
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.73	0.71
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.73	0.71
4:F:171:ASP:O	4:F:175:GLU:HG2	1.89	0.71
2:B:392:SER:O	2:B:396:THR:HG23	1.90	0.70
2:D:406:HIS:HA	2:D:409:THR:CG2	2.21	0.70
4:F:39:LEU:HD21	4:F:41:LEU:HD23	1.73	0.70
2:D:406:HIS:HA	2:D:409:THR:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:503:LOC:H2A	9:B:503:LOC:H4B	1.74	0.70
2:D:35:SER:OG	2:D:60:LYS:HE3	1.92	0.70
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.73	0.69
1:A:339:ARG:HB3	1:A:341:ILE:CD1	2.22	0.69
2:B:240:THR:HB	2:B:318:ILE:HD11	1.74	0.69
2:B:352:LYS:HG3	9:B:503:LOC:C16	2.23	0.69
2:B:230:LEU:HD23	10:B:504:EP:H321	1.75	0.68
2:D:402:LYS:CA	2:D:405:LEU:HD11	2.23	0.68
2:D:136:GLN:HA	2:D:167:ASN:O	1.94	0.68
4:F:143:GLU:HG3	4:F:144:GLY:N	2.07	0.68
2:D:180:THR:O	2:D:183:GLU:HG3	1.94	0.68
1:C:209:ILE:HD11	1:C:302:MET:SD	2.34	0.68
1:A:223:THR:HG22	1:A:226:ASN:OD1	1.94	0.67
2:B:250:ALA:HB1	9:B:503:LOC:H7	1.75	0.66
4:F:304:THR:CG2	4:F:311:SER:HB2	2.21	0.66
1:C:177:VAL:HG12	1:C:177:VAL:O	1.95	0.66
4:F:138:ARG:HB2	4:F:145:ASN:HD21	1.61	0.65
1:A:339:ARG:HB3	1:A:341:ILE:HD12	1.78	0.65
2:B:156:LYS:HE2	3:E:76:ARG:NE	2.10	0.65
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.79	0.65
4:F:341:LYS:HD2	4:F:341:LYS:O	1.96	0.65
2:B:179:ASP:HB3	1:C:352:LYS:HG3	1.79	0.64
1:A:334:THR:O	1:A:337:THR:HG22	1.96	0.64
2:B:136:GLN:HA	2:B:167:ASN:O	1.97	0.64
12:C:501:VLB:H511	12:C:501:VLB:H763	1.79	0.64
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.37	0.64
2:B:158:ARG:HD3	15:B:622:HOH:O	1.97	0.63
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.33	0.63
1:A:251:ASP:OD1	1:A:254:GLU:HG3	1.97	0.63
2:D:244:PHE:CD2	2:D:358:ILE:HD11	2.34	0.63
2:D:402:LYS:HB3	2:D:405:LEU:HD11	1.81	0.63
4:F:178:GLN:HA	4:F:178:GLN:OE1	1.98	0.63
1:A:372:GLN:HA	1:A:372:GLN:HE21	1.63	0.62
4:F:138:ARG:HD2	4:F:145:ASN:OD1	1.99	0.62
4:F:151:SER:HB2	4:F:179:VAL:O	2.00	0.62
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.80	0.62
1:A:223:THR:HG23	1:A:225:THR:N	2.14	0.62
2:B:298:SER:HB2	2:B:307:PRO:HD2	1.81	0.61
1:A:223:THR:HG23	1:A:225:THR:H	1.64	0.61
4:F:1:MET:CE	4:F:28:LYS:HB2	2.30	0.61
2:D:334:ASN:OD1	2:D:338:LYS:HE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:O	4:F:91:CYS:HB2	1.99	0.61
4:F:14:TYR:CA	4:F:17:VAL:HG12	2.27	0.61
4:F:192:LEU:HD11	4:F:262:MET:CE	2.29	0.61
2:B:369:ARG:HG3	2:B:369:ARG:HH11	1.66	0.60
1:A:335:ILE:O	1:A:339:ARG:HB2	2.01	0.60
2:B:69:ASP:O	2:B:94:PHE:HA	2.02	0.60
1:A:261:PRO:HD2	15:A:612:HOH:O	2.02	0.60
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.84	0.59
2:D:286:LEU:HD12	2:D:286:LEU:O	2.01	0.59
4:F:101:TYR:HD2	4:F:126:ASP:HB2	1.67	0.59
2:D:405:LEU:HD12	2:D:405:LEU:H	1.66	0.59
1:C:320:ARG:HA	1:C:356:ASN:O	2.03	0.59
1:C:177:VAL:HG11	1:C:224:TYR:CE1	2.38	0.59
2:D:402:LYS:HB3	2:D:405:LEU:CD1	2.33	0.59
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.84	0.58
2:B:40:SER:OG	2:B:42:LEU:CD1	2.42	0.58
9:B:503:LOC:H4B	9:B:503:LOC:C2	2.33	0.58
11:B:505:POU:H2	11:B:505:POU:H30	1.85	0.58
2:D:132:LEU:O	2:D:164:ARG:NH1	2.36	0.58
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.85	0.58
2:D:63:PRO:HD3	2:D:86:ILE:HG12	1.86	0.58
2:B:191:VAL:O	2:B:195:VAL:HG13	2.04	0.58
1:C:1:MET:HG2	1:C:2:ARG:H	1.68	0.58
4:F:345:GLU:CG	4:F:374:ILE:HG21	2.33	0.58
1:A:293:ASN:OD1	1:A:339:ARG:NH1	2.37	0.58
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.84	0.58
1:A:174:ALA:HB3	1:A:177:VAL:HG23	1.86	0.57
1:C:229[B]:ARG:HD3	1:C:363:VAL:HG21	1.86	0.57
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.04	0.57
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.85	0.57
2:B:295:MET:SD	2:B:375:ALA:HB1	2.44	0.57
1:C:48:SER:HB3	1:C:243:ARG:O	2.04	0.57
4:F:14:TYR:HA	4:F:17:VAL:CG1	2.30	0.57
1:A:209:ILE:HD11	1:A:302:MET:SD	2.45	0.57
4:F:131:PHE:HE2	4:F:182:ILE:HG21	1.67	0.57
1:A:1:MET:HA	1:A:1:MET:CE	2.34	0.57
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.87	0.56
1:A:175:PRO:HA	1:A:179:THR:HG22	1.87	0.56
1:C:27:GLU:HG2	1:C:361:THR:CG2	2.35	0.56
1:C:224:TYR:HE2	2:D:247[A]:GLN:HE22	1.52	0.56
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.56
2:D:244:PHE:CE2	2:D:358:ILE:HD11	2.40	0.56
1:A:26:LEU:HD21	1:A:364:PRO:HD3	1.86	0.56
4:F:184:LYS:HD2	4:F:185:TYR:N	2.20	0.56
4:F:19:ARG:HD3	4:F:19:ARG:N	2.20	0.56
2:D:137:LEU:HD21	2:D:139:HIS:CD2	2.40	0.55
1:A:255:PHE:O	1:A:259:LEU:HB2	2.06	0.55
2:B:278:ARG:HG3	2:B:279:GLY:HA3	1.89	0.55
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.88	0.55
4:F:296[A]:MET:SD	4:F:380:HIS:ND1	2.80	0.55
1:A:214:ARG:HG2	1:A:219:ILE:O	2.07	0.55
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.37	0.55
1:A:319:TYR:CD1	1:A:375:VAL:HG22	2.42	0.55
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.88	0.55
4:F:14:TYR:HD1	4:F:17:VAL:HG11	1.72	0.55
2:D:402:LYS:CB	2:D:405:LEU:HD11	2.37	0.55
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.07	0.55
2:B:219:LEU:HD21	10:B:504:EP:H533	1.88	0.55
3:E:6:MET:O	3:E:6:MET:HG3	2.06	0.55
4:F:358:VAL:HG23	4:F:359:PHE:CD2	2.41	0.55
1:A:48:SER:O	1:A:51:THR:HG23	2.06	0.55
4:F:39:LEU:CD2	4:F:41:LEU:HD23	2.37	0.54
4:F:39:LEU:HD21	4:F:41:LEU:CD2	2.37	0.54
1:A:177:VAL:O	1:A:177:VAL:HG22	2.08	0.54
2:B:171:VAL:HA	2:B:204:ILE:O	2.08	0.54
2:B:240:THR:CB	2:B:318:ILE:HD11	2.37	0.54
4:F:259:GLY:O	4:F:261:GLU:HG3	2.08	0.54
2:D:70:LEU:HG	2:D:145:THR:HG23	1.89	0.54
4:F:213:ILE:HG22	4:F:378:LEU:HD12	1.88	0.54
1:A:26:LEU:HD21	1:A:364:PRO:CD	2.38	0.53
1:A:338:LYS:O	1:A:338:LYS:HG2	2.09	0.53
1:A:56:THR:HG21	1:A:60:LYS:HB3	1.91	0.53
2:B:48:ARG:HH21	2:B:245:PRO:HA	1.72	0.53
4:F:292:ARG:O	4:F:296[B]:MET:HB2	2.08	0.53
1:A:293:ASN:HD21	1:A:339:ARG:HH12	1.55	0.53
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.91	0.53
12:C:501:VLB:H262	12:C:501:VLB:N1	2.24	0.53
2:D:405:LEU:O	2:D:409:THR:HG22	2.07	0.53
2:D:371:LEU:HD11	10:D:503:EP:H62	1.90	0.53
4:F:102:PRO:HB3	4:F:173:ILE:O	2.09	0.53
1:A:377:MET:HE3	1:A:379:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.24	0.53
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.91	0.53
1:C:27:GLU:HG2	1:C:361:THR:HG22	1.91	0.53
1:C:417:GLU:HB3	15:C:601:HOH:O	2.08	0.53
1:A:56:THR:CG2	1:A:60:LYS:HB3	2.39	0.53
2:B:230:LEU:HD23	10:B:504:EP:C32	2.38	0.53
2:B:297:ASP:OD1	11:B:505:POU:H9	2.09	0.53
1:C:293:ASN:HD21	1:C:339:ARG:HH12	1.53	0.52
2:D:67:LEU:N	2:D:67:LEU:HD12	2.24	0.52
1:C:251:ASP:OD1	1:C:252:LEU:N	2.42	0.52
2:D:276:THR:OG1	2:D:281:GLN:HG2	2.09	0.52
1:A:180:ALA:O	1:A:183:GLU:HG3	2.10	0.52
2:B:369:ARG:HG3	2:B:369:ARG:NH1	2.21	0.52
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.92	0.52
2:D:360:PRO:C	2:D:369:ARG:HA	2.30	0.52
3:E:109:LYS:HE2	3:E:113:GLU:OE2	2.10	0.52
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.44	0.52
2:B:219:LEU:HD21	10:B:504:EP:C53	2.39	0.52
2:B:318:ILE:HG23	2:B:376:THR:HB	1.90	0.52
4:F:73:ARG:HB2	4:F:76:SER:OG	2.09	0.52
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.45	0.51
2:D:295:MET:CG	2:D:377:PHE:HB2	2.39	0.51
2:D:396:THR:O	2:D:400:ARG:HB2	2.10	0.51
4:F:213:ILE:CG2	4:F:378:LEU:HD12	2.40	0.51
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.45	0.51
2:D:403:ALA:O	2:D:404:PHE:HB2	2.09	0.51
2:D:404:PHE:HE2	13:D:504:BKF:C13	2.24	0.51
2:B:156:LYS:HE2	3:E:76:ARG:CZ	2.40	0.51
4:F:129:GLU:OE1	4:F:129:GLU:HA	2.10	0.51
1:A:101:ASN:ND2	2:B:254:LYS:HE2	2.25	0.51
1:C:271:THR:HG22	1:C:272:TYR:N	2.25	0.51
2:D:402:LYS:HA	2:D:405:LEU:HD11	1.93	0.51
2:B:229:HIS:ND1	10:B:504:EP:H382	2.26	0.51
4:F:222:ARG:O	4:F:241:THR:HB	2.10	0.51
1:C:177:VAL:CG1	1:C:224:TYR:CE1	2.94	0.51
4:F:346:LEU:O	4:F:350:ILE:HG13	2.11	0.50
2:B:82:PRO:O	2:B:83:PHE:HB2	2.11	0.50
12:C:501:VLB:O32	12:C:501:VLB:C73	2.59	0.50
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.93	0.50
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.93	0.50
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:THR:OG1	4:F:37:PHE:HA	2.11	0.50
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.50
1:A:282:TYR:O	1:A:283:HIS:HB2	2.11	0.50
1:C:60:LYS:HB2	1:C:60:LYS:NZ	2.25	0.50
2:D:360:PRO:C	2:D:369:ARG:CA	2.80	0.50
1:A:56:THR:CG2	1:A:60:LYS:H	2.23	0.50
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.50
1:A:136:LEU:HD12	1:A:136:LEU:N	2.27	0.50
1:A:175:PRO:HA	1:A:179:THR:CG2	2.42	0.49
1:C:271:THR:HG22	1:C:272:TYR:H	1.76	0.49
2:D:7:ILE:O	2:D:137:LEU:HA	2.11	0.49
2:B:97:SER:O	1:C:2:ARG:NH2	2.46	0.49
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.95	0.49
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.48	0.49
2:B:42:LEU:C	2:B:45:GLN:N	2.66	0.49
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.94	0.49
12:C:501:VLB:H763	12:C:501:VLB:C51	2.42	0.49
2:D:181:VAL:HG22	13:D:504:BKF:O09	2.13	0.49
4:F:4:PHE:O	4:F:29:ARG:HA	2.13	0.49
4:F:18:SER:HA	4:F:21:LEU:HD12	1.94	0.49
4:F:71:LEU:HD22	4:F:298:ILE:HD13	1.94	0.49
2:B:229:HIS:CE1	10:B:504:EP:C27	2.96	0.49
2:D:306:ASP:OD1	2:D:308:ARG:HB2	2.13	0.49
4:F:344:ALA:O	4:F:346:LEU:N	2.42	0.49
1:A:154:MET:HE2	1:A:154:MET:HA	1.94	0.48
2:B:270:PRO:O	2:B:302:MET:HB2	2.13	0.48
2:B:332:MET:O	2:B:336:GLN:HG3	2.13	0.48
1:C:177:VAL:O	1:C:177:VAL:CG1	2.61	0.48
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.48	0.48
4:F:61:LEU:HD22	4:F:358:VAL:HG21	1.95	0.48
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.95	0.48
1:A:338:LYS:O	1:A:339:ARG:HD2	2.13	0.48
2:B:305[B]:CYS:O	2:B:307:PRO:HD3	2.13	0.48
1:A:245:ASP:O	3:E:16:SER:HB2	2.13	0.48
4:F:198:LYS:HG2	4:F:199:PHE:H	1.79	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.28	0.48
2:D:112:ALA:HB1	3:E:134:ARG:HH21	1.77	0.48
4:F:350:ILE:O	4:F:354:ALA:HB3	2.14	0.48
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.43	0.48
1:A:286:LEU:N	1:A:286:LEU:HD22	2.27	0.48
1:A:36:MET:HG2	1:A:61:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:PRO:HB3	12:C:501:VLB:C65	2.43	0.48
4:F:79:LYS:O	4:F:83:THR:OG1	2.22	0.48
1:A:56:THR:HG22	1:A:60:LYS:O	2.14	0.48
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.48
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.79	0.48
1:C:298:PRO:HD2	15:C:605:HOH:O	2.13	0.48
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.14	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
1:A:291:ILE:CD1	1:A:375:VAL:HG23	2.42	0.47
2:B:269:MET:HE3	2:B:301:MET:HG3	1.95	0.47
2:B:278:ARG:HG3	2:B:279:GLY:CA	2.44	0.47
1:C:298:PRO:O	1:C:301:GLN:HG2	2.14	0.47
2:D:356:CYS:SG	2:D:358:ILE:CD1	3.02	0.47
2:B:42:LEU:HD22	2:B:358:ILE:HD11	1.96	0.47
1:A:319:TYR:CE1	1:A:375:VAL:HG22	2.50	0.47
2:D:146:GLY:O	2:D:150:GLY:HA3	2.15	0.47
2:D:402:LYS:C	2:D:405:LEU:HD11	2.35	0.47
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.97	0.47
4:F:246:GLN:HG2	4:F:260:ASN:OD1	2.14	0.47
2:D:86:ILE:HG12	2:D:86:ILE:O	2.14	0.47
4:F:17:VAL:HG23	4:F:351:VAL:HG13	1.95	0.47
2:B:119:LEU:HB3	2:B:123:ARG:NH1	2.29	0.47
4:F:351:VAL:O	4:F:356:SER:HB2	2.15	0.46
1:A:81:GLY:O	1:A:84:ARG:HD3	2.15	0.46
4:F:32:LYS:HB2	4:F:32:LYS:HE3	1.72	0.46
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.50	0.46
2:D:70:LEU:H	2:D:145:THR:HG21	1.81	0.46
4:F:19:ARG:N	4:F:19:ARG:CD	2.79	0.46
2:B:35:SER:OG	2:B:60:LYS:HE2	2.15	0.46
2:B:178:SER:OG	2:B:183:GLU:OE2	2.21	0.46
2:D:105:LYS:HB3	2:D:110:GLU:HG3	1.98	0.46
1:A:284:GLU:CD	1:A:284:GLU:H	2.20	0.46
10:D:503:EP:C24	10:D:503:EP:H61	2.46	0.46
1:A:286:LEU:O	1:A:373:ARG:NH1	2.47	0.46
2:B:72:PRO:O	2:B:75:MET:HB2	2.16	0.46
2:B:352:LYS:HG3	9:B:503:LOC:C17	2.46	0.46
4:F:15:ALA:O	4:F:19:ARG:HD3	2.16	0.46
4:F:19:ARG:HA	4:F:22:LEU:HD12	1.97	0.46
2:D:413:MET:HE2	2:D:418:PHE:CE1	2.52	0.45
4:F:28:LYS:HD3	4:F:30:LEU:HD21	1.96	0.45
4:F:216:TYR:OH	4:F:342:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:ALA:HA	3:E:60:ARG:NH1	2.32	0.45
3:E:134:ARG:NH1	3:E:134:ARG:HG3	2.31	0.45
3:E:135:LYS:O	3:E:139:LEU:HG	2.16	0.45
4:F:262:MET:HB3	4:F:262:MET:HE3	1.64	0.45
2:D:234:THR:OG1	2:D:302:MET:CE	2.64	0.45
2:D:413:MET:CE	2:D:418:PHE:CE1	2.99	0.45
1:A:137:VAL:HG21	1:A:154:MET:CE	2.46	0.45
1:A:304:LYS:HB3	4:F:54:HIS:HE1	1.80	0.45
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.98	0.45
2:D:182:VAL:HG11	13:D:504:BKF:O34	2.17	0.45
4:F:351:VAL:HG12	4:F:355:ILE:HD12	1.99	0.45
2:B:42:LEU:O	2:B:45:GLN:N	2.50	0.45
2:D:274:PRO:HB2	10:D:503:EP:C16	2.46	0.45
4:F:204:TRP:CZ2	4:F:338:CYS:HA	2.51	0.45
2:D:88:ARG:HD2	2:D:90:ASP:OD1	2.17	0.45
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.98	0.45
2:B:371:LEU:HD21	10:B:504:EP:H10	1.99	0.45
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.99	0.45
1:A:26:LEU:CD2	1:A:364:PRO:HD3	2.47	0.45
4:F:40:MET:CE	4:F:52:LEU:HD11	2.47	0.45
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.47	0.45
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.47	0.45
2:B:278:ARG:HA	2:B:279:GLY:HA2	1.64	0.45
2:B:400:ARG:HD2	15:B:621:HOH:O	2.17	0.45
2:D:413:MET:HE2	2:D:418:PHE:HE1	1.82	0.45
2:B:250:ALA:HB1	9:B:503:LOC:C7	2.46	0.44
2:B:303:ALA:O	2:B:305[A]:CYS:N	2.47	0.44
2:D:167:ASN:HD22	2:D:200:GLU:HB2	1.82	0.44
1:C:141:PHE:HB3	1:C:187:SER:OG	2.17	0.44
1:A:355:ILE:O	3:E:17:GLY:HA3	2.18	0.44
1:A:337:THR:HG23	1:A:338:LYS:N	2.33	0.44
1:C:250:VAL:HG23	1:C:255:PHE:CE2	2.53	0.44
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.99	0.44
1:A:176[B]:GLN:HB2	1:A:177:VAL:HG21	1.99	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.44
2:D:147:SER:O	2:D:151:THR:HG23	2.18	0.44
2:D:276:THR:OG1	10:D:503:EP:C16	2.66	0.44
2:D:234:THR:OG1	2:D:302:MET:HE2	2.18	0.44
2:D:244:PHE:CE2	2:D:358:ILE:CD1	3.01	0.44
4:F:200:ASP:OD1	4:F:222:ARG:HD2	2.17	0.44
1:A:292:THR:HG22	1:A:335:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:HE2	2:D:247[A]:GLN:NE2	2.16	0.43
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.99	0.43
2:B:119:LEU:HB3	2:B:123:ARG:HH12	1.83	0.43
1:C:1:MET:CG	1:C:131:GLY:HA3	2.48	0.43
1:C:85:GLN:HB2	15:C:609:HOH:O	2.18	0.43
4:F:39:LEU:CD2	4:F:41:LEU:CD2	2.96	0.43
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.54	0.43
1:A:325:PRO:O	1:A:329:ASN:OD1	2.36	0.43
2:B:179:ASP:HB2	1:C:352:LYS:HZ2	1.83	0.43
1:C:1:MET:HB2	1:C:1:MET:HE2	1.72	0.43
1:C:47:ASP:O	1:C:50:ASN:HB2	2.18	0.43
2:D:22:GLU:HG3	2:D:83:PHE:CD1	2.53	0.43
4:F:226:GLU:HG3	4:F:237:THR:CG2	2.48	0.43
1:C:251:ASP:HB3	15:C:620:HOH:O	2.18	0.43
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.45	0.43
1:C:217:LEU:HD21	1:C:368:LEU:HD23	2.01	0.43
2:D:399:PHE:CE1	2:D:405:LEU:HD21	2.53	0.43
4:F:221:LEU:O	4:F:261:GLU:HA	2.19	0.43
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.01	0.43
4:F:71:LEU:HD22	4:F:298:ILE:CD1	2.49	0.43
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.52	0.43
2:D:83:PHE:O	2:D:86:ILE:CG2	2.61	0.43
1:A:293:ASN:ND2	1:A:339:ARG:HH12	2.17	0.43
4:F:8:ASP:HB2	4:F:43:GLU:HA	2.01	0.43
1:A:26:LEU:HB3	1:A:361:THR:HG21	2.01	0.42
1:A:176[A]:GLN:C	1:A:177:VAL:HG22	2.39	0.42
1:A:241:SER:HB2	1:A:249:ASN:O	2.19	0.42
2:D:291:LEU:HD11	2:D:373:MET:HB3	2.01	0.42
1:A:339:ARG:HB3	1:A:341:ILE:HD11	1.98	0.42
1:A:176[A]:GLN:HG2	4:F:56:PRO:HB3	2.00	0.42
1:A:285:GLN:HA	1:A:285:GLN:OE1	2.19	0.42
4:F:14:TYR:CD1	4:F:17:VAL:HG11	2.52	0.42
2:B:75:MET:SD	2:B:92:PHE:HD2	2.41	0.42
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.19	0.42
2:D:272:PHE:O	2:D:300:ASN:ND2	2.44	0.42
4:F:81:ILE:HD12	4:F:94:PHE:CD2	2.54	0.42
4:F:314:LEU:HD22	4:F:350:ILE:HD11	2.01	0.42
2:B:3:GLU:OE1	2:B:130:ASP:N	2.52	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.42
2:B:293:GLN:O	11:B:505:POU:H4	2.20	0.42
1:C:217:LEU:O	1:C:218:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:PRO:C	2:D:369:ARG:N	2.73	0.42
4:F:299:GLU:N	4:F:300:PRO:HD2	2.35	0.42
1:A:176[B]:GLN:O	1:A:177:VAL:HG13	2.20	0.42
1:A:179:THR:O	2:B:352:LYS:NZ	2.52	0.42
1:A:245:ASP:OD2	3:E:15:THR:OG1	2.37	0.42
2:B:358:ILE:N	2:B:358:ILE:HD12	2.35	0.42
2:B:405:LEU:HD12	2:B:405:LEU:HA	1.80	0.42
1:C:68:VAL:HG21	1:C:118:VAL:HG21	2.02	0.42
4:F:305:LYS:O	4:F:306:HIS:HB2	2.19	0.42
10:B:504:EP:C6	10:B:504:EP:C75	2.98	0.42
1:C:27:GLU:HG2	1:C:361:THR:HG21	2.02	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.19	0.42
2:B:402:LYS:HG3	2:B:405:LEU:CD2	2.49	0.42
4:F:208:ASP:HB2	15:F:502:HOH:O	2.19	0.42
4:F:345:GLU:O	4:F:349:GLY:N	2.47	0.42
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.02	0.41
2:B:308:ARG:HE	11:B:505:POU:H8	1.85	0.41
1:C:156:ARG:HD2	1:C:156:ARG:HA	1.83	0.41
1:A:36:MET:CG	1:A:36:MET:O	2.68	0.41
1:C:250:VAL:CG2	1:C:255:PHE:CZ	3.03	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.41
2:B:147:SER:OG	2:B:190:SER:OG	2.24	0.41
4:F:15:ALA:O	4:F:19:ARG:NE	2.53	0.41
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.03	0.41
2:B:392:SER:HB2	2:B:425:MET:HE2	2.03	0.41
1:C:255:PHE:CE2	1:C:318:LEU:HD11	2.55	0.41
2:D:197:ASN:OD1	3:E:122:ARG:NH2	2.52	0.41
3:E:106:GLU:HA	3:E:106:GLU:OE1	2.20	0.41
4:F:284:LEU:HA	4:F:284:LEU:HD23	1.80	0.41
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.55	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.20	0.41
10:D:503:EP:H433	10:D:503:EP:C27	2.50	0.41
11:B:505:POU:H2	11:B:505:POU:C14	2.49	0.41
1:C:99:ALA:HB3	1:C:144:GLY:HA3	2.03	0.41
4:F:80:LEU:O	4:F:84:SER:OG	2.22	0.41
1:A:2:ARG:HG3	1:A:2:ARG:HH11	1.85	0.41
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.56	0.41
2:B:2:ARG:HH21	2:B:130:ASP:HB2	1.85	0.41
2:D:414:ASP:OD1	2:D:416:MET:HG2	2.21	0.41
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.03	0.41
1:A:88:HIS:N	1:A:91:GLN:OE1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG23	2:B:352:LYS:HZ2	1.86	0.41
1:A:283:HIS:NE2	1:A:369:ALA:HB1	2.36	0.41
1:C:168:GLU:OE2	1:C:194:THR:HG21	2.21	0.41
1:C:209:ILE:CD1	1:C:302:MET:SD	3.07	0.41
2:D:39:ASP:OD1	2:D:39:ASP:N	2.53	0.41
2:D:112:ALA:O	2:D:115:VAL:HG12	2.20	0.41
2:D:295:MET:SD	2:D:375:ALA:HB1	2.61	0.41
1:A:36:MET:CG	1:A:39:ASP:HB2	2.51	0.41
1:C:225:THR:O	1:C:229[A]:ARG:HG3	2.21	0.41
2:D:161:TYR:HB3	2:D:164:ARG:HG3	2.02	0.41
4:F:77:LEU:O	4:F:81:ILE:HG13	2.21	0.41
4:F:178:GLN:OE1	4:F:178:GLN:CA	2.68	0.41
2:D:349:ASN:O	2:D:352:LYS:HE2	2.21	0.40
3:E:138:GLU:HA	3:E:141:GLU:HB2	2.02	0.40
4:F:40:MET:HE3	4:F:52:LEU:HD11	2.03	0.40
4:F:173:ILE:CD1	4:F:180:HIS:HB2	2.52	0.40
4:F:207:VAL:O	4:F:312:PHE:HB2	2.22	0.40
4:F:226:GLU:HG3	4:F:237:THR:HG22	2.01	0.40
1:C:55:GLU:HA	1:C:60:LYS:O	2.21	0.40
3:E:47:LEU:HD23	3:E:47:LEU:O	2.22	0.40
2:B:179:ASP:CB	1:C:352:LYS:HG3	2.49	0.40
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.39	0.40
2:D:63:PRO:CD	2:D:86:ILE:HG12	2.51	0.40
4:F:226:GLU:CG	4:F:237:THR:HG22	2.51	0.40
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.86	0.40
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.57	0.40
2:D:60:LYS:HD2	2:D:60:LYS:HA	1.78	0.40
2:D:210:TYR:CD1	2:D:222:PRO:HG2	2.57	0.40
2:D:345:GLU:CD	2:D:345:GLU:H	2.25	0.40
3:E:53:LYS:HE2	3:E:53:LYS:HB3	1.95	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)
2:B:113:GLU:OE2	1:C:283:HIS:NE2[4_555]	1.62	0.58

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	436/440 (99%)	420 (96%)	16 (4%)	0	100	100
1	C	442/440 (100%)	426 (96%)	16 (4%)	0	100	100
2	B	428/430 (100%)	413 (96%)	15 (4%)	0	100	100
2	D	427/430 (99%)	414 (97%)	13 (3%)	0	100	100
3	E	120/138 (87%)	119 (99%)	1 (1%)	0	100	100
4	F	321/381 (84%)	304 (95%)	17 (5%)	0	100	100
All	All	2174/2259 (96%)	2096 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	371/371 (100%)	360 (97%)	11 (3%)	41	68
1	C	375/371 (101%)	370 (99%)	5 (1%)	69	87
2	B	371/371 (100%)	366 (99%)	5 (1%)	69	87
2	D	369/371 (100%)	355 (96%)	14 (4%)	33	58
3	E	111/123 (90%)	110 (99%)	1 (1%)	78	92
4	F	298/339 (88%)	286 (96%)	12 (4%)	31	56
All	All	1895/1946 (97%)	1847 (98%)	48 (2%)	47	73

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	96	LYS
1	A	178	SER
1	A	193	THR
1	A	256	GLN
1	A	280	LYS
1	A	329	ASN
1	A	339	ARG
1	A	346	TRP
1	A	381	THR
1	A	437	VAL
2	B	48	ARG
2	B	139	HIS
2	B	402	LYS
2	B	414	ASP
2	B	430	SER
1	C	46	ASP
1	C	120	ASP
1	C	283	HIS
1	C	339	ARG
1	C	430	LYS
2	D	15	GLN
2	D	85	GLN
2	D	133	GLN
2	D	155	SER
2	D	207	GLU
2	D	282	GLN
2	D	284	ARG
2	D	286	LEU
2	D	302	MET
2	D	308	ARG
2	D	322	ARG
2	D	405	LEU
2	D	422	GLU
2	D	426	ASN
3	E	6	MET
4	F	32	LYS
4	F	46	ARG
4	F	143	GLU
4	F	164	SER
4	F	197	ARG
4	F	217	ARG

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Mol	Chain	Res	Type
4	F	224	SER
4	F	262	MET
4	F	353	VAL
4	F	356	SER
4	F	357	SER
4	F	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	285	GLN
1	A	372	GLN
1	C	293	ASN
2	D	139	HIS
4	F	260	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\#\|Z\|>2$
13	BKF	D	504	-	45,47,47	0.63	2 (4%)	53,71,71	0.53	0
5	GTP	A	501	6	26,34,34	0.99	2 (7%)	32,54,54	0.69	1 (3%)
10	EP	D	503	-	32,36,36	0.28	0	39,53,53	0.54	0
12	VLB	C	501	-	63,67,67	1.76	16 (25%)	79,108,108	2.38	26 (32%)
11	POU	B	505	-	37,39,39	0.24	0	44,57,57	0.48	0
14	ACP	F	401	-	27,33,33	0.89	1 (3%)	32,52,52	0.80	2 (6%)
10	EP	B	504	-	32,36,36	0.24	0	39,53,53	0.59	0
8	GDP	B	501	6	24,30,30	1.02	3 (12%)	30,47,47	0.67	1 (3%)
8	GDP	D	501	6	24,30,30	0.99	2 (8%)	30,47,47	0.66	1 (3%)
5	GTP	C	502	6	26,34,34	1.02	3 (11%)	32,54,54	0.69	1 (3%)
9	LOC	B	503	-	31,31,31	0.48	0	44,44,44	0.38	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
13	BKF	D	504	-	4/4/17/17	21/49/76/76	0/2/4/4
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
10	EP	D	503	-	3/3/12/12	6/49/55/55	0/2/3/3
12	VLB	C	501	-	-	15/38/131/131	0/7/9/9
11	POU	B	505	-	4/4/14/14	23/54/76/76	1/1/2/2
14	ACP	F	401	-	-	0/15/38/38	0/3/3/3
10	EP	B	504	-	4/4/12/12	17/49/55/55	0/2/3/3
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3
5	GTP	C	502	6	-	6/18/38/38	0/3/3/3
9	LOC	B	503	-	-	0/12/25/25	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	501	VLB	C57-N56	5.12	1.59	1.47
12	C	501	VLB	C68-C73	-3.87	1.50	1.53
12	C	501	VLB	C58-C59	-3.84	1.45	1.52
12	C	501	VLB	C19-N9	3.18	1.52	1.47
12	C	501	VLB	O75-C76	-3.02	1.38	1.45
13	D	504	BKF	C27-C26	-2.83	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	501	VLB	C5-C6	-2.82	1.45	1.51
12	C	501	VLB	O27-C3	-2.75	1.37	1.42
8	B	501	GDP	C5-C6	-2.73	1.41	1.47
5	C	502	GTP	C5-C6	-2.69	1.41	1.47
5	A	501	GTP	C5-C6	-2.68	1.42	1.47
8	D	501	GDP	C5-C6	-2.66	1.42	1.47
12	C	501	VLB	C70-C54	2.53	1.57	1.53
12	C	501	VLB	O25-C26	-2.50	1.39	1.45
12	C	501	VLB	O32-C16	2.49	1.41	1.37
12	C	501	VLB	C57-C58	-2.42	1.45	1.52
14	F	401	ACP	PB-O2B	-2.42	1.50	1.56
12	C	501	VLB	C68-C67	-2.31	1.51	1.53
13	D	504	BKF	C21-N20	-2.30	1.42	1.46
12	C	501	VLB	O32-C33	-2.23	1.36	1.42
12	C	501	VLB	C69-C52	2.19	1.55	1.52
12	C	501	VLB	C5-C19	-2.16	1.48	1.53
5	C	502	GTP	C8-N7	-2.16	1.31	1.35
8	B	501	GDP	C8-N7	-2.15	1.31	1.35
8	D	501	GDP	C8-N7	-2.13	1.31	1.35
12	C	501	VLB	C59-C67	-2.11	1.36	1.39
5	A	501	GTP	C8-N7	-2.09	1.31	1.35
5	C	502	GTP	C5-C4	-2.02	1.37	1.43
8	B	501	GDP	C5-C4	-2.02	1.37	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	501	VLB	O25-C23-C3	6.46	123.08	112.22
12	C	501	VLB	C52-C69-N56	6.24	121.05	111.28
12	C	501	VLB	C57-C58-C59	5.63	124.94	114.30
12	C	501	VLB	C58-C57-N56	5.43	125.56	113.44
12	C	501	VLB	O72-C54-C70	-4.87	100.35	108.75
12	C	501	VLB	O75-C73-C68	4.34	117.84	111.32
12	C	501	VLB	C19-C5-C6	4.30	112.68	108.28
12	C	501	VLB	O75-C73-O74	-4.27	116.44	123.93
12	C	501	VLB	C13-C18-N1	3.85	115.35	110.98
12	C	501	VLB	C63-C64-C65	-3.85	114.55	120.08
12	C	501	VLB	C22-N1-C18	-3.67	109.10	120.84
12	C	501	VLB	O25-C23-O24	-3.62	117.59	123.93
12	C	501	VLB	O32-C16-C15	3.55	120.21	116.58
12	C	501	VLB	C22-N1-C2	-3.38	110.96	119.21
12	C	501	VLB	C17-C18-N1	-3.27	123.05	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	501	VLB	O32-C16-C17	-3.21	118.59	124.12
12	C	501	VLB	C62-C61-C60	-3.00	116.73	120.89
12	C	501	VLB	O24-C23-C3	-2.99	119.29	123.94
12	C	501	VLB	C3-C2-N1	-2.92	108.79	112.81
12	C	501	VLB	C18-N1-C2	-2.75	105.33	109.03
12	C	501	VLB	C53-C52-C69	2.73	111.91	108.72
12	C	501	VLB	O28-C29-C30	2.34	115.39	111.09
12	C	501	VLB	C61-C60-C65	2.33	121.25	118.17
14	F	401	ACP	C5-C6-N6	2.28	123.82	120.35
14	F	401	ACP	O1G-PG-C3B	-2.18	106.53	111.24
12	C	501	VLB	C33-O32-C16	-2.08	114.38	117.53
12	C	501	VLB	C2-C12-C19	2.08	117.58	114.07
12	C	501	VLB	C21-C20-C5	-2.06	111.82	115.79
8	B	501	GDP	O6-C6-C5	2.03	128.34	124.37
5	C	502	GTP	O6-C6-C5	2.03	128.33	124.37
8	D	501	GDP	O6-C6-C5	2.03	128.33	124.37
5	A	501	GTP	O6-C6-C5	2.00	128.29	124.37

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	504	EP	C27
10	B	504	EP	C41
10	B	504	EP	C3
10	B	504	EP	C24
10	D	503	EP	C27
10	D	503	EP	C41
10	D	503	EP	C24
11	B	505	POU	C3
11	B	505	POU	C8
11	B	505	POU	C23
11	B	505	POU	C2
13	D	504	BKF	C15
13	D	504	BKF	C21
13	D	504	BKF	C22
13	D	504	BKF	C16

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O1A
10	B	504	EP	C5-C10-C12-N20
10	B	504	EP	C5-C3-O2-C75
10	B	504	EP	O26-C27-C32-C35
10	B	504	EP	C51-C57-C59-C60
10	B	504	EP	O58-C57-C59-C60
10	B	504	EP	C59-C68-C72-C75
10	B	504	EP	O70-C68-C72-C75
10	B	504	EP	C72-C75-O2-C3
11	B	505	POU	C25-C21-C22-C23
11	B	505	POU	C15-C21-C22-C23
11	B	505	POU	C21-C22-C23-C26
11	B	505	POU	C11-C12-C13-C14
11	B	505	POU	C11-C12-C13-O13
11	B	505	POU	C14-C13-O13-C20
11	B	505	POU	O1-C1-C2-C3
11	B	505	POU	O15-C1-C2-C3
11	B	505	POU	O2-C2-C3-C4
11	B	505	POU	O2-C2-C3-O3
11	B	505	POU	C1-C2-C3-C4
11	B	505	POU	C1-C2-C3-O3
12	C	501	VLB	O72-C54-C70-C71
12	C	501	VLB	C55-C54-C70-C71
12	C	501	VLB	C53-C54-C70-C71
12	C	501	VLB	C58-C57-N56-C69
12	C	501	VLB	C51-C68-C73-O75
12	C	501	VLB	C15-C68-C73-O74
12	C	501	VLB	C15-C68-C73-O75
12	C	501	VLB	C68-C73-O75-C76
12	C	501	VLB	O74-C73-O75-C76
12	C	501	VLB	C3-C23-O25-C26
13	D	504	BKF	C12-C14-C15-C16
13	D	504	BKF	C12-C14-C15-C33
13	D	504	BKF	O34-C14-C15-C33
13	D	504	BKF	C14-C15-C16-O17
13	D	504	BKF	C14-C15-C16-C31
13	D	504	BKF	C33-C15-C16-O17

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Mol	Chain	Res	Type	Atoms
13	D	504	BKF	C33-C15-C16-C31
13	D	504	BKF	C31-C21-C22-O29
13	D	504	BKF	C22-C23-C24-C25
13	D	504	BKF	C01-C02-O42-C43
13	D	504	BKF	C10-C08-N07-C06
13	D	504	BKF	O09-C08-N07-C06
13	D	504	BKF	C10-C08-N07-C41
13	D	504	BKF	O09-C08-N07-C41
13	D	504	BKF	O35-C11-C12-C14
12	C	501	VLB	O24-C23-O25-C26
10	B	504	EP	O76-C75-O2-C3
13	D	504	BKF	C03-C02-O42-C43
10	D	503	EP	C32-C35-C38-C41
11	B	505	POU	C3-C4-C5-O9
11	B	505	POU	O15-C1-C2-O2
10	B	504	EP	C35-C38-C41-C43
11	B	505	POU	C14-C15-C21-C25
11	B	505	POU	O1-C1-C2-O2
10	D	503	EP	C35-C38-C41-C43
11	B	505	POU	C24-C23-C26-C27
10	B	504	EP	C24-C27-C32-C35
10	D	503	EP	C68-C72-C75-O76
11	B	505	POU	C14-C15-C21-C22
10	D	503	EP	C68-C72-C75-O2
10	B	504	EP	C32-C35-C38-C41
10	D	503	EP	O76-C75-O2-C3
8	D	501	GDP	C5'-O5'-PA-O3A
11	B	505	POU	C12-C13-O13-C20
10	D	503	EP	C72-C75-O2-C3
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
13	D	504	BKF	C08-C10-C11-C12
13	D	504	BKF	O34-C14-C15-C16
10	B	504	EP	C51-C57-C59-C64
11	B	505	POU	C3-C4-C5-C6
8	D	501	GDP	PB-O3A-PA-O2A
10	B	504	EP	C41-C47-C51-C57
12	C	501	VLB	O25-C23-C3-C4
11	B	505	POU	O15-C15-C21-C25
11	B	505	POU	O15-C15-C21-C22
10	B	504	EP	C27-C32-C35-C38

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Mol	Chain	Res	Type	Atoms
12	C	501	VLB	C67-C68-C73-O75
13	D	504	BKF	C12-C11-O35-C36
11	B	505	POU	C26-C23-C24-O24
5	A	501	GTP	PB-O3A-PA-O2A
12	C	501	VLB	C67-C68-C73-O74
10	B	504	EP	O2-C3-C5-C6
10	B	504	EP	C38-C41-C47-O49
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	502	GTP	PB-O3A-PA-O1A
5	C	502	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
13	D	504	BKF	C10-C11-C12-O34
13	D	504	BKF	N07-C08-C10-C11
5	A	501	GTP	PB-O3B-PG-O1G
12	C	501	VLB	C58-C57-N56-C55

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	505	POU	C5-C6-C7-C8-C9-O9

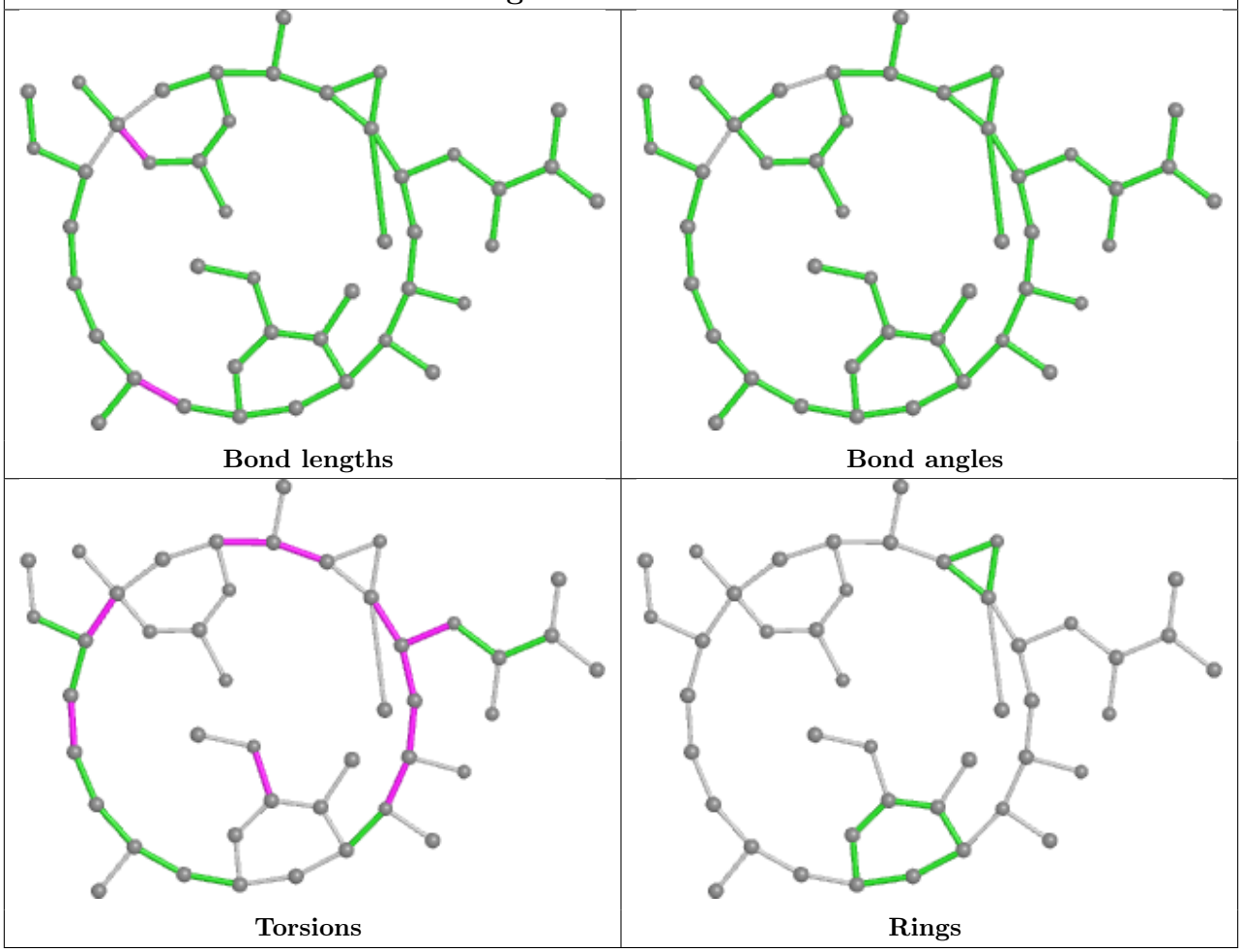
6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	504	BKF	3	0
10	D	503	EP	5	0
12	C	501	VLB	5	0
11	B	505	POU	6	0
10	B	504	EP	9	0
9	B	503	LOC	6	0

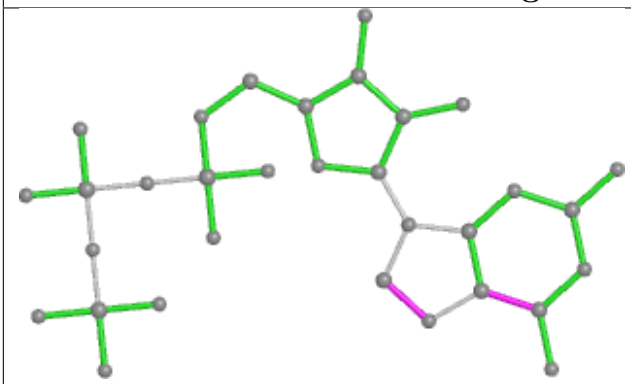
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

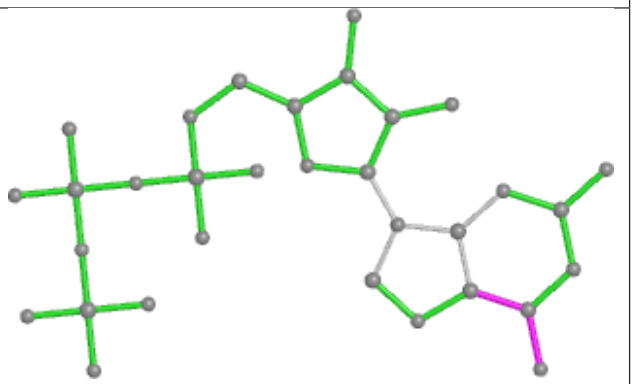
Ligand BKF D 504



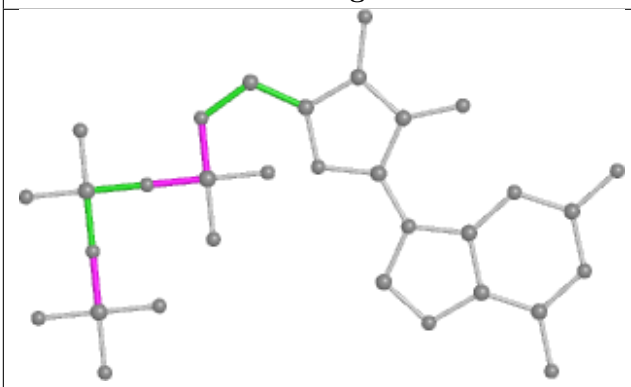
Ligand GTP A 501



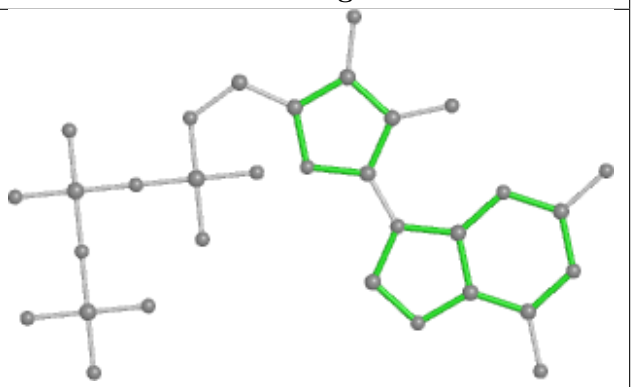
Bond lengths



Bond angles

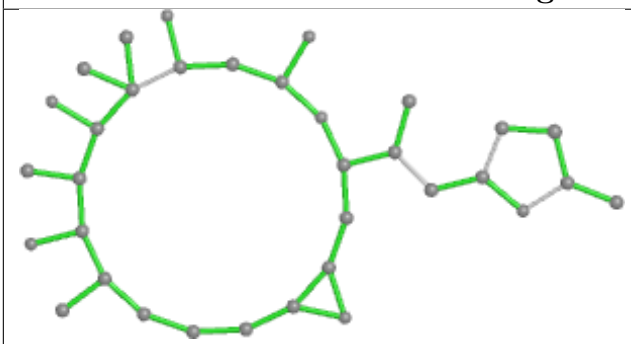


Torsions



Rings

Ligand EP D 503



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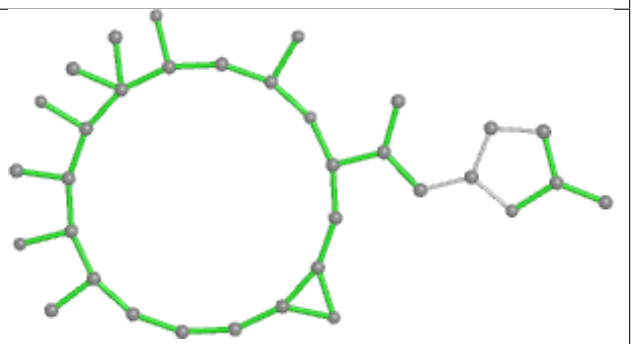
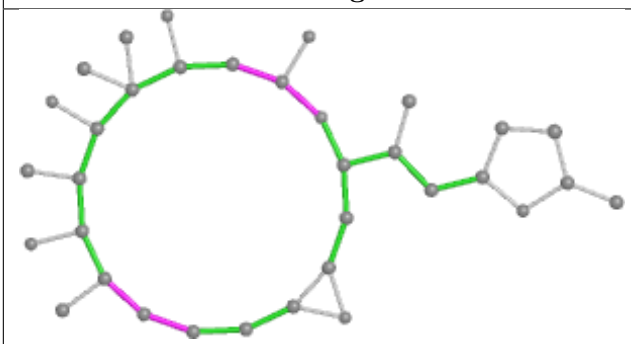
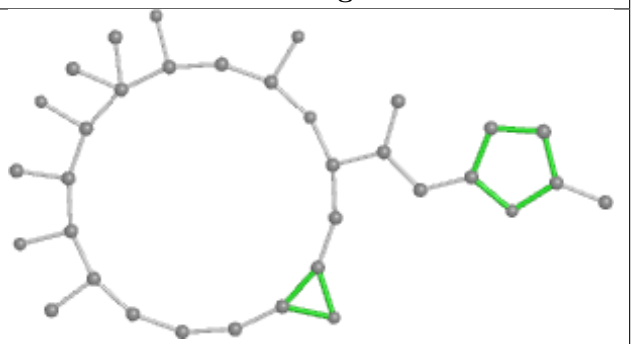


Bond angles

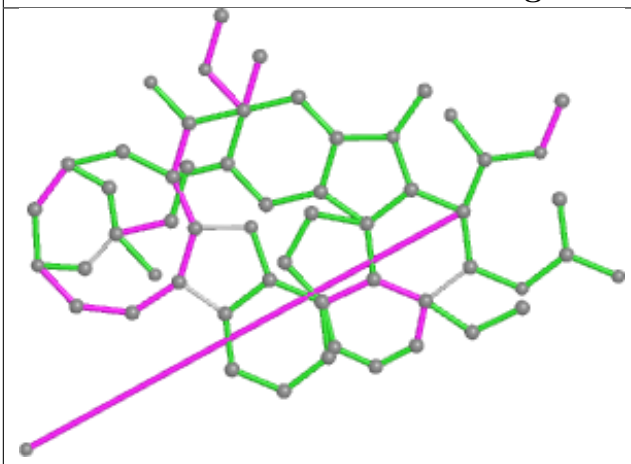


Torsions

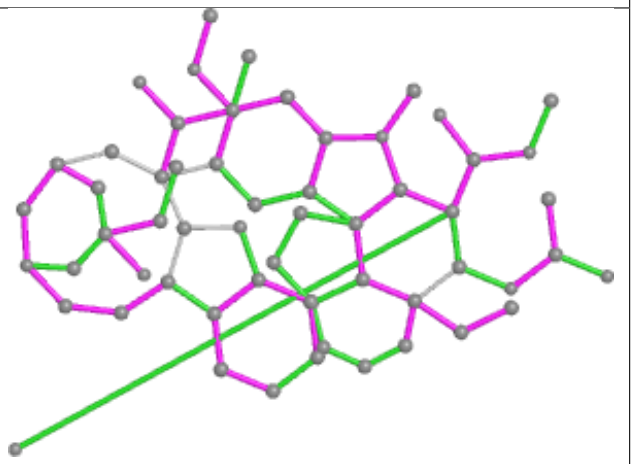


Rings

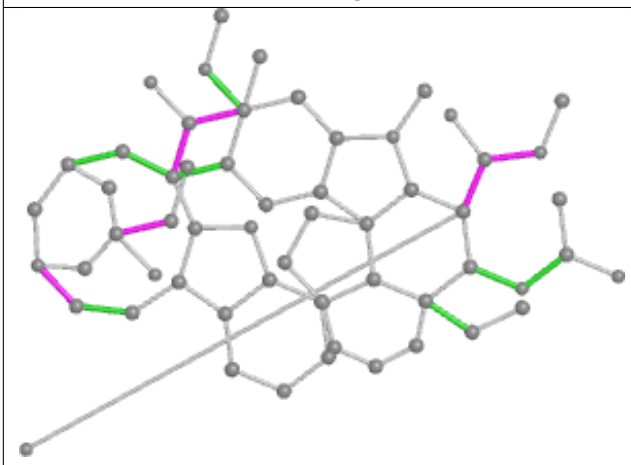
Ligand VLB C 501



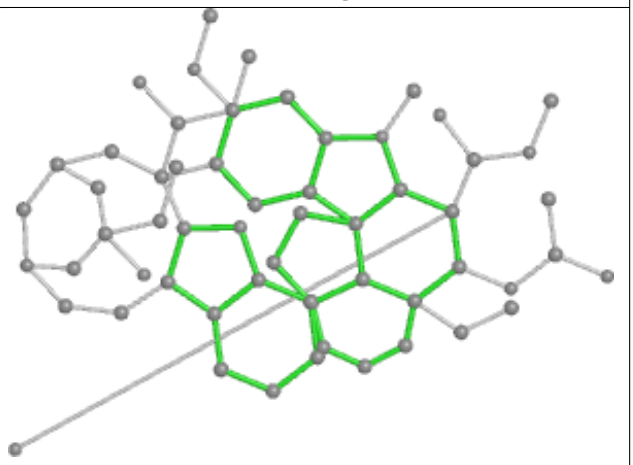
Bond lengths



Bond angles

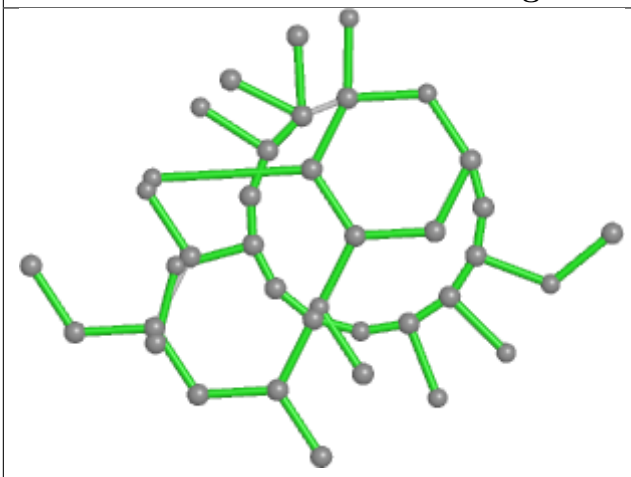


Torsions

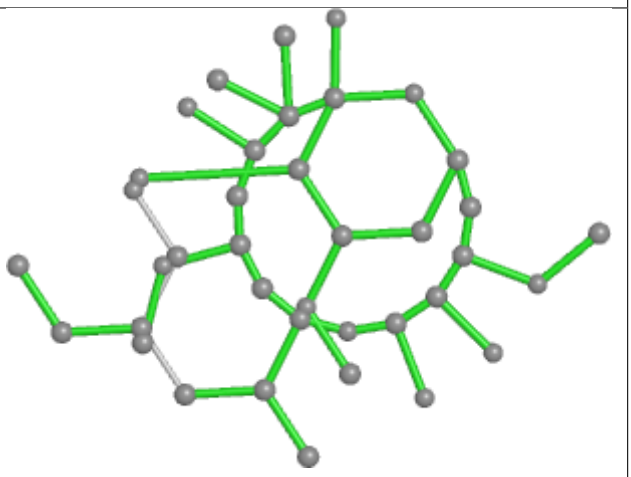


Rings

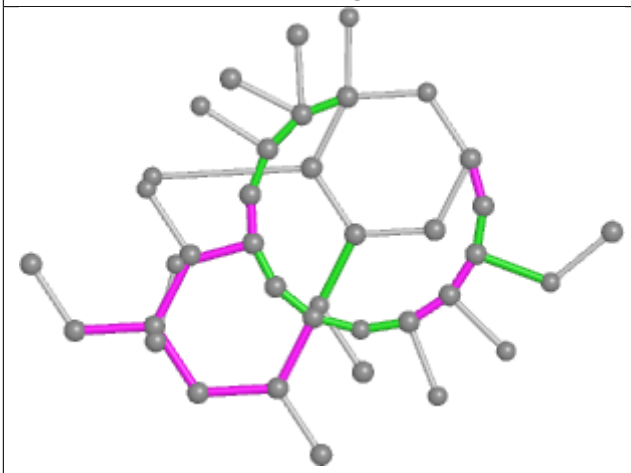
Ligand POU B 505



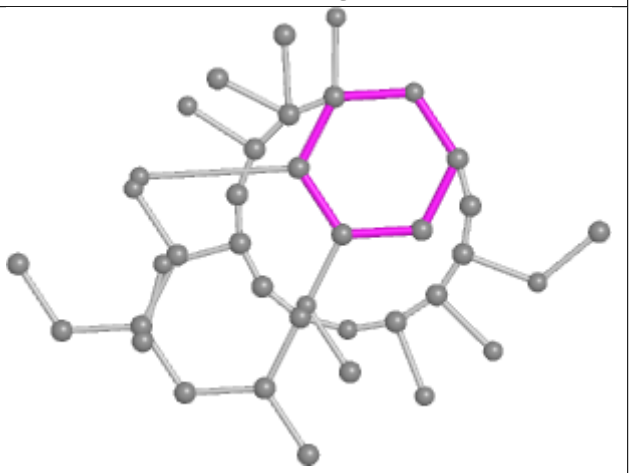
Bond lengths



Bond angles

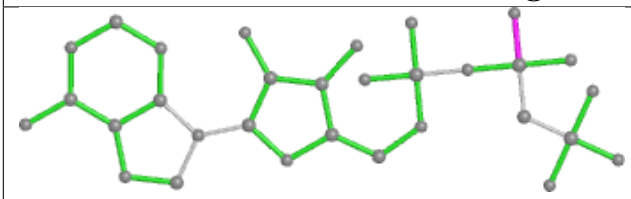


Torsions

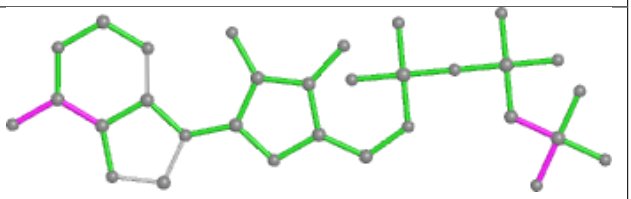


Rings

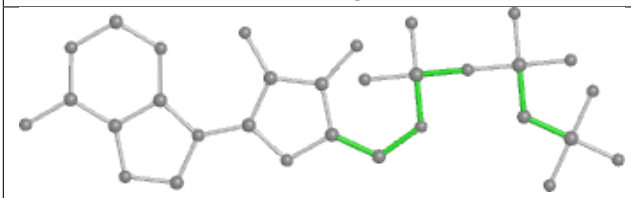
Ligand ACP F 401



Bond lengths



Bond angles



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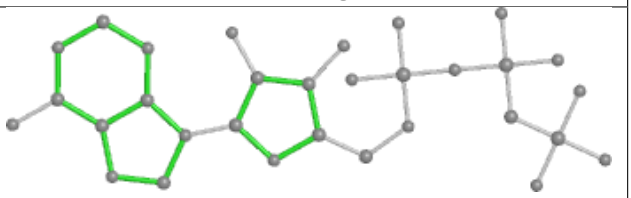
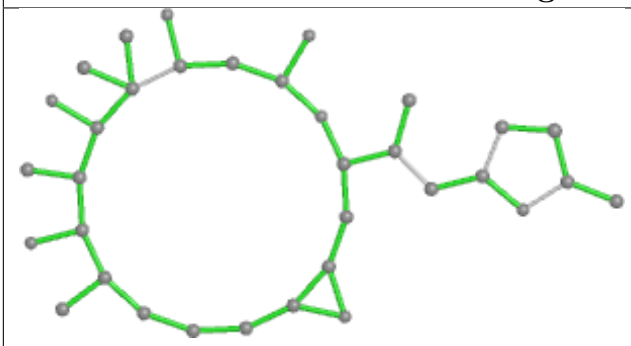
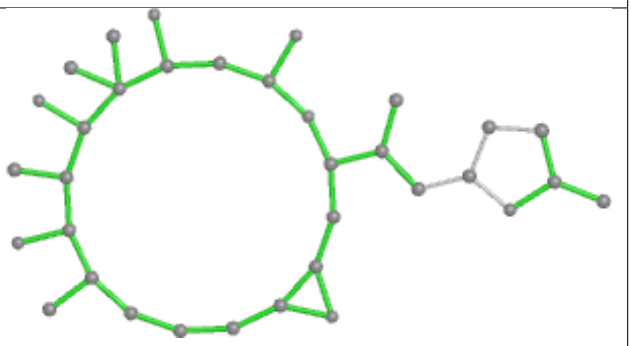


Rings

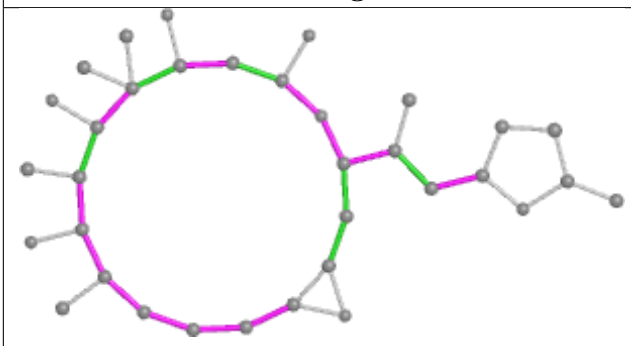
Ligand EP B 504



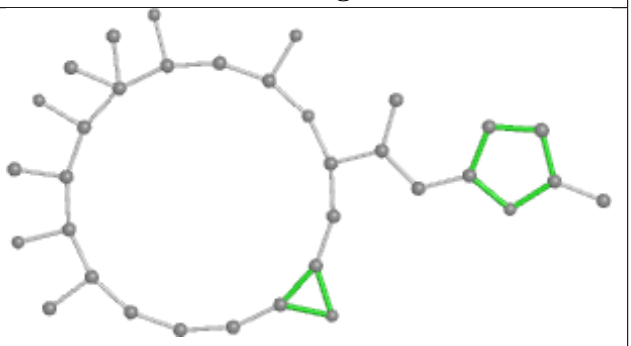
Bond lengths



Bond angles

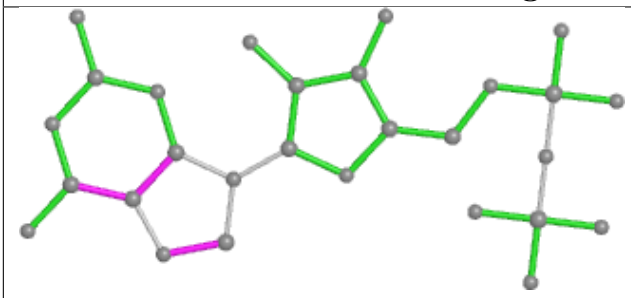


Torsions

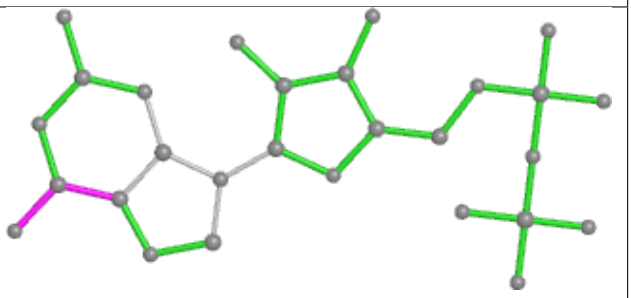


Rings

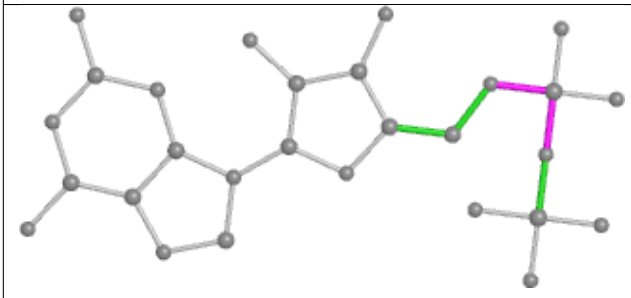
Ligand GDP B 501



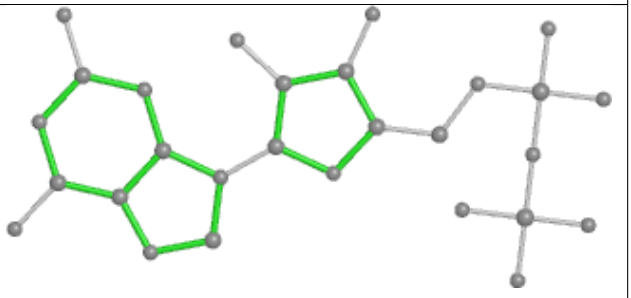
Bond lengths



Bond angles

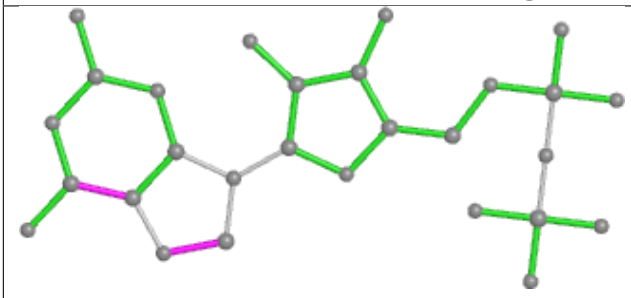


Torsions

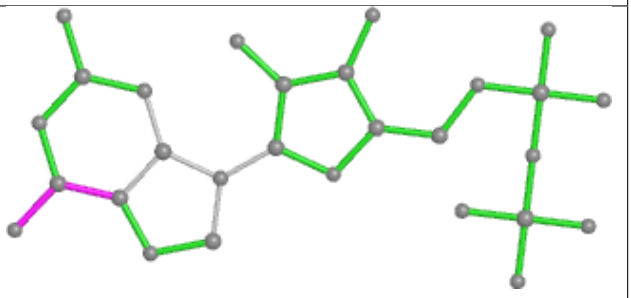


Rings

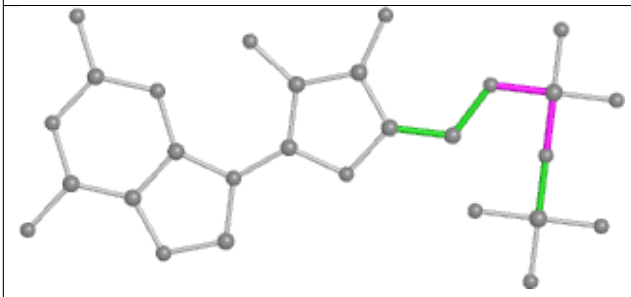
Ligand GDP D 501



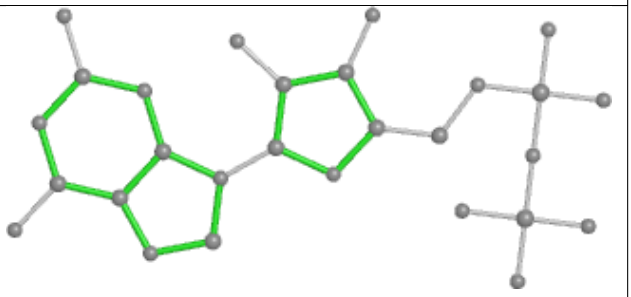
Bond lengths



Bond angles

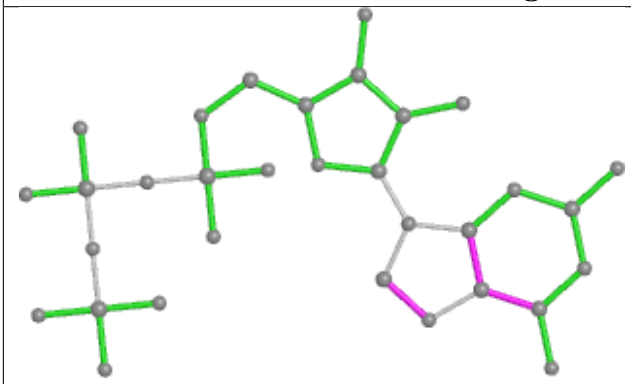


Torsions

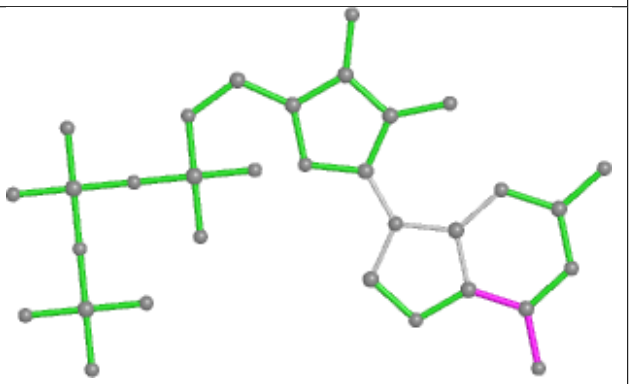


Rings

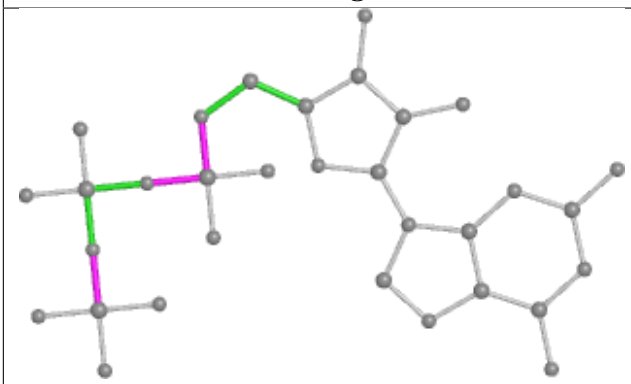
Ligand GTP C 502



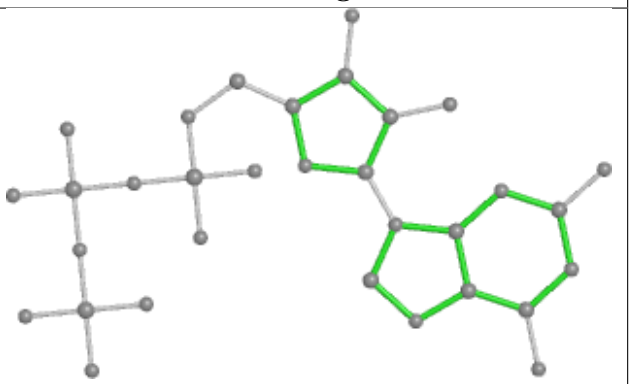
Bond lengths



Bond angles

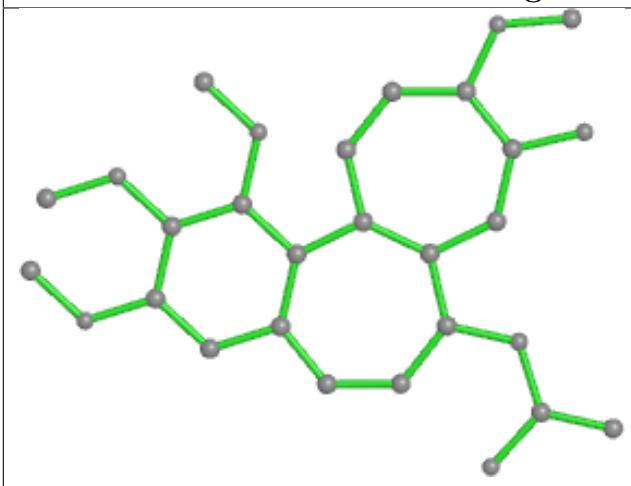


Torsions

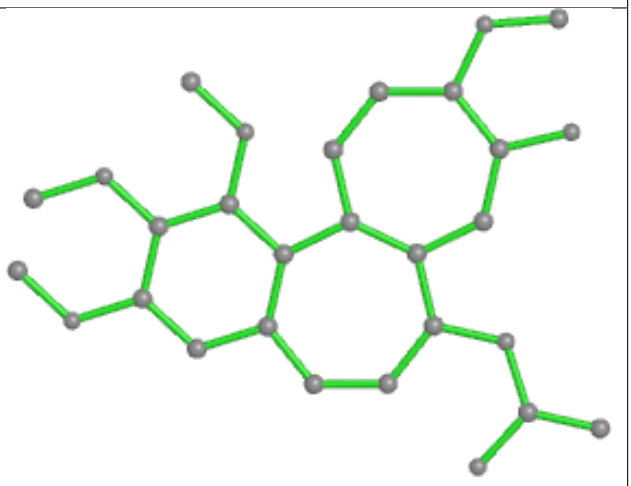


Rings

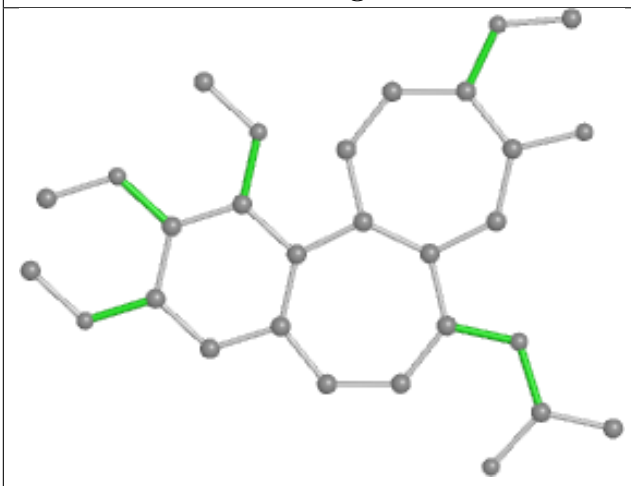
Ligand LOC B 503



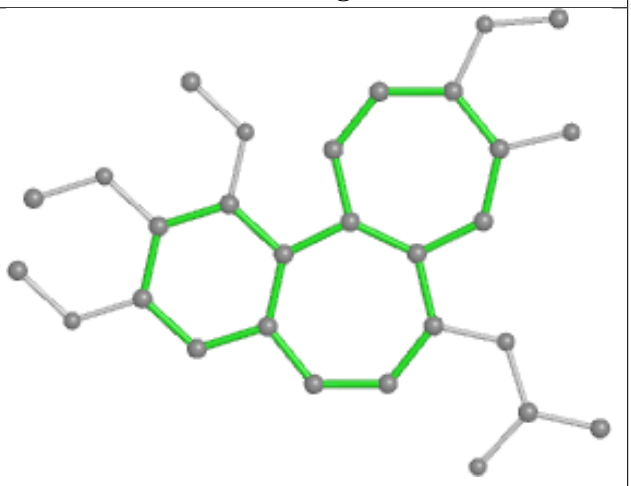
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
2	D	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	176[A]:GLN	C	177:VAL	N	5.41
1	A	176[B]:GLN	C	177:VAL	N	5.38
1	D	360:PRO	C	369:ARG	N	2.73
1	B	42:LEU	C	45:GLN	N	2.66

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

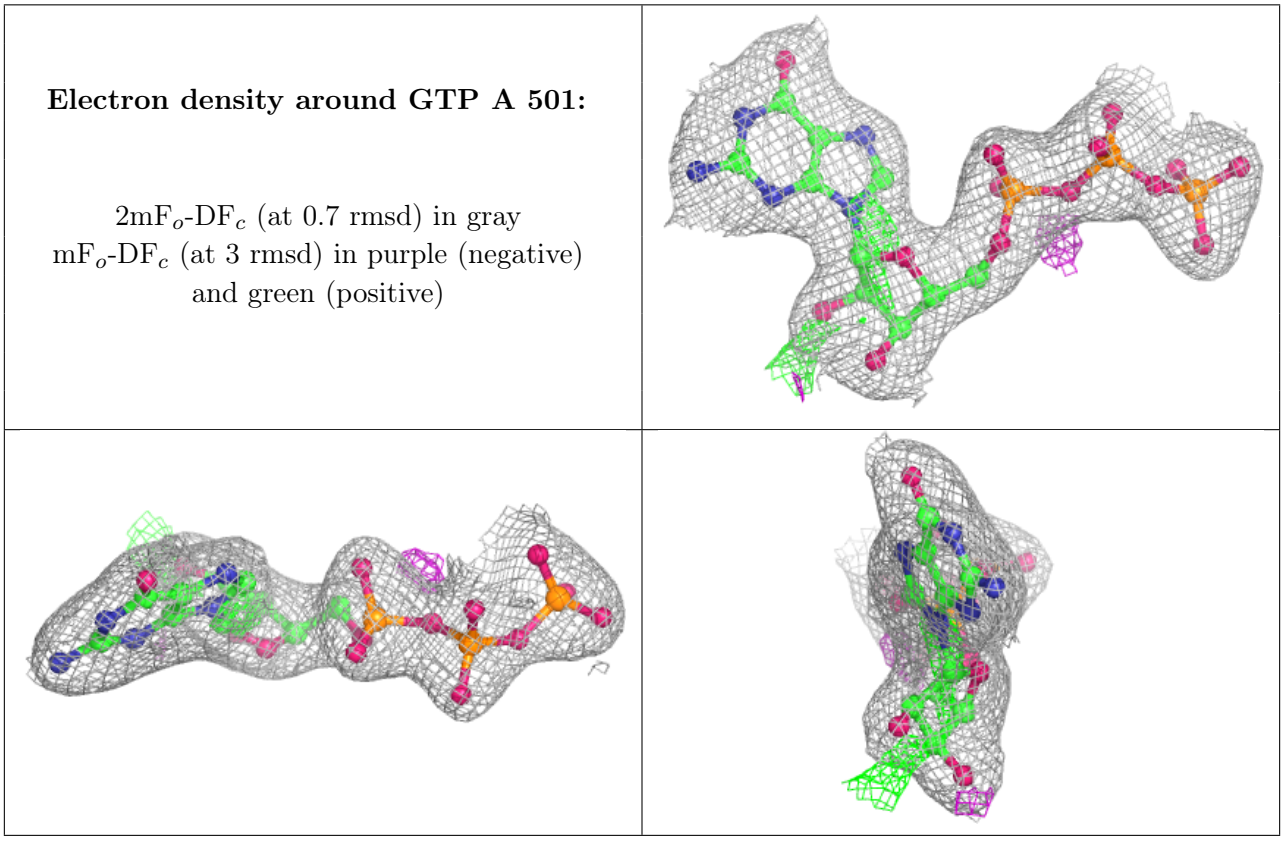
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

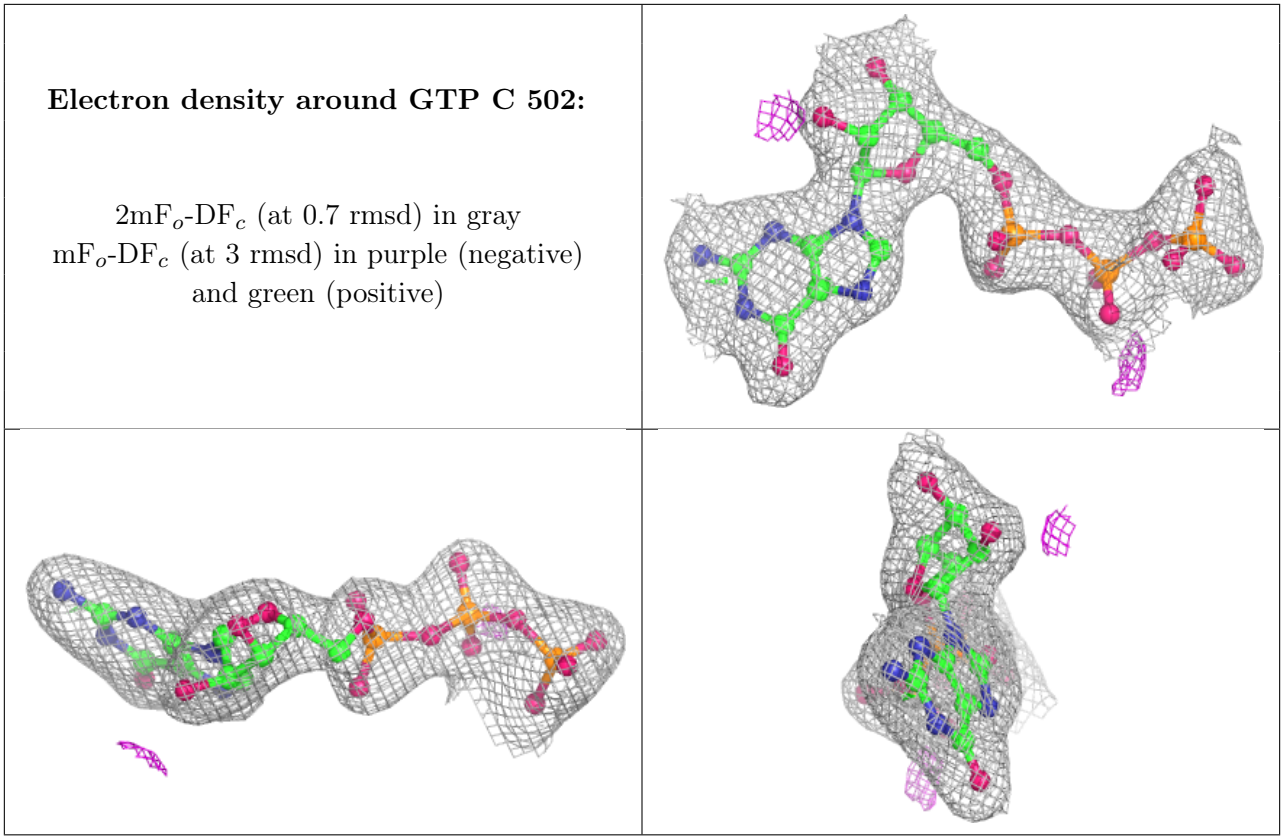
Electron density around GTP A 501:

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



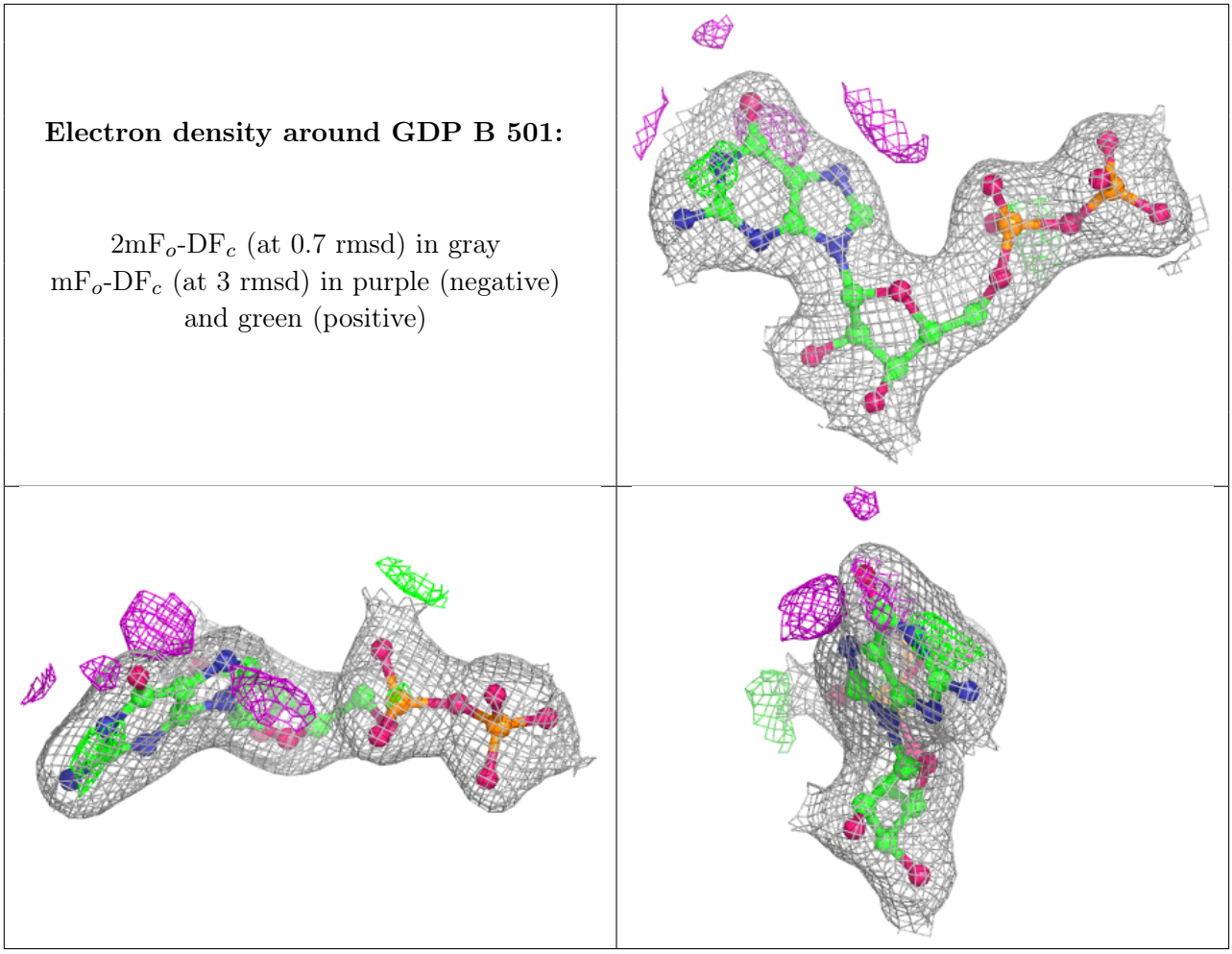
Electron density around GTP C 502:

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



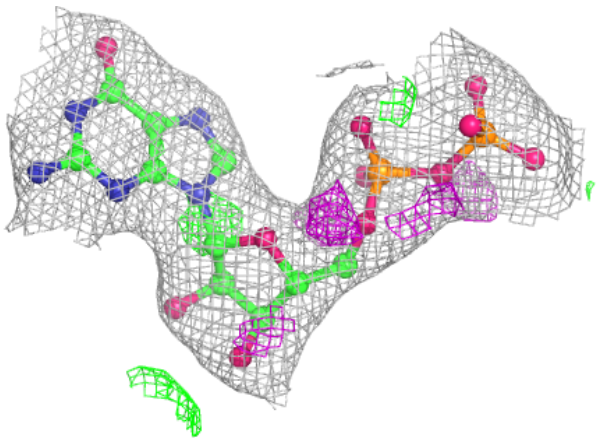
Electron density around GDP B 501:

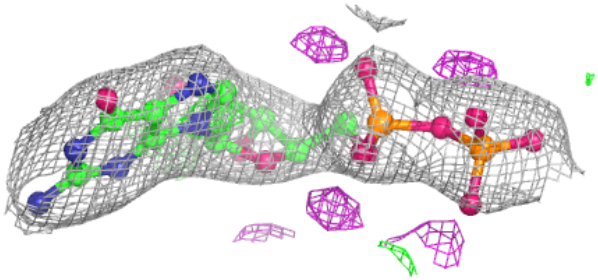
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

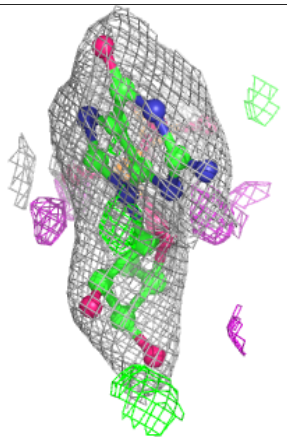


Electron density around GDP D 501:

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

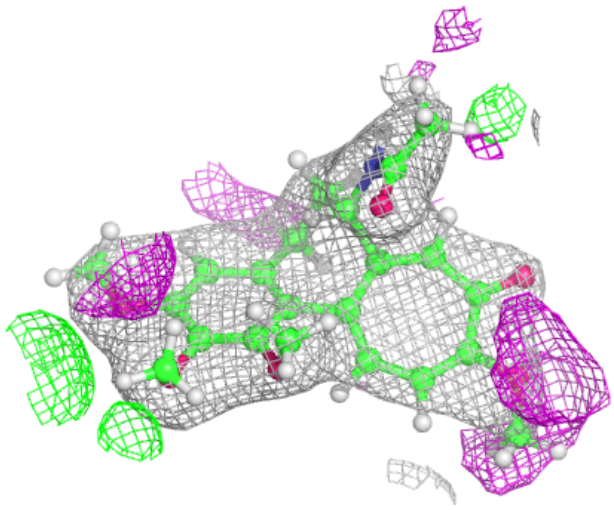


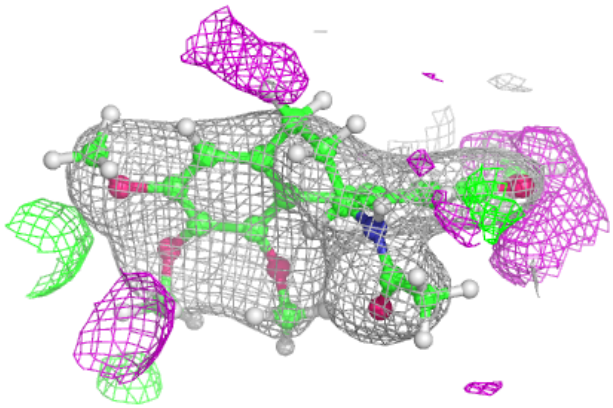


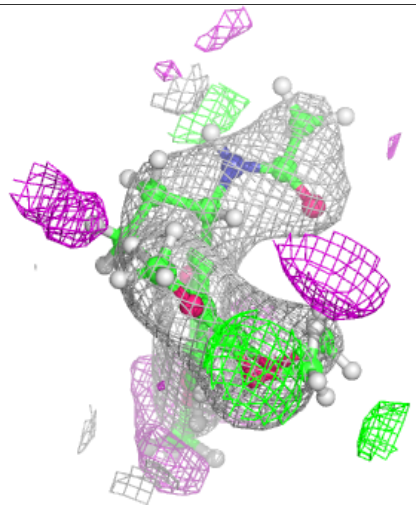


Electron density around LOC B 503:

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

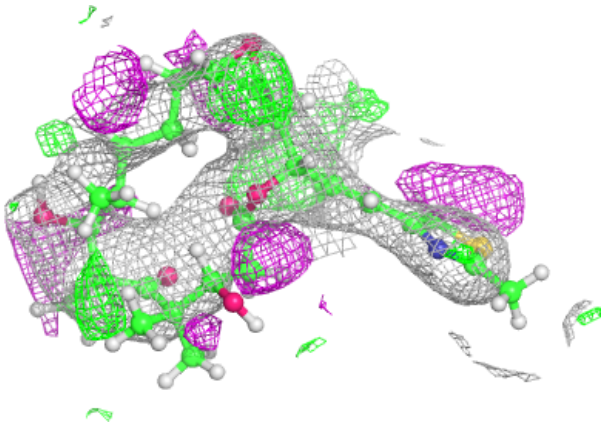


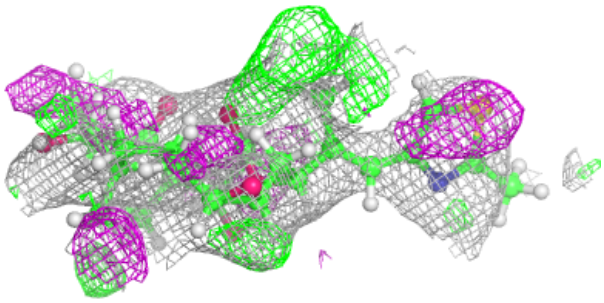


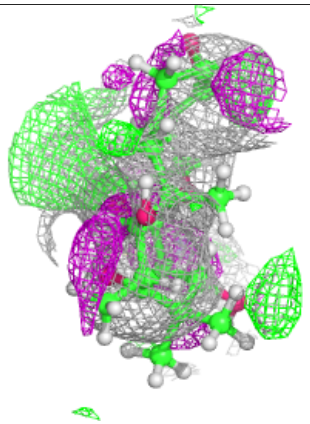


Electron density around EP B 504:

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

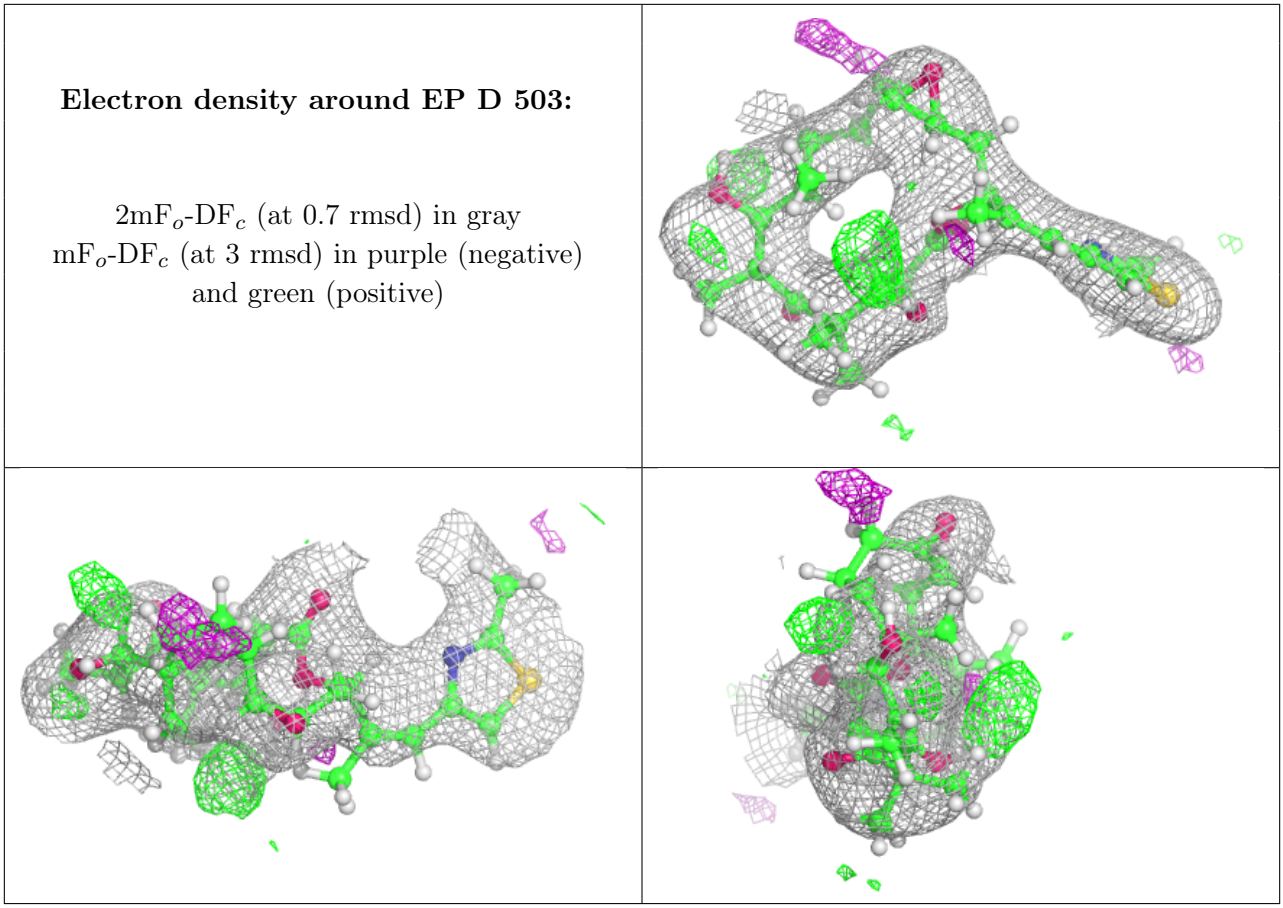






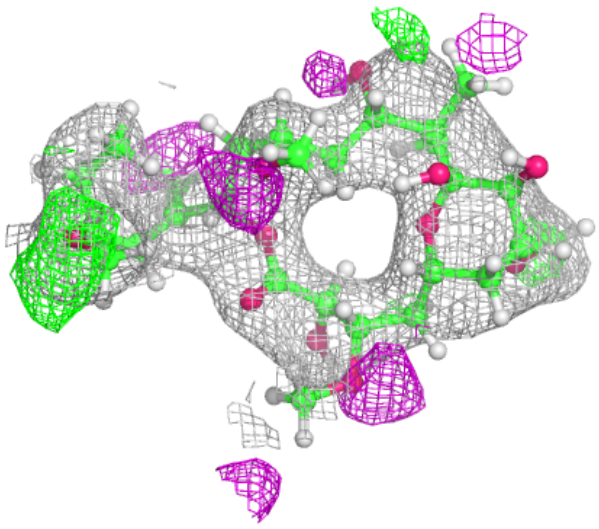
Electron density around EP D 503:

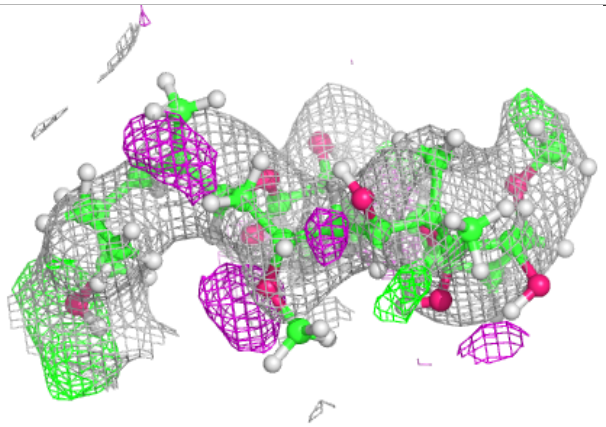
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

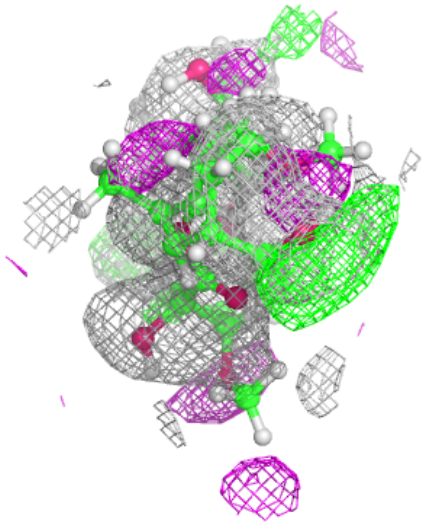


Electron density around POU B 505:

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

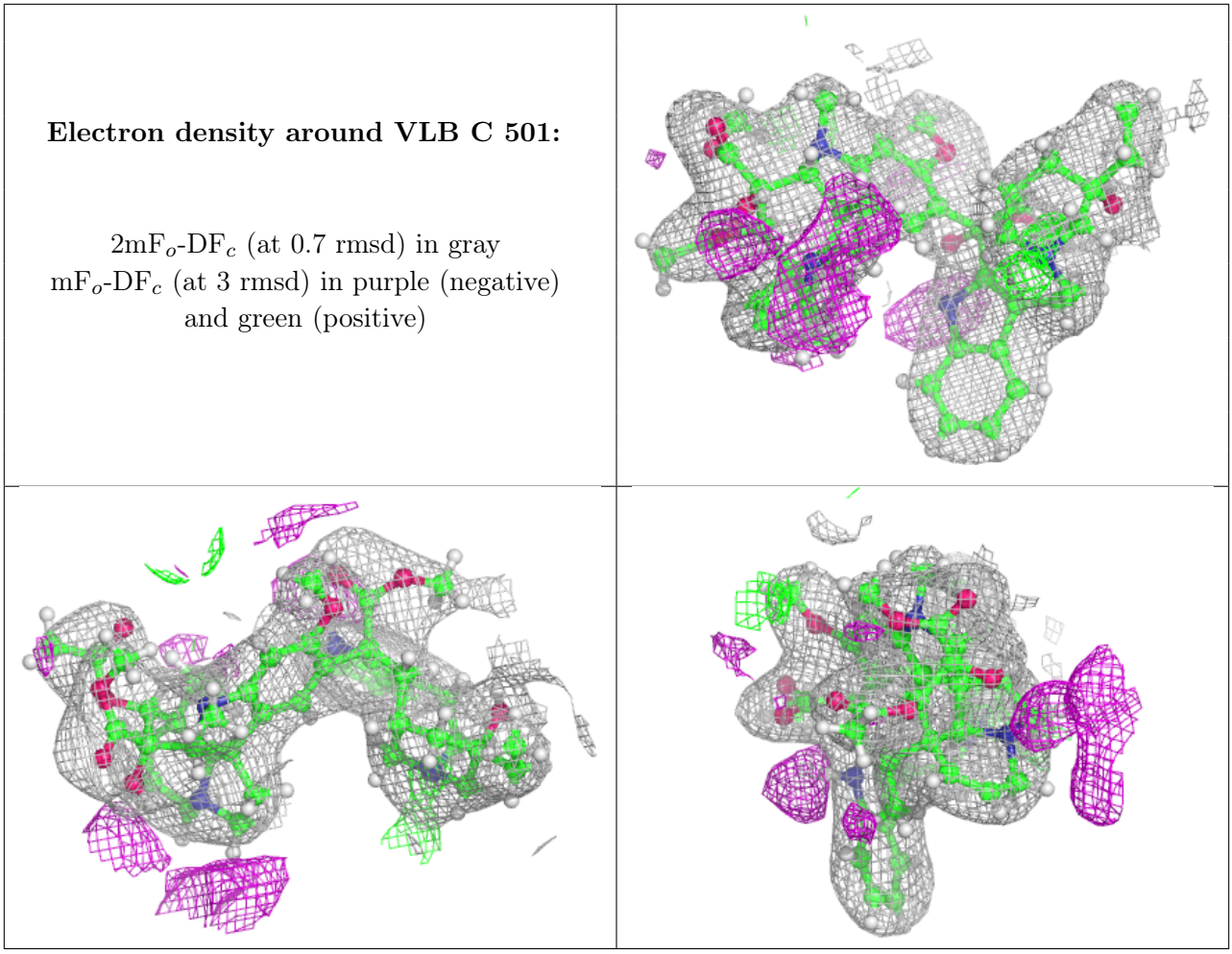






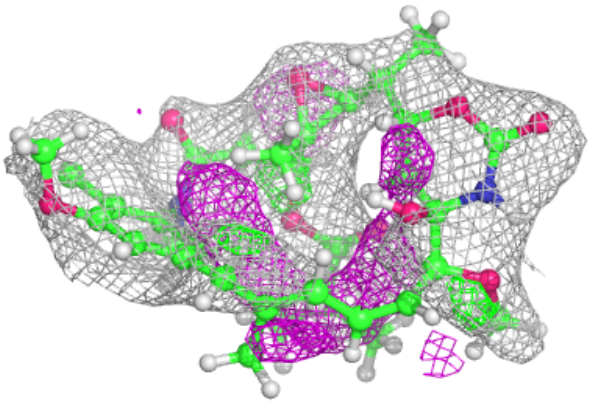
Electron density around VLB C 501:

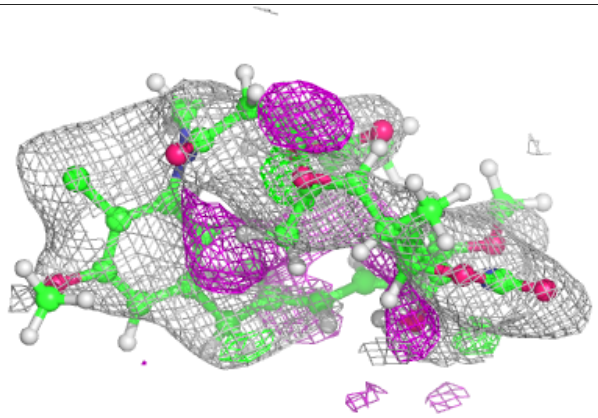
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

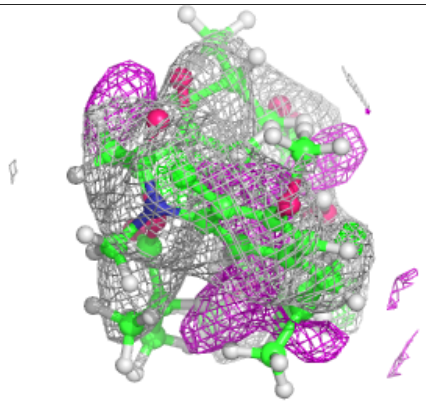


Electron density around BKF D 504:

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

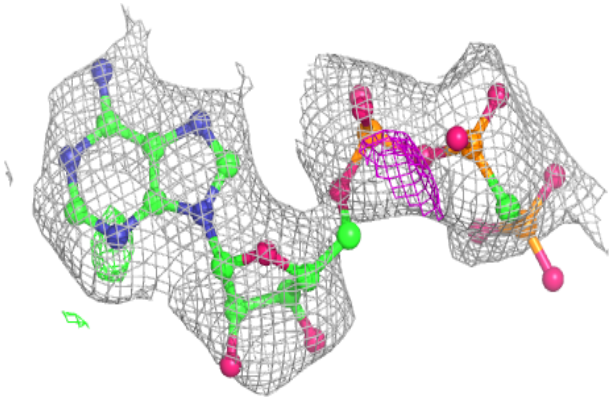


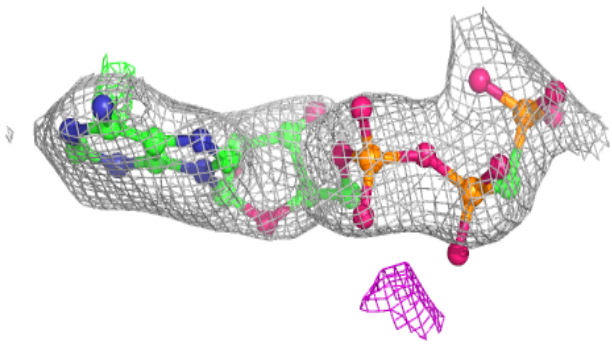


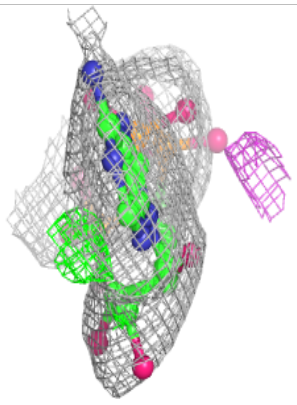


Electron density around ACP F 401:

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







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.