



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:11 PM EDT

PDB ID : 5JCB / pdb_00005jcb
Title : Microtubule depolymerizing agent podophyllotoxin derivative YJTSF1
Authors : Guan, Z.; Zhao, W.; Yin, P.
Deposited on : 2016-04-14
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

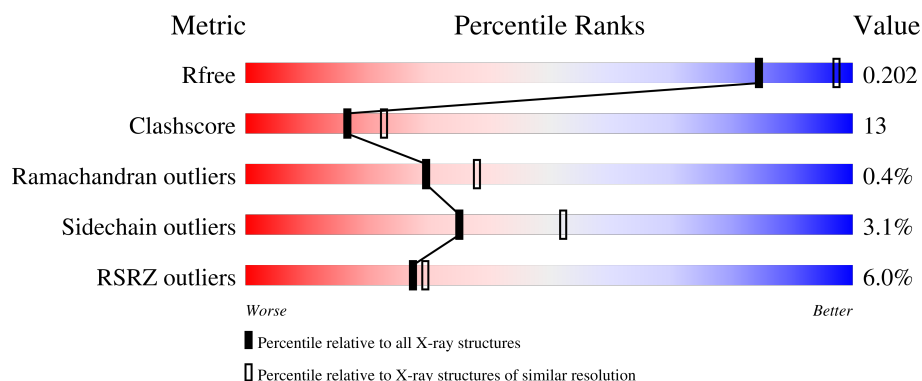
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	3% 78% 18% ..
1	C	451	3% 77% 20% ..
2	B	445	4% 72% 21% • 5%
2	D	445	6% 69% 23% • 6%
3	E	152	6% 65% 13% • 20%

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Mol	Chain	Length	Quality of chain
4	F	388	

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
13	NV4	D	507	-	-	X	-
7	GOL	C	501	-	-	X	-
7	GOL	C	504	-	-	X	-
8	IMD	A	505	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 18127 atoms, of which 13 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	12	0
			3482	2213	585	659	25			
1	C	440	Total	C	N	O	S	0	9	0
			3481	2204	587	667	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	11	0
			3382	2129	570	657	26			
2	D	418	Total	C	N	O	S	0	5	0
			3316	2089	561	638	28			

- Molecule 3 is a protein called Stathmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1010	624	182	198	6			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP F2Z508
E	146	LEU	-	expression tag	UNP F2Z508
E	147	GLU	-	expression tag	UNP F2Z508
E	148	HIS	-	expression tag	UNP F2Z508
E	149	HIS	-	expression tag	UNP F2Z508
E	150	HIS	-	expression tag	UNP F2Z508
E	151	HIS	-	expression tag	UNP F2Z508
E	152	HIS	-	expression tag	UNP F2Z508
E	153	HIS	-	expression tag	UNP F2Z508
E	154	HIS	-	expression tag	UNP F2Z508

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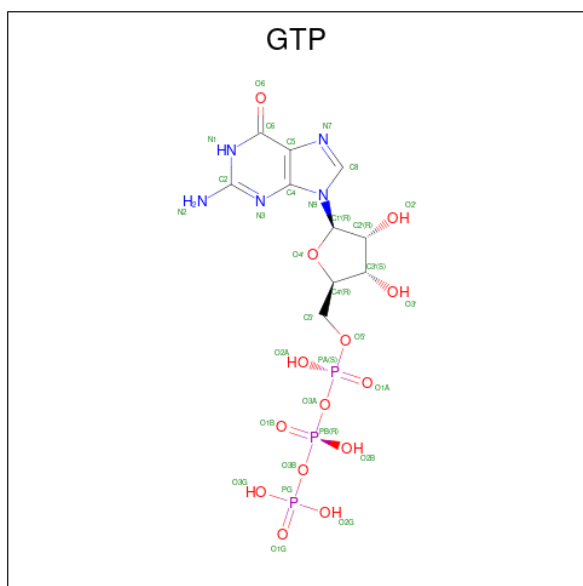
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Chain	Residue	Modelled	Actual	Comment	Reference
E	155	HIS	-	expression tag	UNP F2Z508

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	312	Total	C	N	O	S	0	4	0
			2577	1673	428	462	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: MG) (formula: Mg).

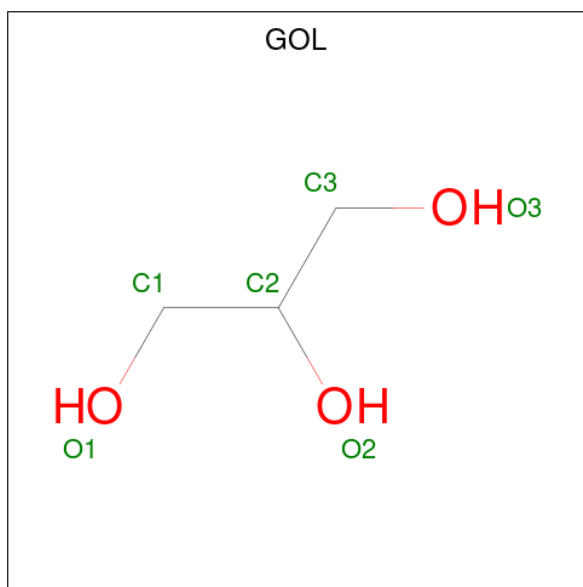
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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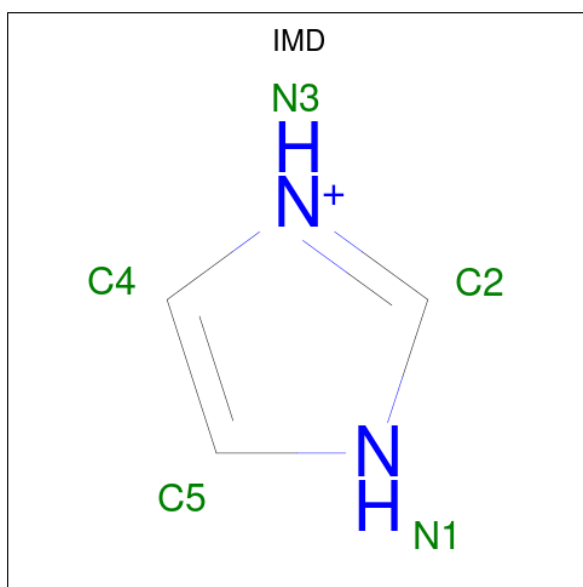
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Mg	0	0
			2	2		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O		0	0
			6	3	3			
7	A	1	Total	C	O		0	0
			6	3	3			
7	C	1	Total	C	O		0	0
			6	3	3			
7	C	1	Total	C	O		0	0
			6	3	3			
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	D	1	Total	C	O		0	0
			6	3	3			
7	D	1	Total	C	O		0	0
			6	3	3			
7	D	1	Total	C	O		0	0
			6	3	3			

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).

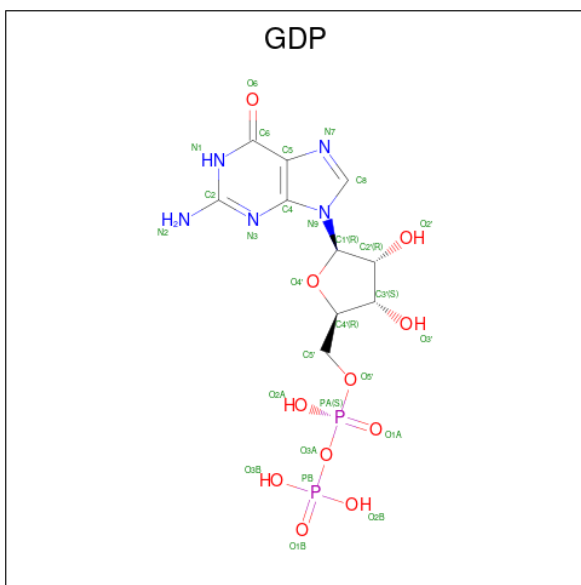


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H N 10 3 5 2	0	0
8	C	1	Total C N 5 3 2	0	0

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

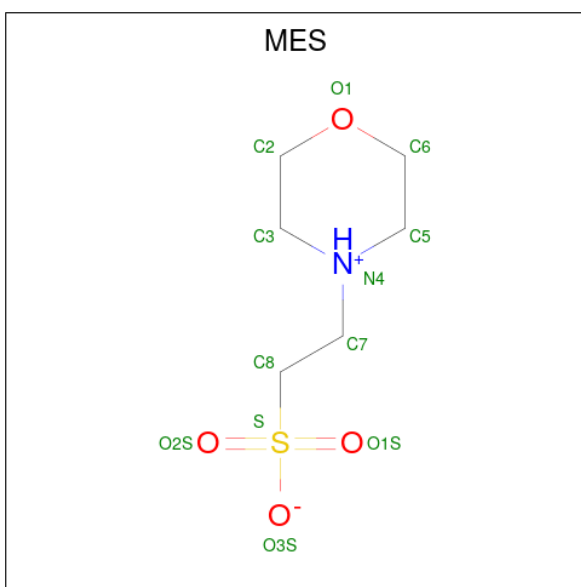


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
10	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

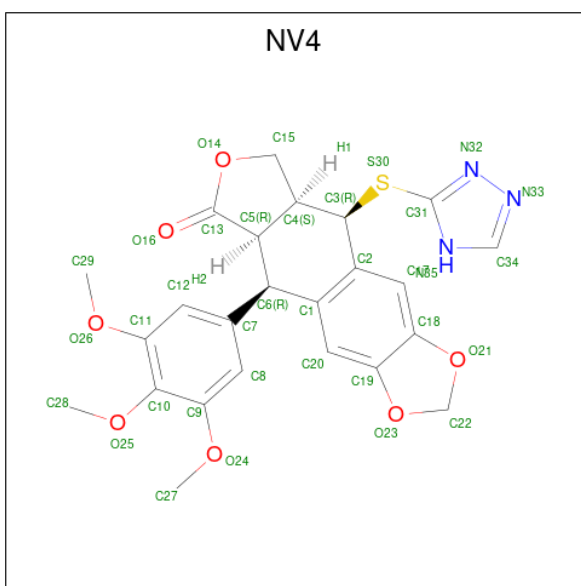
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Na 1 1	0	0
11	C	1	Total Na 1 1	0	0

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



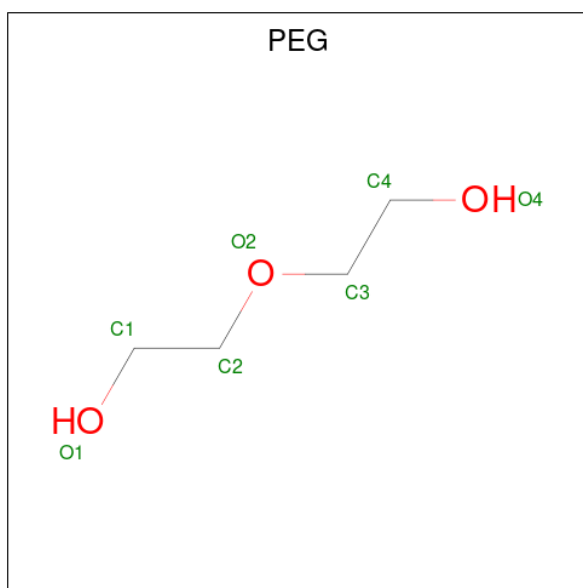
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 13 is (5R,5aR,8aS,9R)-9-[(4H-1,2,4-triazol-3-yl)sulfanyl]-5-(3,4,5-trimethoxyphenyl)-5,8,8a,9-tetrahydro-2H-furo[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one (CCD ID: NV4) (formula: C₂₄H₂₃N₃O₇S).



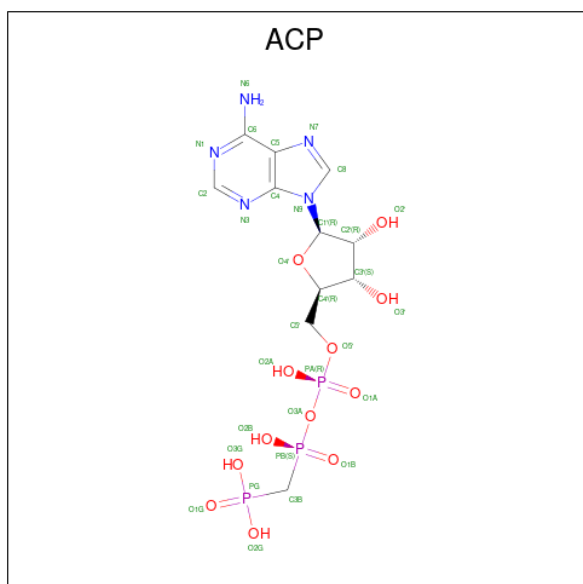
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	N	O	S	0	0
			35	24	3	7	1		
13	D	1	Total	C	N	O	S	0	0
			35	24	3	7	1		

- Molecule 14 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 15 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



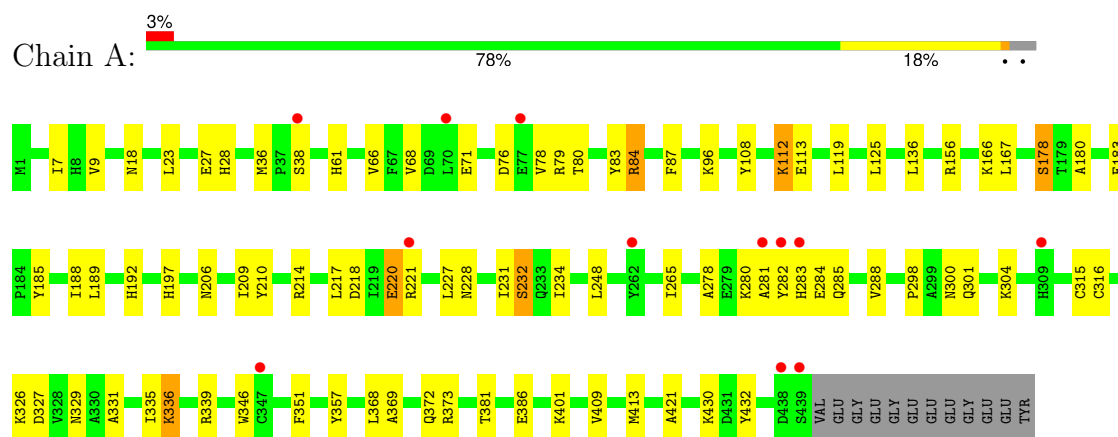
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	115	Total 115	O 115	0	0
16	B	84	Total 84	O 84	0	0
16	C	199	Total 199	O 199	0	0
16	D	66	Total 66	O 66	0	0
16	E	28	Total 28	O 28	0	0
16	F	65	Total 65	O 65	0	0

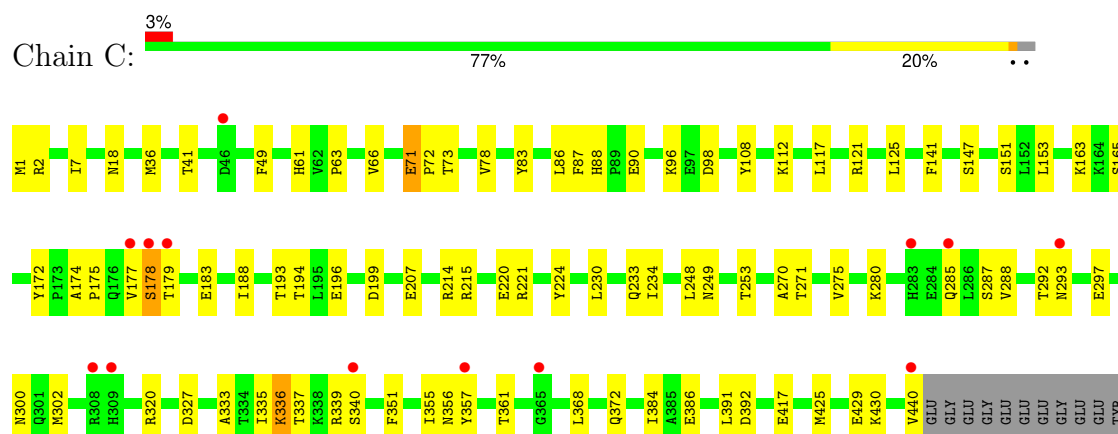
3 Residue-property plots [i](#)

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.

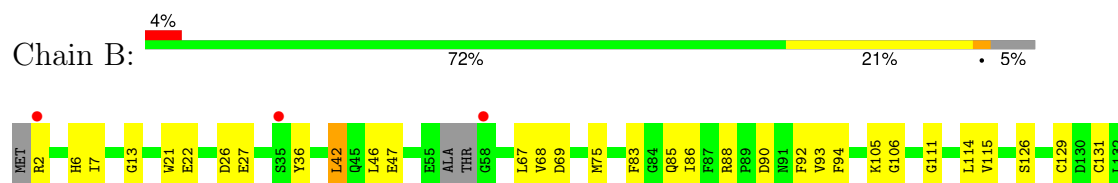
• Molecule 1: Tubulin alpha-1B chain

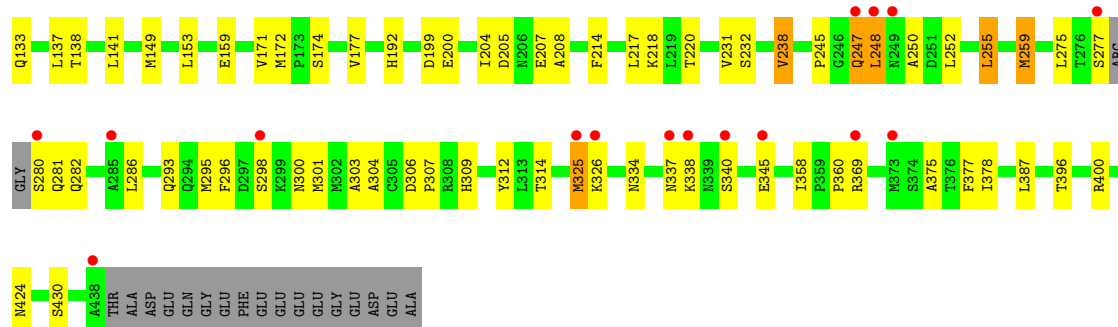


• Molecule 1: Tubulin alpha-1B chain

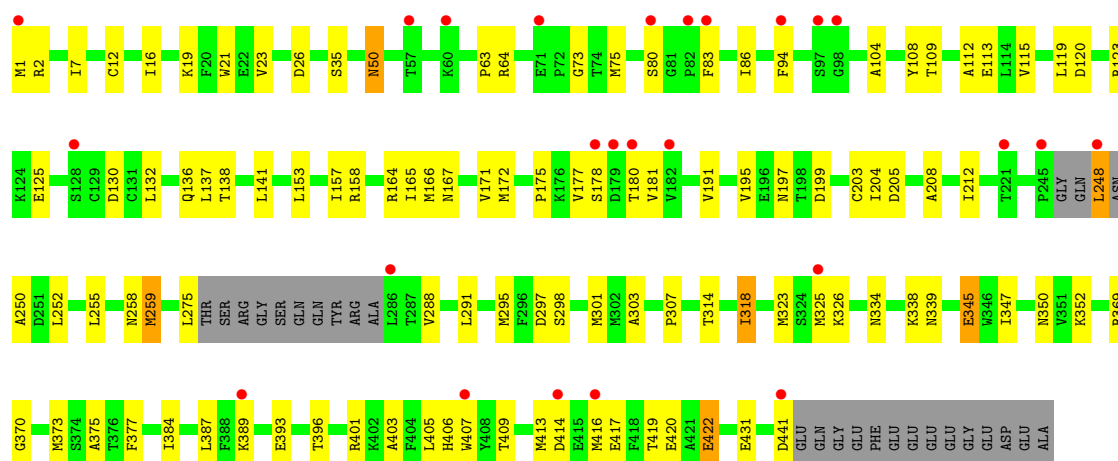


• Molecule 2: Tubulin beta chain

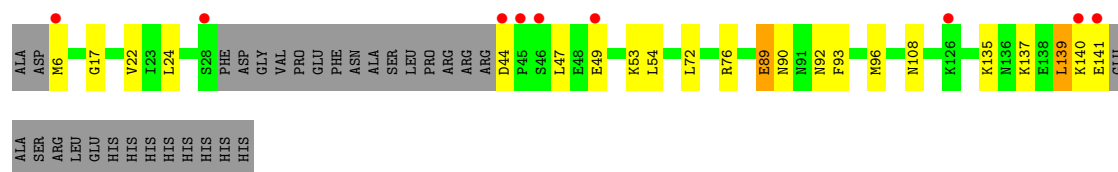




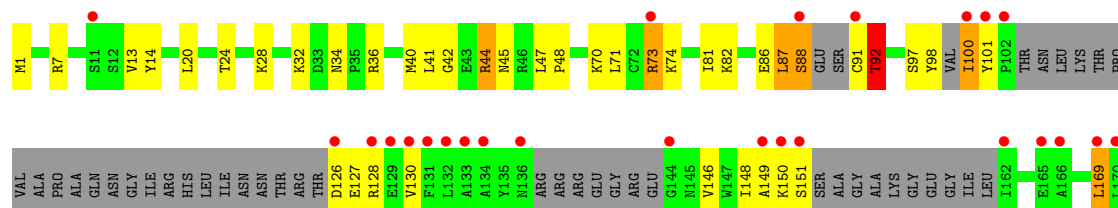
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.36Å 157.25Å 179.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 2.30 47.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.64-2.30) 99.8 (47.64-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.181 , 0.200 0.183 , 0.202	Depositor DCC
R_{free} test set	6501 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18127	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, CA, GTP, PEG, MES, GDP, NV4, ACP, IMD, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/3596	0.53	2/4883 (0.0%)
1	C	0.51	2/3583 (0.1%)	0.61	2/4866 (0.0%)
2	B	0.35	0/3485	0.55	0/4718
2	D	0.38	1/3399 (0.0%)	0.50	0/4602
3	E	0.30	0/1024	0.47	0/1358
4	F	0.38	0/2644	0.53	1/3566 (0.0%)
All	All	0.39	3/17731 (0.0%)	0.54	5/23993 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	288	VAL	CA-CB	12.68	1.61	1.54
1	C	297	GLU	C-O	-5.15	1.17	1.24
1	C	292	THR	C-O	-5.15	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	42	GLY	N-CA-C	7.17	123.48	112.51
1	C	297	GLU	CA-C-N	5.62	125.46	119.28
1	C	297	GLU	C-N-CA	5.62	125.46	119.28
1	A	87	PHE	CA-C-N	-5.03	111.93	123.15
1	A	87	PHE	C-N-CA	-5.03	111.93	123.15

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	3482	0	3434	71	0
1	C	3481	0	3401	85	0
2	B	3382	0	3270	92	0
2	D	3316	0	3213	88	0
3	E	1010	0	1033	25	0
4	F	2577	0	2576	104	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	F	1	0	0	0	0
7	A	12	0	16	2	0
7	C	18	8	24	11	0
7	D	18	0	23	2	0
8	A	5	5	5	4	0
8	C	5	0	5	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
12	B	12	0	12	0	0
13	B	35	0	0	3	0
13	D	35	0	0	9	0
14	C	7	0	10	0	0
15	F	31	0	13	3	0
16	A	115	0	0	10	1
16	B	84	0	0	4	0
16	C	199	0	0	17	1
16	D	66	0	0	7	0
16	E	28	0	0	6	0
16	F	65	0	0	10	0
All	All	18114	13	17083	443	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 (443) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HD2	2:D:325:MET:HB3	1.29	1.09
4:F:100:ILE:HD11	4:F:127:GLU:H	1.15	1.07
1:C:220:GLU:HB3	2:D:326:LYS:HE3	1.46	0.98
2:B:27:GLU:HA	2:B:369:ARG:HH22	1.27	0.98
4:F:32:LYS:H	4:F:32:LYS:HD2	1.24	0.98
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.45	0.98
4:F:254:GLY:O	16:F:501:HOH:O	1.82	0.97
1:C:417:GLU:OE1	16:C:601:HOH:O	1.84	0.94
4:F:91:CYS:O	4:F:92:THR:HB	1.67	0.92
2:B:220:THR:O	16:B:601:HOH:O	1.85	0.92
2:D:175:PRO:HA	2:D:178:SER:HB2	1.51	0.92
2:D:370:GLY:O	16:D:602:HOH:O	1.86	0.91
4:F:100:ILE:HD11	4:F:127:GLU:N	1.84	0.91
1:C:98:ASP:OD1	16:C:602:HOH:O	1.87	0.90
2:D:180:THR:HG22	2:D:181:VAL:H	1.37	0.90
2:D:431:GLU:OE2	16:D:603:HOH:O	1.88	0.89
4:F:73:ARG:HD2	4:F:74:LYS:H	1.35	0.89
1:C:386:GLU:OE2	16:C:603:HOH:O	1.92	0.87
2:B:27:GLU:HA	2:B:369:ARG:NH2	1.88	0.87
3:E:53:LYS:O	16:E:201:HOH:O	1.92	0.87
4:F:247:LYS:HZ1	4:F:259:GLY:HA2	1.39	0.87
7:A:507:GOL:O1	16:A:601:HOH:O	1.95	0.84
4:F:100:ILE:CD1	4:F:127:GLU:H	1.90	0.83
4:F:169:LEU:HD13	4:F:172:PHE:HB3	1.59	0.83
2:B:301:MET:HE1	2:B:307:PRO:CG	2.08	0.83
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.59	0.82
1:A:218:ASP:HB3	16:A:610:HOH:O	1.79	0.82
2:B:159:GLU:OE2	16:B:602:HOH:O	1.97	0.82
1:C:221:ARG:CD	2:D:325:MET:HB3	2.09	0.81
1:C:214:ARG:NH1	16:C:607:HOH:O	2.10	0.80
2:D:323:MET:HB3	2:D:373:MET:HE1	1.63	0.80
4:F:1:MET:SD	4:F:28:LYS:HD3	2.21	0.80
2:B:247:GLN:HG3	2:B:248:LEU:H	1.45	0.80
2:D:370:GLY:C	16:D:602:HOH:O	2.26	0.79
4:F:151:SER:OG	4:F:180:HIS:HA	1.82	0.79
1:C:41:THR:OG1	16:C:604:HOH:O	2.01	0.79
4:F:247:LYS:NZ	4:F:259:GLY:HA2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:359:PHE:O	16:F:504:HOH:O	2.01	0.79
4:F:237:THR:HG21	4:F:249:TYR:HD1	1.48	0.78
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.65	0.78
2:B:42:LEU:H	2:B:42:LEU:HD12	1.50	0.76
2:B:247:GLN:O	16:B:603:HOH:O	2.02	0.76
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.19	0.76
1:C:288:VAL:HG23	7:C:504:GOL:H2	1.67	0.76
4:F:100:ILE:N	4:F:180:HIS:O	2.19	0.75
4:F:150:LYS:HD2	4:F:151:SER:H	1.51	0.75
2:B:340:SER:HB3	4:F:34:ASN:HD21	1.50	0.75
4:F:200:ASP:OD1	4:F:222:ARG:NH2	2.18	0.75
1:C:215:ARG:NH1	16:C:605:HOH:O	2.03	0.74
2:B:281:GLN:HG2	2:B:281:GLN:O	1.88	0.74
3:E:108[B]:ASN:OD1	16:E:202:HOH:O	2.06	0.73
1:A:221:ARG:HG2	2:B:325:MET:HE2	1.70	0.73
4:F:169:LEU:CD1	4:F:172:PHE:HB3	2.19	0.73
1:C:287:SER:HB2	7:C:504:GOL:H12	1.71	0.73
1:C:96:LYS:HE3	2:D:130:ASP:OD1	1.90	0.72
2:B:26:ASP:OD2	2:B:369:ARG:NE	2.21	0.72
4:F:237:THR:HG21	4:F:249:TYR:CD1	2.24	0.72
1:C:214:ARG:NE	16:C:607:HOH:O	2.12	0.71
4:F:73:ARG:HD2	4:F:74:LYS:N	2.05	0.71
4:F:334:GLY:O	16:F:505:HOH:O	2.08	0.70
1:C:18:ASN:OD1	16:C:606:HOH:O	2.09	0.70
2:B:298:SER:HA	2:B:301:MET:HE2	1.72	0.70
1:C:163:LYS:HE2	3:E:93:PHE:CD2	2.27	0.69
2:D:441:ASP:N	16:D:601:HOH:O	1.86	0.69
1:A:288:VAL:H	8:A:505:IMD:HN1	1.41	0.69
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.56	0.69
4:F:32:LYS:HD2	4:F:32:LYS:N	2.04	0.68
4:F:87:LEU:O	4:F:88:SER:HB3	1.93	0.68
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.93	0.68
1:A:228:ASN:O	1:A:232:SER:OG	2.10	0.68
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.57	0.68
1:C:215:ARG:HD2	16:C:605:HOH:O	1.95	0.67
1:A:221:ARG:HG2	2:B:325:MET:HG2	1.76	0.67
1:C:327:ASP:OD2	16:C:608:HOH:O	2.13	0.67
4:F:254:GLY:CA	16:F:501:HOH:O	2.42	0.67
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.77	0.67
1:C:221:ARG:O	1:C:221:ARG:HG2	1.93	0.66
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ILE:HD11	4:F:127:GLU:C	2.21	0.66
1:A:386:GLU:OE2	16:A:602:HOH:O	2.14	0.66
1:C:280:LYS:HD3	16:C:640:HOH:O	1.95	0.66
2:B:340:SER:CB	4:F:34:ASN:HD21	2.08	0.65
2:D:416:MET:O	2:D:420:GLU:HG3	1.96	0.65
2:D:136:GLN:HA	2:D:167:ASN:O	1.97	0.65
4:F:127:GLU:HB2	4:F:130:VAL:CG2	2.27	0.64
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.33	0.64
1:C:271:THR:HG23	1:C:300:ASN:C	2.23	0.64
4:F:188:LYS:HD2	4:F:323:GLU:CD	2.23	0.64
2:B:280:SER:O	2:B:281:GLN:HB3	1.97	0.63
2:B:301:MET:HE1	2:B:307:PRO:HG2	1.80	0.63
2:B:345:GLU:H	2:B:345:GLU:CD	2.06	0.63
4:F:333:ASN:ND2	15:F:402:ACP:O2G	2.27	0.63
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.79	0.63
4:F:193:GLU:HG3	4:F:196:HIS:H	1.65	0.62
2:D:323:MET:HE2	2:D:373:MET:HE2	1.81	0.62
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.82	0.62
1:A:373:ARG:CZ	8:A:505:IMD:H5	2.29	0.62
3:E:92:ASN:O	3:E:96:MET:HG2	2.00	0.62
4:F:169:LEU:HD12	4:F:169:LEU:O	1.98	0.62
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.35	0.62
2:B:105[B]:LYS:NZ	7:C:501:GOL:H31	2.14	0.61
4:F:100:ILE:HG23	4:F:126:ASP:OD2	2.00	0.61
2:B:247:GLN:HG3	2:B:248:LEU:N	2.15	0.61
2:B:250:ALA:HB1	13:B:505:NV4:O16	2.00	0.61
1:A:283:HIS:HD2	1:A:284:GLU:O	1.84	0.61
4:F:341:LYS:CB	16:F:502:HOH:O	2.49	0.61
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.83	0.60
4:F:100:ILE:HD11	4:F:127:GLU:CA	2.32	0.60
2:B:248:LEU:HD11	13:B:505:NV4:S30	2.41	0.60
1:C:1:MET:O	1:C:2:ARG:HB2	2.02	0.60
2:D:352:LYS:HG3	13:D:507:NV4:C17	2.32	0.60
1:A:248:LEU:HD21	1:A:316[B]:CYS:SG	2.42	0.60
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.83	0.60
4:F:100:ILE:HG22	4:F:101:TYR:N	2.16	0.60
2:B:2:ARG:NE	2:B:133:GLN:HG3	2.17	0.60
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.22	0.60
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.20	0.59
2:D:258:ASN:HB3	13:D:507:NV4:C18	2.32	0.59
1:C:339:ARG:O	16:C:609:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.84	0.59
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.67	0.59
1:A:304:LYS:HB2	16:A:614:HOH:O	2.03	0.59
4:F:73:ARG:HH22	4:F:151:SER:C	2.10	0.58
2:B:42:LEU:HD12	2:B:42:LEU:N	2.17	0.58
4:F:184:LYS:HD2	4:F:185:TYR:N	2.18	0.58
2:B:47:GLU:HB3	2:B:245:PRO:HG3	1.84	0.58
2:D:389:LYS:NZ	16:D:604:HOH:O	2.16	0.58
1:A:329:ASN:HB3	3:E:6:MET:HE2	1.86	0.58
2:D:2:ARG:NH2	16:D:605:HOH:O	2.26	0.58
1:C:163:LYS:HE2	3:E:93:PHE:CG	2.38	0.58
1:C:214:ARG:CZ	16:C:607:HOH:O	2.41	0.57
2:D:401:ARG:HE	2:D:403:ALA:HB2	1.68	0.57
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.85	0.57
1:C:253:THR:HB	7:C:501:GOL:H11	1.84	0.57
2:D:50:ASN:H	2:D:50:ASN:ND2	2.02	0.57
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.40	0.57
4:F:148:ILE:HG22	4:F:183:GLN:O	2.04	0.57
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.04	0.57
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.39	0.57
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.70	0.57
2:D:295:MET:CG	2:D:377:PHE:HB2	2.34	0.57
2:B:259:MET:HE3	2:B:314:THR:OG1	2.05	0.56
4:F:100:ILE:HD13	4:F:126:ASP:CG	2.30	0.56
1:C:302:MET:N	1:C:302:MET:HE2	2.20	0.56
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.56
2:D:255:LEU:HD13	13:D:507:NV4:C8	2.35	0.56
2:D:323:MET:HB3	2:D:373:MET:CE	2.32	0.56
2:D:180:THR:HG22	2:D:181:VAL:N	2.16	0.56
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.87	0.56
3:E:6:MET:HE3	3:E:22:VAL:HG21	1.86	0.56
4:F:7:ARG:CD	4:F:40:MET:HE3	2.36	0.56
2:B:42:LEU:H	2:B:42:LEU:CD1	2.17	0.56
1:C:287:SER:HA	7:C:504:GOL:O2	2.06	0.56
4:F:74:LYS:NZ	4:F:150:LYS:HE3	2.20	0.56
4:F:100:ILE:CG2	4:F:101:TYR:N	2.69	0.56
1:A:288:VAL:HG23	8:A:505:IMD:HN1	1.71	0.55
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.88	0.55
4:F:146:VAL:O	4:F:184:LYS:NZ	2.28	0.55
1:C:71:GLU:HG2	1:C:72:PRO:N	2.21	0.55
2:D:203:CYS:SG	2:D:384[B]:ILE:HD11	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:O	2:D:157:ILE:HG13	2.07	0.55
3:E:137:LYS:O	3:E:141:GLU:HG2	2.06	0.55
4:F:149:ALA:HB2	4:F:182:ILE:CD1	2.36	0.55
4:F:255:ARG:HB2	4:F:256:TYR:CD2	2.42	0.55
3:E:135:LYS:NZ	3:E:139:LEU:HD21	2.20	0.55
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.42	0.55
2:D:259:MET:HE3	2:D:314:THR:OG1	2.06	0.55
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.72	0.55
2:B:105[A]:LYS:NZ	7:C:501:GOL:H31	2.22	0.54
1:C:293:ASN:HA	1:C:335:ILE:HD11	1.89	0.54
3:E:89:GLU:OE2	16:E:203:HOH:O	2.18	0.54
4:F:70:LYS:CE	4:F:298:ILE:HD11	2.37	0.54
4:F:151:SER:CB	4:F:180:HIS:HA	2.38	0.54
4:F:150:LYS:O	4:F:151:SER:OG	2.12	0.54
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.89	0.54
4:F:341:LYS:HB3	16:F:502:HOH:O	2.08	0.54
1:A:23:LEU:O	1:A:27:GLU:HG3	2.07	0.54
1:A:206:ASN:HA	1:A:209[B]:ILE:HG12	1.89	0.54
1:A:304:LYS:CB	16:A:614:HOH:O	2.55	0.54
3:E:108[A]:ASN:OD1	16:E:204:HOH:O	2.19	0.54
1:A:221:ARG:CG	2:B:325:MET:HE2	2.38	0.54
2:D:112:ALA:O	2:D:115:VAL:HG12	2.08	0.54
1:C:271:THR:HG23	1:C:300:ASN:O	2.07	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.43	0.54
2:B:396:THR:O	2:B:400:ARG:HG2	2.09	0.53
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.39	0.53
1:A:401:LYS:NZ	16:A:609:HOH:O	2.40	0.53
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.44	0.53
2:D:393:GLU:HA	2:D:396:THR:HG22	1.90	0.53
2:B:238:VAL:HG22	2:B:378:ILE:HG12	1.90	0.53
2:B:105[B]:LYS:HZ2	7:C:501:GOL:H31	1.73	0.53
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.91	0.53
1:C:288:VAL:H	7:C:504:GOL:H12	1.73	0.52
2:D:258:ASN:HB3	13:D:507:NV4:C17	2.38	0.52
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.90	0.52
2:D:248:LEU:HG	2:D:248:LEU:O	2.09	0.52
4:F:247:LYS:HD3	4:F:253:TYR:CE2	2.44	0.52
1:A:220:GLU:CG	2:B:326:LYS:HD2	2.40	0.52
2:D:16:ILE:HD11	2:D:138:THR:HB	1.91	0.52
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.10	0.52
2:D:191:VAL:O	2:D:195:VAL:HG23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:44:ASP:N	16:E:206:HOH:O	2.42	0.52
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.45	0.52
2:D:141:LEU:HD12	2:D:172:MET:SD	2.50	0.52
4:F:98:TYR:O	4:F:181:VAL:HA	2.10	0.52
1:C:440:VAL:HG12	1:C:440:VAL:O	2.09	0.51
2:B:2:ARG:HA	2:B:131:CYS:O	2.10	0.51
1:C:2:ARG:HA	1:C:2:ARG:NE	2.25	0.51
1:A:83:TYR:O	1:A:84:ARG:C	2.54	0.51
1:C:221:ARG:O	1:C:221:ARG:CG	2.57	0.51
2:D:208:ALA:O	2:D:212:ILE:HG13	2.11	0.51
2:B:42:LEU:HB2	2:B:358:ILE:HD11	1.92	0.51
2:D:334:ASN:OD1	2:D:338:LYS:HE2	2.11	0.51
2:B:27:GLU:CA	2:B:369:ARG:NH2	2.68	0.51
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.44	0.51
2:D:409:THR:O	3:E:140:LYS:HE2	2.10	0.51
4:F:100:ILE:CG2	4:F:101:TYR:H	2.25	0.50
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.26	0.50
1:A:79:ARG:O	1:A:84:ARG:HB3	2.11	0.50
2:B:255:LEU:HD22	2:B:259:MET:HG3	1.92	0.50
2:D:158[A]:ARG:NH2	2:D:197:ASN:OD1	2.44	0.50
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.24	0.50
4:F:44:ARG:NH1	16:F:511:HOH:O	2.45	0.50
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.93	0.50
2:D:250:ALA:HB1	13:D:507:NV4:O16	2.11	0.50
2:D:301:MET:HE3	2:D:307:PRO:HG3	1.94	0.50
4:F:217:ARG:HG3	4:F:374:ILE:O	2.12	0.49
1:A:221:ARG:NH1	2:B:325:MET:O	2.45	0.49
4:F:199:PHE:HA	4:F:241:THR:HG21	1.93	0.49
4:F:249:TYR:CD1	4:F:249:TYR:O	2.65	0.49
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.93	0.49
2:D:419:THR:O	2:D:422:GLU:OE1	2.31	0.49
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	1.95	0.49
2:B:217:LEU:HD13	2:B:277:SER:HB3	1.93	0.49
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.48	0.49
2:D:119:LEU:O	2:D:123:ARG:HG3	2.12	0.49
4:F:70:LYS:HE3	4:F:298:ILE:HD11	1.95	0.48
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.13	0.48
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.13	0.48
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.78	0.48
2:D:7:ILE:O	2:D:137:LEU:HD12	2.14	0.48
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HE	2:B:133:GLN:HG3	1.77	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.54	0.48
2:D:158[A]:ARG:NH2	16:D:609:HOH:O	2.47	0.48
2:B:295:MET:SD	2:B:375:ALA:HB1	2.53	0.48
1:C:340:SER:HA	16:C:609:HOH:O	2.13	0.48
4:F:151:SER:HB2	4:F:180:HIS:ND1	2.29	0.48
4:F:193:GLU:HA	4:F:194:PRO:C	2.37	0.48
1:A:178:SER:OG	13:B:505:NV4:N32	2.46	0.48
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.96	0.48
2:D:132:LEU:HD23	2:D:164:ARG:HH11	1.78	0.48
2:B:2:ARG:CZ	2:B:133:GLN:HG3	2.43	0.48
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.48
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.96	0.48
2:D:177:VAL:HG12	2:D:177:VAL:O	2.14	0.48
3:E:44:ASP:N	3:E:44:ASP:OD1	2.46	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.12	0.48
1:A:298:PRO:HA	1:A:301:GLN:CD	2.39	0.48
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.95	0.48
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.49	0.48
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.48
4:F:169:LEU:HD11	4:F:172:PHE:CD2	2.49	0.48
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.95	0.47
1:C:220:GLU:CB	2:D:326:LYS:HE3	2.31	0.47
2:D:7:ILE:O	2:D:137:LEU:HA	2.14	0.47
4:F:127:GLU:HB2	4:F:130:VAL:HG22	1.96	0.47
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.95	0.47
2:B:301:MET:HE1	2:B:307:PRO:HG3	1.93	0.47
1:A:285:GLN:OE1	1:A:372[B]:GLN:HG3	2.14	0.47
1:C:179:THR:HA	1:C:183:GLU:OE1	2.14	0.47
2:B:83:PHE:O	2:B:86:ILE:HG22	2.14	0.47
4:F:82:LYS:NZ	4:F:97:SER:O	2.28	0.47
1:A:192:HIS:CG	1:A:421:ALA:HA	2.49	0.47
2:D:318:ILE:HG12	13:D:507:NV4:C28	2.44	0.47
4:F:150:LYS:HD2	4:F:151:SER:N	2.25	0.47
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.49	0.47
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.50	0.47
1:C:196[B]:GLU:HG2	16:C:666:HOH:O	2.15	0.47
1:C:230:LEU:O	1:C:234:ILE:HD12	2.14	0.47
2:D:339:ASN:CB	7:D:506:GOL:H32	2.45	0.47
1:C:287:SER:HB2	7:C:504:GOL:C1	2.43	0.47
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.47
4:F:341:LYS:N	16:F:502:HOH:O	1.86	0.46
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.46
2:B:286:LEU:N	2:B:286:LEU:HD12	2.31	0.46
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.50	0.46
3:E:137:LYS:HG3	3:E:140:LYS:NZ	2.30	0.46
2:B:301:MET:HE1	2:B:307:PRO:CD	2.45	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.46
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.46	0.46
2:D:109:THR:O	2:D:113:GLU:OE1	2.34	0.46
2:D:416:MET:HE2	2:D:420:GLU:OE2	2.15	0.46
2:D:248:LEU:HD23	2:D:250:ALA:HB2	1.96	0.46
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	1.98	0.46
1:C:270:ALA:HB3	1:C:302:MET:HG2	1.98	0.46
1:A:304:LYS:CG	16:A:614:HOH:O	2.63	0.46
1:C:336:LYS:HE2	16:C:785:HOH:O	2.14	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.46
1:C:108:TYR:O	1:C:112:LYS:HG2	2.16	0.45
2:D:158[B]:ARG:NH2	2:D:199:ASP:OD2	2.49	0.45
4:F:247:LYS:HA	4:F:253:TYR:CD1	2.51	0.45
2:D:275:LEU:HA	2:D:275:LEU:HD23	1.82	0.45
2:D:339:ASN:CG	7:D:506:GOL:H32	2.41	0.45
1:C:2:ARG:NH2	16:C:619:HOH:O	2.49	0.45
1:A:185:TYR:O	1:A:189:LEU:HG	2.17	0.45
2:B:259:MET:HE2	2:B:259:MET:HB3	1.69	0.45
1:C:392:ASP:OD2	1:C:429:GLU:OE1	2.35	0.45
2:D:75:MET:CE	2:D:94:PHE:HD2	2.28	0.45
4:F:100:ILE:HD13	4:F:126:ASP:HB3	1.99	0.45
4:F:274:ALA:C	4:F:275[A]:LEU:HD22	2.42	0.45
1:A:112:LYS:HG3	3:E:54:LEU:HB3	1.99	0.45
3:E:49:GLU:OE2	3:E:53:LYS:HE2	2.17	0.45
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.47	0.44
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.17	0.44
1:C:288:VAL:CG2	7:C:504:GOL:H2	2.43	0.44
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.35	0.44
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.52	0.44
2:B:2:ARG:NH2	2:B:133:GLN:HG3	2.31	0.44
1:A:327:ASP:OD2	16:A:603:HOH:O	2.21	0.44
2:D:318:ILE:CG1	13:D:507:NV4:C28	2.96	0.44
13:D:507:NV4:C28	13:D:507:NV4:O24	2.65	0.44
4:F:169:LEU:HD13	4:F:169:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.50	0.44
1:A:209[B]:ILE:HG13	1:A:210:TYR:N	2.32	0.44
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.49	0.44
4:F:184:LYS:HD2	4:F:184:LYS:C	2.43	0.44
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.89	0.44
2:B:208:ALA:HB2	2:B:304:ALA:N	2.33	0.44
1:C:177:VAL:O	1:C:178:SER:C	2.61	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.00	0.44
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.48	0.44
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.18	0.44
1:C:165:SER:HA	1:C:199:ASP:OD2	2.18	0.44
2:D:352:LYS:HA	2:D:352:LYS:HD3	1.78	0.44
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.99	0.43
4:F:127:GLU:HB2	4:F:130:VAL:HG21	1.99	0.43
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.18	0.43
1:C:177:VAL:CG1	1:C:224:TYR:CE1	3.01	0.43
2:D:318:ILE:HD11	13:D:507:NV4:C28	2.48	0.43
2:B:68:VAL:HA	2:B:93:VAL:O	2.18	0.43
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.48	0.43
1:A:346:TRP:H	1:A:346:TRP:CD1	2.35	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.43
4:F:322:ASP:OD1	4:F:322:ASP:C	2.62	0.43
2:B:199:ASP:C	2:B:200:GLU:HG3	2.44	0.43
1:C:83:TYR:CD2	1:C:86:LEU:HD22	2.53	0.43
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.48	0.43
2:D:166:MET:HE2	2:D:166:MET:HB2	1.92	0.43
2:D:259:MET:HE2	2:D:259:MET:HB3	1.90	0.43
1:A:288:VAL:N	8:A:505:IMD:HN1	2.12	0.43
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.01	0.43
4:F:230:SER:O	4:F:230:SER:OG	2.33	0.43
1:A:28:HIS:O	1:A:36:MET:HE3	2.18	0.43
2:D:345:GLU:CD	2:D:345:GLU:H	2.26	0.43
1:A:66[A]:VAL:HG23	1:A:125:LEU:HD12	2.01	0.43
1:A:280:LYS:HE2	1:A:283:HIS:ND1	2.34	0.43
2:B:295:MET:HE3	2:B:296:PHE:CE1	2.54	0.43
2:B:334:ASN:O	2:B:338:LYS:HG2	2.18	0.43
1:C:175:PRO:HA	1:C:179:THR:HG21	2.01	0.43
1:C:177:VAL:HG11	1:C:224:TYR:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:335:ILE:HG13	2.19	0.42
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.54	0.42
4:F:100:ILE:HD13	4:F:126:ASP:CB	2.49	0.42
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.54	0.42
2:D:295:MET:HE2	2:D:295:MET:HB3	1.80	0.42
1:A:221:ARG:HG2	2:B:325:MET:CE	2.45	0.42
2:B:115:VAL:HG23	2:B:153:LEU:HD23	2.01	0.42
2:B:387:LEU:C	2:B:387:LEU:HD23	2.43	0.42
4:F:330:ILE:HA	4:F:330:ILE:HD13	1.77	0.42
1:A:218:ASP:CB	16:A:610:HOH:O	2.55	0.42
1:A:300:ASN:OD1	7:A:504:GOL:H12	2.20	0.42
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.65	0.42
2:D:297:ASP:OD1	2:D:298:SER:N	2.53	0.42
2:D:334:ASN:CG	2:D:338:LYS:HE2	2.45	0.42
3:E:90:ASN:ND2	16:E:205:HOH:O	2.29	0.42
4:F:247:LYS:CE	4:F:259:GLY:HA2	2.49	0.42
1:A:304:LYS:HG3	16:A:614:HOH:O	2.19	0.42
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.42
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.84	0.42
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.85	0.42
2:B:298:SER:HA	2:B:301:MET:CE	2.46	0.42
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.54	0.42
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.35	0.42
4:F:1:MET:HE2	4:F:1:MET:HB2	1.87	0.42
2:D:19:LYS:O	2:D:23:VAL:HG23	2.20	0.42
4:F:241:THR:OG1	15:F:402:ACP:O3'	2.38	0.42
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.43	0.41
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.44	0.41
4:F:81:ILE:O	4:F:87:LEU:O	2.38	0.41
4:F:242:ASN:OD1	15:F:402:ACP:H5'1	2.20	0.41
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	2.02	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.41
2:B:218:LYS:HA	2:B:218:LYS:HD3	1.69	0.41
1:C:333:ALA:O	1:C:337:THR:HG23	2.19	0.41
2:B:214:PHE:CD1	2:B:220:THR:HA	2.56	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.41
1:C:248:LEU:HD12	1:C:357:TYR:CZ	2.55	0.41
4:F:247:LYS:HZ1	4:F:259:GLY:CA	2.23	0.41
4:F:271:LEU:HD23	4:F:275[B]:LEU:HD12	2.01	0.41
2:B:22[B]:GLU:HG3	2:B:83:PHE:CE1	2.56	0.41
2:B:301:MET:HE3	2:B:301:MET:HB2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.41
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	0.41
4:F:209:HIS:HA	4:F:311:SER:O	2.20	0.41
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.56	0.41
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.51	0.41
4:F:13:VAL:HG23	16:F:524:HOH:O	2.21	0.41
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.74	0.41
2:B:75:MET:N	16:B:614:HOH:O	2.41	0.41
2:B:105[A]:LYS:HZ1	7:C:501:GOL:H31	1.86	0.41
1:C:1:MET:O	1:C:2:ARG:CB	2.69	0.41
1:C:141:PHE:O	1:C:147:SER:HB3	2.19	0.41
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	2.02	0.41
2:D:291:LEU:HG	2:D:375:ALA:HB2	2.02	0.41
3:E:47:LEU:HD12	3:E:47:LEU:O	2.21	0.41
4:F:14:TYR:CD1	4:F:41:LEU:HD22	2.56	0.41
4:F:47:LEU:HD23	4:F:48:PRO:HD2	2.03	0.41
4:F:188:LYS:HD3	4:F:188:LYS:HA	1.94	0.41
2:D:414:ASP:OD1	2:D:414:ASP:N	2.54	0.41
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.51	0.41
2:B:192:HIS:ND1	2:B:424[B]:ASN:ND2	2.67	0.40
1:C:177:VAL:HG11	1:C:224:TYR:CE1	2.55	0.40
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.40
2:D:83:PHE:O	2:D:86:ILE:HG22	2.20	0.40
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.24	0.40
2:B:36:TYR:CD2	2:B:46:LEU:HD11	2.56	0.40
2:B:126:SER:O	2:B:129:CYS:HB2	2.21	0.40
1:C:248:LEU:HD13	1:C:355:ILE:HD12	2.03	0.40
4:F:188:LYS:HD2	4:F:323:GLU:OE2	2.21	0.40
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	2.03	0.40
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.22	0.40
4:F:191:LEU:HD23	4:F:191:LEU:HA	1.86	0.40
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.34	0.40
1:A:315[A]:CYS:HG	1:A:351:PHE:HE2	1.63	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
1:C:351:PHE:N	1:C:351:PHE:CD1	2.89	0.40
4:F:14:TYR:OH	16:F:506:HOH:O	2.21	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)
16:A:665:HOH:O	16:C:677:HOH:O[3_554]	1.70	0.50

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	449/451 (100%)	437 (97%)	10 (2%)	2 (0%)	30	38
1	C	447/451 (99%)	434 (97%)	12 (3%)	1 (0%)	43	55
2	B	428/445 (96%)	414 (97%)	12 (3%)	2 (0%)	24	31
2	D	416/445 (94%)	407 (98%)	8 (2%)	1 (0%)	43	55
3	E	119/152 (78%)	118 (99%)	1 (1%)	0	100	100
4	F	296/388 (76%)	288 (97%)	6 (2%)	2 (1%)	18	23
All	All	2155/2332 (92%)	2098 (97%)	49 (2%)	8 (0%)	30	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA
2	D	73	GLY
4	F	92	THR
4	F	255	ARG
1	A	178	SER
2	B	177	VAL
1	C	178	SER
2	B	360	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/379 (101%)	367 (96%)	15 (4%)	28	43
1	C	380/379 (100%)	375 (99%)	5 (1%)	61	77
2	B	377/383 (98%)	365 (97%)	12 (3%)	34	51
2	D	367/383 (96%)	358 (98%)	9 (2%)	42	60
3	E	111/136 (82%)	109 (98%)	2 (2%)	51	70
4	F	285/346 (82%)	270 (95%)	15 (5%)	20	30
All	All	1902/2006 (95%)	1844 (97%)	58 (3%)	35	53

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	71	GLU
1	A	84	ARG
1	A	96	LYS
1	A	112	LYS
1	A	113	GLU
1	A	188	ILE
1	A	220	GLU
1	A	232	SER
1	A	234	ILE
1	A	282	TYR
1	A	326	LYS
1	A	336	LYS
1	A	381	THR
1	A	430	LYS
2	B	42	LEU
2	B	85	GLN
2	B	232	SER
2	B	238	VAL
2	B	247	GLN
2	B	248	LEU
2	B	255	LEU
2	B	259	MET
2	B	282	GLN
2	B	293	GLN
2	B	325	MET
2	B	430	SER

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Mol	Chain	Res	Type
1	C	71	GLU
1	C	336	LYS
1	C	361	THR
1	C	384	ILE
1	C	430	LYS
2	D	1	MET
2	D	35	SER
2	D	50	ASN
2	D	80	SER
2	D	248	LEU
2	D	259	MET
2	D	318	ILE
2	D	345	GLU
2	D	422	GLU
3	E	89	GLU
3	E	139	LEU
4	F	44	ARG
4	F	45	ASN
4	F	73	ARG
4	F	86	GLU
4	F	87	LEU
4	F	88	SER
4	F	92	THR
4	F	100	ILE
4	F	128	ARG
4	F	169	LEU
4	F	193	GLU
4	F	222	ARG
4	F	230	SER
4	F	248	GLU
4	F	377	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	88	HIS
1	A	283	HIS
2	B	101	ASN
2	B	136	GLN
2	B	436	GLN
1	C	85	GLN

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Mol	Chain	Res	Type
2	D	11	GLN
2	D	37	HIS
2	D	426	ASN
3	E	12	ASN
3	E	136	ASN
4	F	196	HIS
4	F	269	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 11 are monoatomic - leaving 19 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	NV4	D	507	-	38,40,40	1.98	9 (23%)	52,59,59	2.82	19 (36%)
5	GTP	C	502	6	33,34,34	1.16	3 (9%)	50,54,54	1.59	9 (18%)
8	IMD	A	505	-	5,5,5	0.56	0	5,5,5	0.66	0
12	MES	B	504	-	12,12,12	2.14	1 (8%)	15,16,16	2.10	4 (26%)
7	GOL	D	504	-	5,5,5	0.34	0	5,5,5	0.86	0
10	GDP	B	501	6	29,30,30	1.38	5 (17%)	45,47,47	1.89	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	IMD	C	508	-	5,5,5	0.80	0	5,5,5	0.41	0
7	GOL	C	501	-	5,5,5	0.37	0	5,5,5	0.42	0
14	PEG	C	505	-	6,6,6	0.52	0	5,5,5	0.40	0
7	GOL	D	505	-	5,5,5	0.36	0	5,5,5	0.54	0
7	GOL	C	509	-	5,5,5	0.41	0	5,5,5	0.54	0
7	GOL	A	507	-	5,5,5	0.35	0	5,5,5	0.26	0
5	GTP	A	501	6	33,34,34	0.79	0	50,54,54	1.63	13 (26%)
10	GDP	D	501	6	29,30,30	1.20	3 (10%)	45,47,47	1.72	6 (13%)
7	GOL	C	504	-	5,5,5	0.41	0	5,5,5	0.24	0
7	GOL	D	506	-	5,5,5	0.40	0	5,5,5	0.80	0
7	GOL	A	504	-	5,5,5	0.45	0	5,5,5	0.49	0
15	ACP	F	402	6	31,33,33	3.53	12 (38%)	47,52,52	2.20	13 (27%)
13	NV4	B	505	-	38,40,40	2.02	9 (23%)	52,59,59	2.58	15 (28%)

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	NV4	D	507	-	-	4/14/49/49	0/6/6/6
5	GTP	C	502	6	-	7/22/38/38	0/3/3/3
8	IMD	A	505	-	-	-	0/1/1/1
12	MES	B	504	-	-	1/6/14/14	0/1/1/1
7	GOL	D	504	-	-	2/4/4/4	-
10	GDP	B	501	6	-	5/16/32/32	0/3/3/3
8	IMD	C	508	-	-	-	0/1/1/1
7	GOL	C	501	-	-	2/4/4/4	-
14	PEG	C	505	-	-	1/4/4/4	-
7	GOL	D	505	-	-	3/4/4/4	-
7	GOL	C	509	-	-	2/4/4/4	-
7	GOL	A	507	-	-	3/4/4/4	-
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
10	GDP	D	501	6	-	5/16/32/32	0/3/3/3
7	GOL	C	504	-	-	1/4/4/4	-
7	GOL	D	506	-	-	2/4/4/4	-
7	GOL	A	504	-	-	4/4/4/4	-
15	ACP	F	402	6	-	8/19/38/38	0/3/3/3
13	NV4	B	505	-	-	2/14/49/49	0/6/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	402	ACP	O4'-C1'	8.69	1.62	1.42
15	F	402	ACP	PB-O3A	7.86	1.67	1.58
15	F	402	ACP	C6-N6	7.52	1.53	1.34
12	B	504	MES	C8-S	-7.27	1.67	1.77
15	F	402	ACP	O4'-C4'	-7.15	1.29	1.45
15	F	402	ACP	C2'-C1'	-7.08	1.31	1.53
13	B	505	NV4	C1-C2	5.93	1.50	1.40
13	D	507	NV4	C1-C2	5.77	1.50	1.40
13	B	505	NV4	O14-C13	5.10	1.46	1.35
13	B	505	NV4	C3-S30	-4.90	1.78	1.83
13	D	507	NV4	C3-S30	-4.72	1.78	1.83
15	F	402	ACP	PA-O3A	4.42	1.64	1.59
13	D	507	NV4	O14-C13	4.38	1.44	1.35
13	D	507	NV4	C9-C10	4.12	1.49	1.41
13	D	507	NV4	C11-C10	3.99	1.49	1.41
13	B	505	NV4	C11-C10	3.91	1.49	1.41
15	F	402	ACP	O2'-C2'	3.52	1.51	1.43
13	B	505	NV4	C9-C10	3.51	1.48	1.41
10	D	501	GDP	C5-C4	3.16	1.47	1.38
15	F	402	ACP	PB-O2B	-3.13	1.48	1.56
5	C	502	GTP	PB-O3A	-3.12	1.56	1.59
13	B	505	NV4	O25-C10	2.98	1.43	1.38
13	D	507	NV4	O25-C10	2.87	1.43	1.38
10	B	501	GDP	PA-O3A	2.86	1.62	1.59
10	B	501	GDP	C6-N1	-2.81	1.33	1.38
15	F	402	ACP	C5-N7	-2.74	1.34	1.39
5	C	502	GTP	C2-N3	2.73	1.39	1.33
13	B	505	NV4	C19-C18	2.70	1.45	1.39
10	B	501	GDP	C5-C4	2.67	1.46	1.38
15	F	402	ACP	O3'-C3'	-2.57	1.36	1.43
10	B	501	GDP	PB-O2B	-2.54	1.45	1.54
10	B	501	GDP	C5-N7	-2.52	1.34	1.39
13	D	507	NV4	C19-C18	2.51	1.45	1.39
5	C	502	GTP	PA-O3A	2.50	1.62	1.59
10	D	501	GDP	C6-N1	-2.40	1.34	1.38
13	D	507	NV4	C31-N32	2.35	1.34	1.31
10	D	501	GDP	PA-O3A	2.26	1.61	1.59
13	B	505	NV4	C31-N32	2.12	1.34	1.31
13	B	505	NV4	C1-C6	-2.08	1.48	1.51
15	F	402	ACP	C8-N7	2.04	1.35	1.31
13	D	507	NV4	C7-C6	-2.03	1.50	1.52
15	F	402	ACP	C2-N3	2.01	1.37	1.33

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	505	NV4	C31-N32-N33	-10.59	102.62	111.43
13	D	507	NV4	C31-N32-N33	-10.00	103.11	111.43
13	D	507	NV4	C9-C10-C11	-6.98	112.76	119.56
13	D	507	NV4	O25-C10-C11	-6.66	110.58	120.12
15	F	402	ACP	N6-C6-N1	-6.44	104.03	118.38
13	B	505	NV4	C9-C10-C11	-6.42	113.31	119.56
10	B	501	GDP	C5-C4-N3	-6.20	118.52	128.39
12	B	504	MES	C5-N4-C3	6.07	121.92	108.84
10	D	501	GDP	C5-C4-N3	-5.74	119.26	128.39
10	B	501	GDP	C2-N3-C4	5.36	121.54	112.30
15	F	402	ACP	C5-C4-N3	-5.31	119.40	126.72
15	F	402	ACP	C5-C6-N6	5.27	136.33	123.29
15	F	402	ACP	N3-C2-N1	-5.23	120.66	128.58
13	B	505	NV4	C7-C6-C5	5.12	121.95	113.22
5	A	501	GTP	C2-N3-C4	4.97	120.85	112.30
5	C	502	GTP	C5-C4-N3	-4.90	120.59	128.39
10	B	501	GDP	N9-C4-N3	4.76	135.47	125.95
13	D	507	NV4	O25-C10-C9	-4.74	113.33	120.12
10	D	501	GDP	C2-N3-C4	4.65	120.30	112.30
13	D	507	NV4	C15-C4-C5	4.65	108.94	101.73
13	B	505	NV4	O25-C10-C9	-4.44	113.75	120.12
10	D	501	GDP	N9-C4-N3	4.41	134.77	125.95
5	C	502	GTP	C2-N3-C4	4.39	119.86	112.30
5	A	501	GTP	C5-C4-N3	-4.38	121.42	128.39
13	D	507	NV4	C3-C4-C5	4.23	119.87	111.69
13	B	505	NV4	C15-C4-C5	4.19	108.23	101.73
13	B	505	NV4	C4-C5-C6	3.99	120.94	113.15
13	D	507	NV4	C27-O24-C9	3.95	123.31	117.51
13	D	507	NV4	C4-C5-C6	3.87	120.69	113.15
15	F	402	ACP	N9-C8-N7	-3.85	108.48	113.94
13	B	505	NV4	O16-C13-C5	-3.81	124.54	129.38
10	D	501	GDP	C6-C5-N7	3.48	136.63	130.29
13	B	505	NV4	C3-C4-C5	3.36	118.18	111.69
13	D	507	NV4	O16-C13-C5	-3.31	125.17	129.38
13	D	507	NV4	C1-C6-C5	3.30	112.00	106.57
15	F	402	ACP	C2-N3-C4	3.26	119.80	111.83
13	D	507	NV4	C22-O23-C19	3.19	109.59	105.32
13	D	507	NV4	C2-C1-C6	3.17	122.62	114.39
12	B	504	MES	O1S-S-C8	3.09	111.40	106.73
10	B	501	GDP	C6-C5-N7	3.08	135.90	130.29
10	B	501	GDP	O6-C6-C5	-3.02	118.57	126.53
5	C	502	GTP	N9-C4-N3	2.95	131.85	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	402	ACP	C5-N7-C8	2.95	108.08	103.45
13	B	505	NV4	C2-C1-C6	2.95	122.04	114.39
13	B	505	NV4	C22-O23-C19	2.94	109.26	105.32
5	C	502	GTP	N9-C8-N7	-2.94	107.94	113.40
15	F	402	ACP	N3-C4-N9	2.92	132.14	127.17
13	D	507	NV4	C12-C11-C10	2.90	123.45	120.22
15	F	402	ACP	PB-O3A-PA	-2.84	123.09	132.37
5	C	502	GTP	C8-N7-C5	2.83	109.31	104.26
15	F	402	ACP	C3'-C2'-C1'	2.80	106.77	101.46
13	B	505	NV4	C22-O21-C18	2.77	109.02	105.32
13	D	507	NV4	C22-O21-C18	2.72	108.97	105.32
13	D	507	NV4	O24-C9-C10	2.71	119.78	115.14
15	F	402	ACP	C4-C5-N7	-2.67	107.52	110.58
13	B	505	NV4	O14-C13-O16	2.64	124.24	121.43
5	A	501	GTP	N9-C8-N7	-2.62	108.55	113.40
5	C	502	GTP	C2-N1-C6	-2.61	120.38	125.11
5	C	502	GTP	C5-C6-N1	2.60	119.87	113.25
13	D	507	NV4	C9-C8-C7	2.55	123.80	119.86
15	F	402	ACP	C6-C5-C4	2.55	120.65	117.18
5	A	501	GTP	N1-C2-N3	-2.52	118.70	123.32
13	B	505	NV4	O26-C11-C12	-2.52	119.74	124.08
5	A	501	GTP	C5'-C4'-C3'	-2.51	106.18	115.21
5	A	501	GTP	C8-N7-C5	2.51	108.73	104.26
5	A	501	GTP	C4-C5-N7	-2.48	106.74	110.67
10	D	501	GDP	C4-C5-N7	-2.47	106.76	110.67
15	F	402	ACP	C5-C4-N9	2.43	108.46	105.81
5	A	501	GTP	N2-C2-N1	2.42	121.86	116.76
13	D	507	NV4	O24-C9-C8	-2.42	119.92	124.08
10	B	501	GDP	C4-C5-N7	-2.39	106.89	110.67
5	A	501	GTP	C6-C5-N7	2.38	134.61	130.29
13	D	507	NV4	O26-C11-C12	-2.36	120.01	124.08
13	D	507	NV4	C29-O26-C11	2.33	120.93	117.51
5	A	501	GTP	O2B-PB-O3A	2.27	113.40	107.27
12	B	504	MES	O2S-S-O1S	-2.26	106.48	113.82
5	C	502	GTP	O2B-PB-O3A	2.12	113.01	107.27
5	A	501	GTP	O2A-PA-O3A	2.12	113.00	107.27
5	A	501	GTP	N9-C4-N3	2.11	130.17	125.95
10	B	501	GDP	C8-N7-C5	2.08	107.97	104.26
10	B	501	GDP	C5-C6-N1	2.07	118.53	113.25
5	A	501	GTP	O3A-PA-O1A	-2.07	104.49	110.70
13	B	505	NV4	C29-O26-C11	2.06	120.53	117.51
10	D	501	GDP	C5-C6-N1	2.06	118.49	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	505	NV4	C27-O24-C9	2.05	120.52	117.51
5	C	502	GTP	O6-C6-C5	-2.03	121.17	126.53
12	B	504	MES	C2-C3-N4	2.02	113.19	110.12

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
7	A	507	GOL	O1-C1-C2-C3
7	D	504	GOL	O1-C1-C2-C3
10	B	501	GDP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O1A
13	B	505	NV4	N32-C31-S30-C3
13	D	507	NV4	N32-C31-S30-C3
15	F	402	ACP	PB-C3B-PG-O1G
15	F	402	ACP	PB-C3B-PG-O2G
15	F	402	ACP	PB-C3B-PG-O3G
15	F	402	ACP	PG-C3B-PB-O1B
15	F	402	ACP	PG-C3B-PB-O3A
15	F	402	ACP	O4'-C4'-C5'-O5'
13	D	507	NV4	C10-C9-O24-C27
13	D	507	NV4	C11-C10-O25-C28
13	D	507	NV4	C8-C9-O24-C27
7	A	504	GOL	O2-C2-C3-O3
15	F	402	ACP	C3'-C4'-C5'-O5'
7	A	504	GOL	O1-C1-C2-C3
7	A	504	GOL	C1-C2-C3-O3
7	C	501	GOL	O1-C1-C2-C3
7	C	509	GOL	C1-C2-C3-O3
7	D	505	GOL	C1-C2-C3-O3
7	D	506	GOL	C1-C2-C3-O3
7	A	504	GOL	O1-C1-C2-O2
7	A	507	GOL	O1-C1-C2-O2

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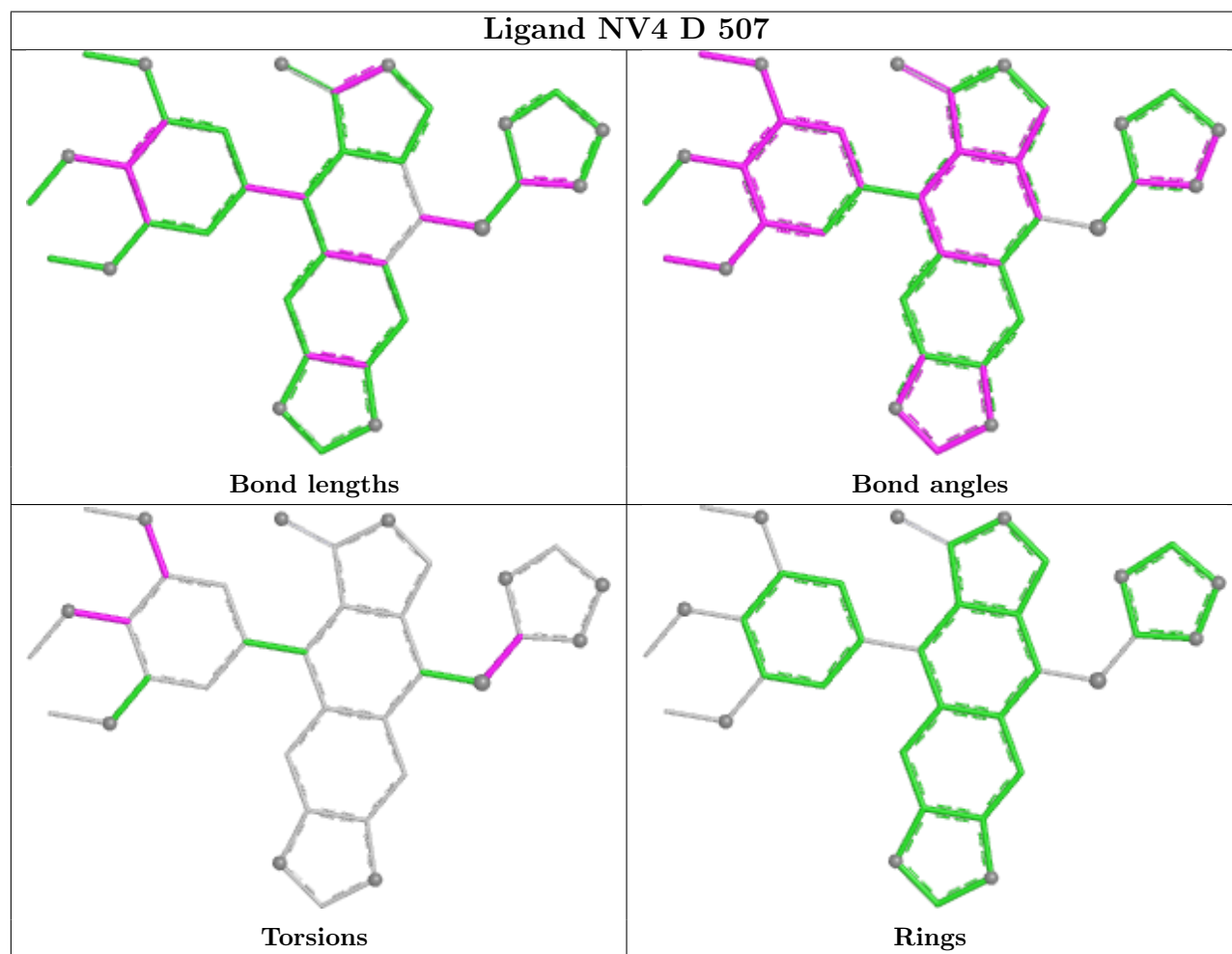
Mol	Chain	Res	Type	Atoms
7	C	509	GOL	O2-C2-C3-O3
7	D	504	GOL	O1-C1-C2-O2
12	B	504	MES	C8-C7-N4-C3
7	C	501	GOL	O1-C1-C2-O2
7	D	506	GOL	O2-C2-C3-O3
13	B	505	NV4	C11-C10-O25-C28
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O2A
15	F	402	ACP	PG-C3B-PB-O2B
7	D	505	GOL	O1-C1-C2-C3
5	A	501	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O2A
5	C	502	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
7	A	507	GOL	C1-C2-C3-O3
7	C	504	GOL	O2-C2-C3-O3
10	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O3G
5	C	502	GTP	PB-O3A-PA-O1A
5	C	502	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O1A
14	C	505	PEG	O1-C1-C2-O2
7	D	505	GOL	O2-C2-C3-O3
5	A	501	GTP	PB-O3A-PA-O1A
10	B	501	GDP	PB-O3A-PA-O1A

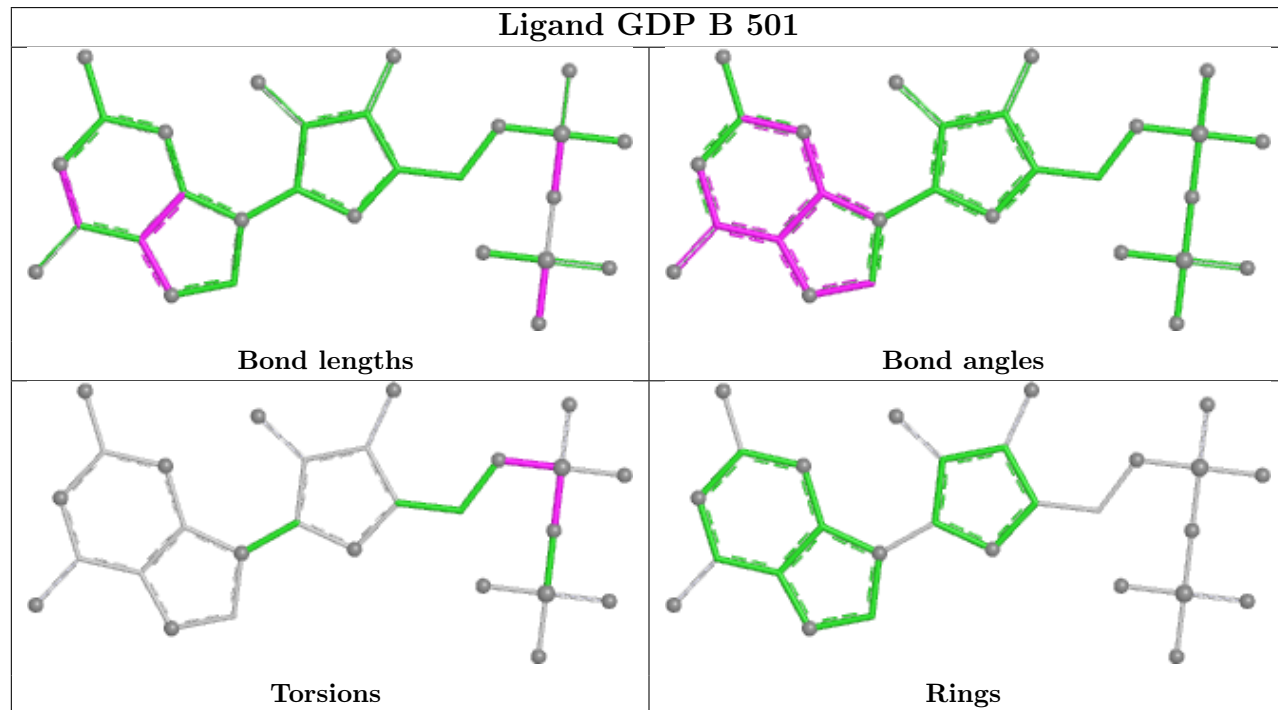
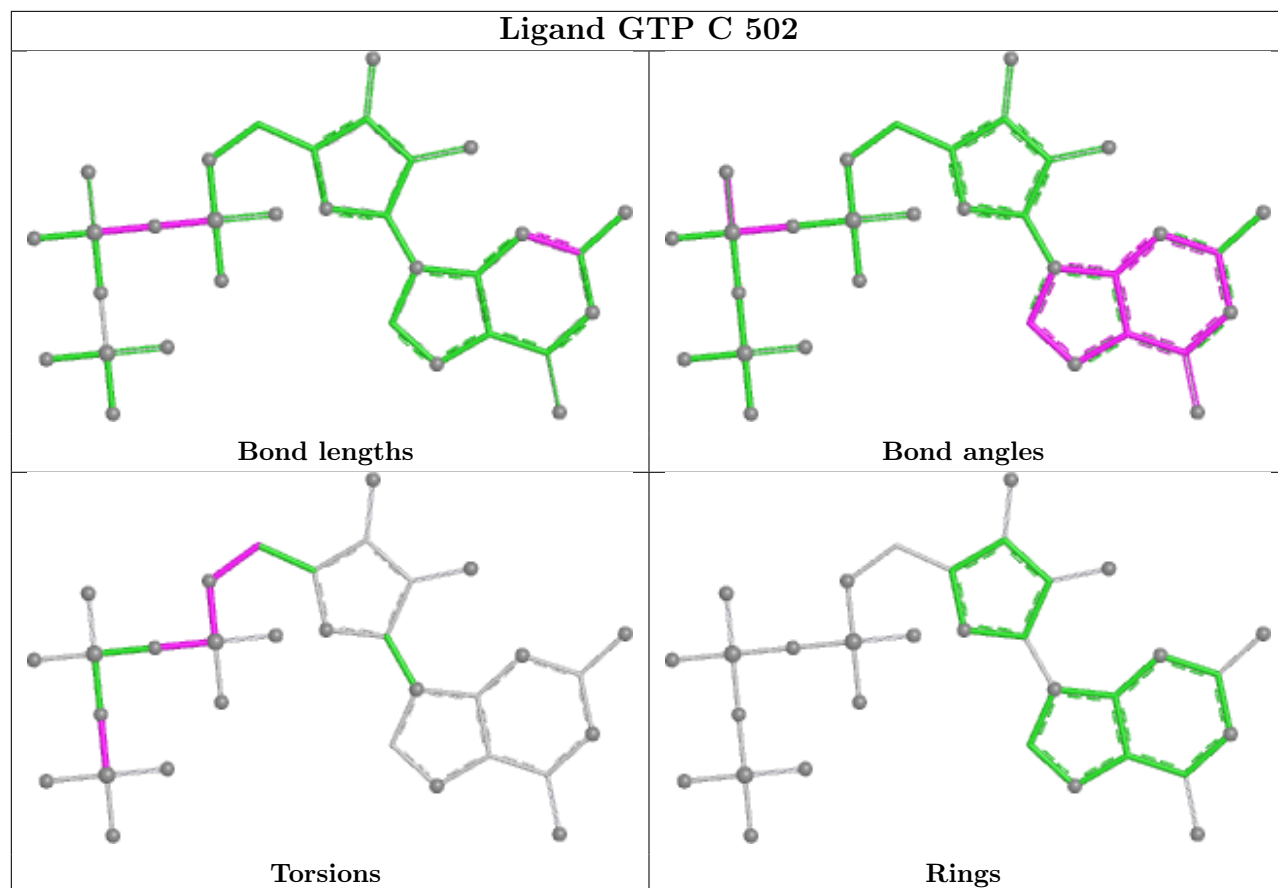
There are no ring outliers.

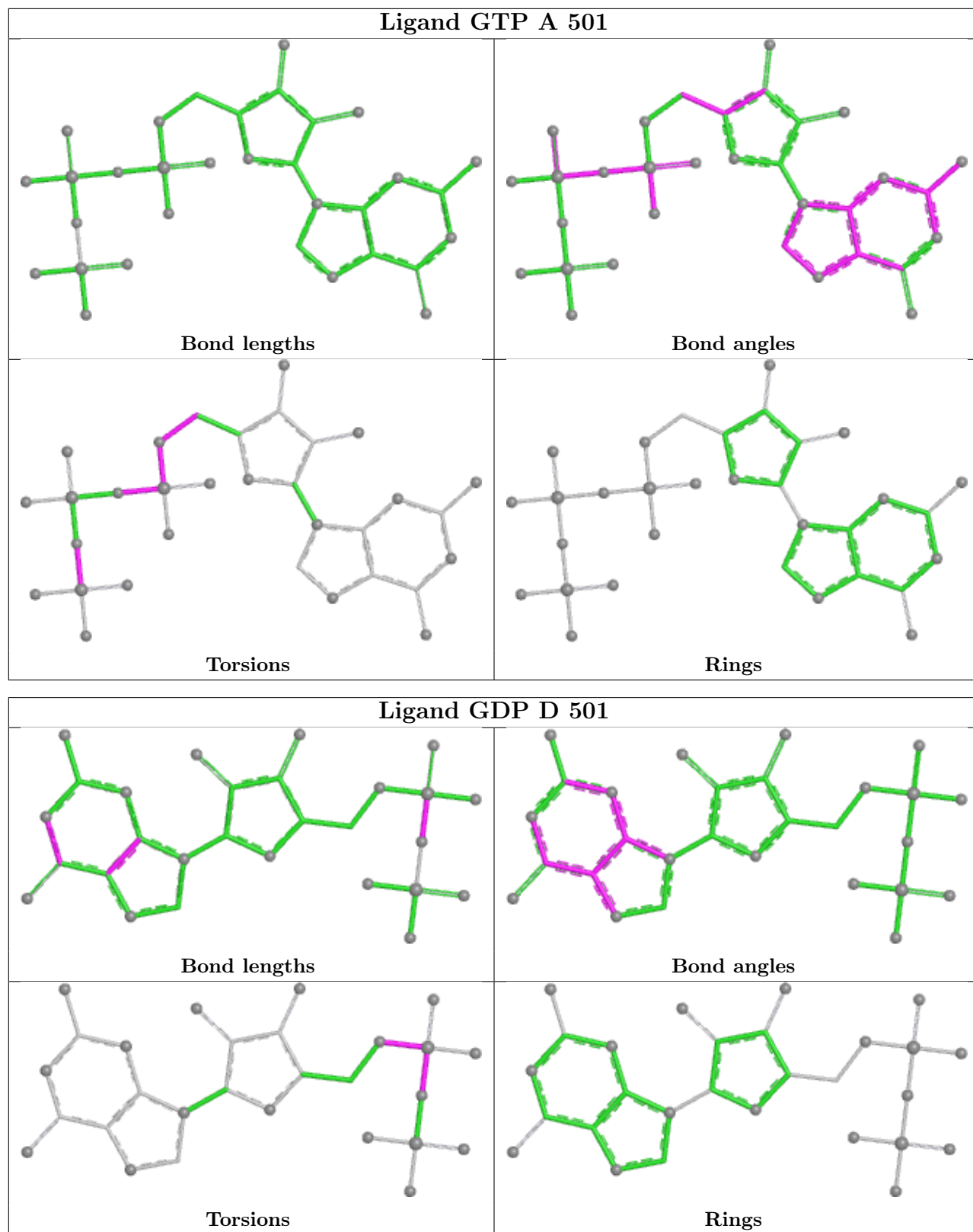
10 monomers are involved in 35 short contacts:

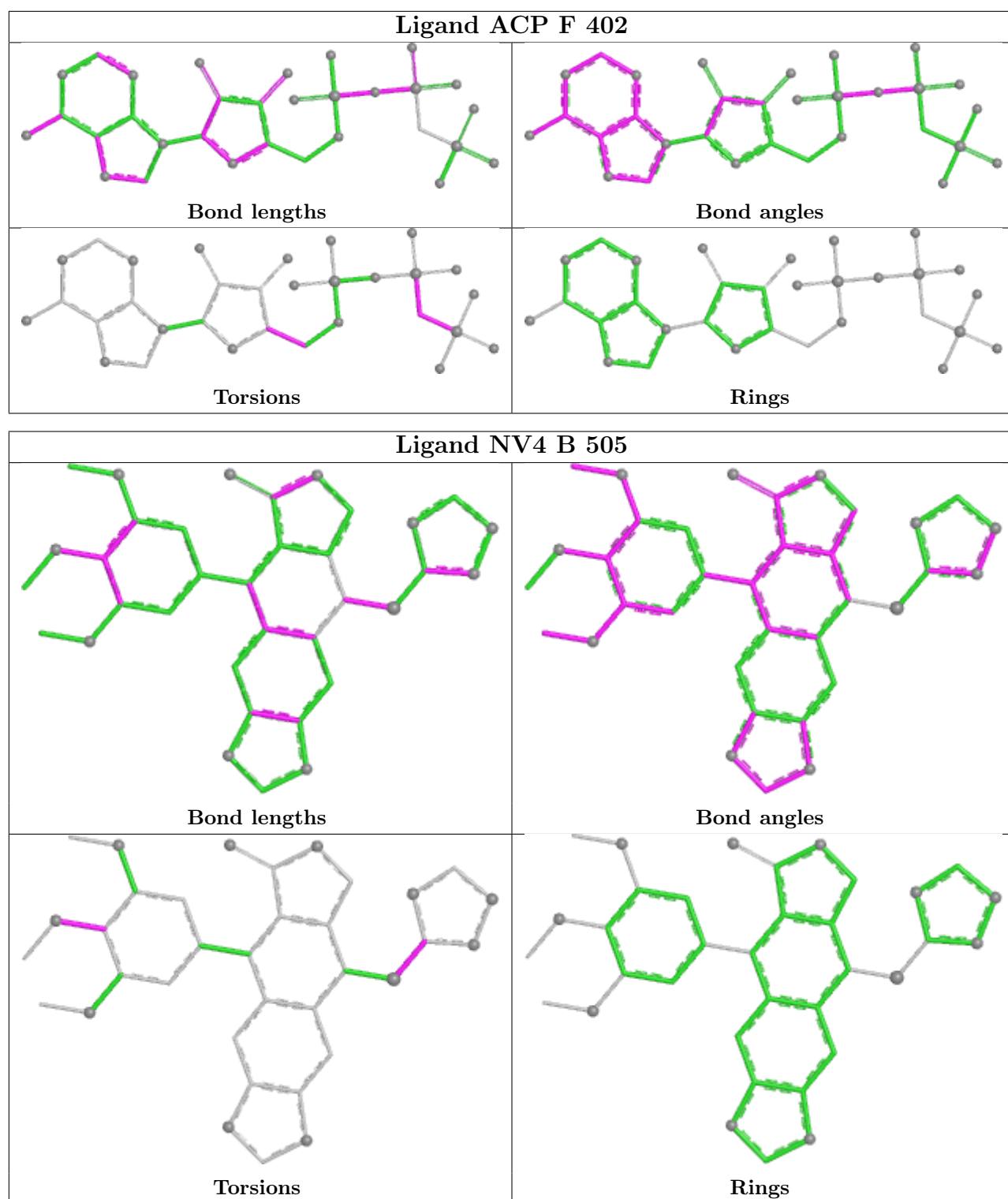
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	507	NV4	9	0
8	A	505	IMD	4	0
7	C	501	GOL	5	0
7	A	507	GOL	1	0
10	D	501	GDP	1	0
7	C	504	GOL	6	0
7	D	506	GOL	2	0
7	A	504	GOL	1	0
15	F	402	ACP	3	0
13	B	505	NV4	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	-0.07	12 (2%)	56	58	18, 41, 75, 126	12 (2%)
1	C	440/451 (97%)	-0.35	13 (2%)	52	54	16, 31, 61, 98	9 (2%)
2	B	423/445 (95%)	0.11	19 (4%)	38	40	15, 40, 80, 114	12 (2%)
2	D	418/445 (93%)	0.21	25 (5%)	27	29	21, 48, 84, 126	7 (1%)
3	E	121/152 (79%)	0.33	9 (7%)	20	22	20, 53, 90, 106	2 (1%)
4	F	312/388 (80%)	0.87	52 (16%)	4	5	26, 61, 113, 144	4 (1%)
All	All	2153/2332 (92%)	0.12	130 (6%)	27	29	15, 44, 87, 144	46 (2%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	253	TYR	6.3
1	A	282	TYR	5.2
4	F	173	ILE	5.1
2	D	180	THR	5.0
4	F	169	LEU	4.9
4	F	151	SER	4.9
4	F	102	PRO	4.8
4	F	249	TYR	4.6
2	D	179	ASP	4.5
4	F	181	VAL	4.4
2	B	285	ALA	4.3
2	D	1	MET	4.3
4	F	236	LYS	4.3
2	D	248	LEU	4.3
4	F	100	ILE	4.2
2	B	438	ALA	4.0
4	F	162	ILE	4.0
1	C	178	SER	4.0
4	F	134	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	407	TRP	3.9
4	F	231	ALA	3.8
2	D	57	THR	3.8
1	A	438	ASP	3.7
4	F	91	CYS	3.7
4	F	132	LEU	3.7
4	F	88	SER	3.6
2	B	58	GLY	3.6
2	B	337	ASN	3.6
4	F	166	ALA	3.4
4	F	136	ASN	3.4
4	F	131	PHE	3.3
2	B	280	SER	3.1
4	F	126	ASP	3.1
2	B	277	SER	3.1
1	C	340	SER	3.1
4	F	255	ARG	3.0
4	F	170	LEU	3.0
4	F	172	PHE	2.9
2	B	247	GLN	2.9
2	D	94	PHE	2.9
2	B	345	GLU	2.9
2	D	416	MET	2.9
4	F	144	GLY	2.9
1	A	221	ARG	2.9
4	F	180	HIS	2.9
4	F	238	CYS	2.9
4	F	244	CYS	2.9
2	B	325	MET	2.9
4	F	247	LYS	2.8
2	B	340	SER	2.8
4	F	240	LEU	2.8
2	D	82	PRO	2.8
2	D	182	VAL	2.8
4	F	130	VAL	2.8
1	C	179	THR	2.8
3	E	28	SER	2.8
4	F	101	TYR	2.8
4	F	186	LEU	2.8
4	F	182	ILE	2.7
1	A	281	ALA	2.7
1	C	357	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	283	HIS	2.7
2	D	325	MET	2.7
2	D	178	SER	2.7
1	C	283	HIS	2.6
2	D	286	LEU	2.6
4	F	171	ASP	2.6
4	F	241	THR	2.6
4	F	306	HIS	2.6
3	E	45	PRO	2.6
1	A	262	TYR	2.6
2	D	441	ASP	2.5
4	F	198	LYS	2.5
2	B	338	LYS	2.5
1	A	309	HIS	2.5
1	C	285	GLN	2.5
2	D	60	LYS	2.4
2	D	221[A]	THR	2.4
2	D	83	PHE	2.4
3	E	141	GLU	2.4
2	D	128	SER	2.4
4	F	129	GLU	2.4
4	F	133	ALA	2.4
4	F	149	ALA	2.4
3	E	46	SER	2.4
4	F	128	ARG	2.4
1	A	439	SER	2.3
2	D	97	SER	2.3
1	C	177	VAL	2.3
1	A	70	LEU	2.3
4	F	259	GLY	2.3
2	B	298	SER	2.3
2	B	248	LEU	2.3
3	E	140	LYS	2.3
1	C	308	ARG	2.3
2	B	369	ARG	2.3
2	D	389	LYS	2.2
4	F	217	ARG	2.2
4	F	165	GLU	2.2
2	B	326	LYS	2.2
2	B	373	MET	2.2
1	C	365	GLY	2.2
2	B	35	SER	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	228	TYR	2.2
1	C	440	VAL	2.2
1	A	347	CYS	2.2
2	D	80	SER	2.2
1	C	293	ASN	2.1
1	A	77	GLU	2.1
1	C	309	HIS	2.1
4	F	239	HIS	2.1
3	E	49	GLU	2.1
4	F	242	ASN	2.1
4	F	150	LYS	2.1
1	C	46	ASP	2.1
2	B	249	ASN	2.1
2	D	414	ASP	2.1
4	F	254	GLY	2.1
3	E	6	MET	2.1
1	A	38	SER	2.0
4	F	11	SER	2.0
2	D	71	GLU	2.0
2	D	245	PRO	2.0
2	B	2	ARG	2.0
2	D	98	GLY	2.0
4	F	226	GLU	2.0
3	E	44	ASP	2.0
4	F	73	ARG	2.0
4	F	194	PRO	2.0
3	E	126	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

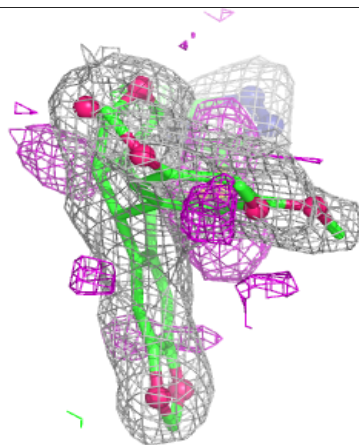
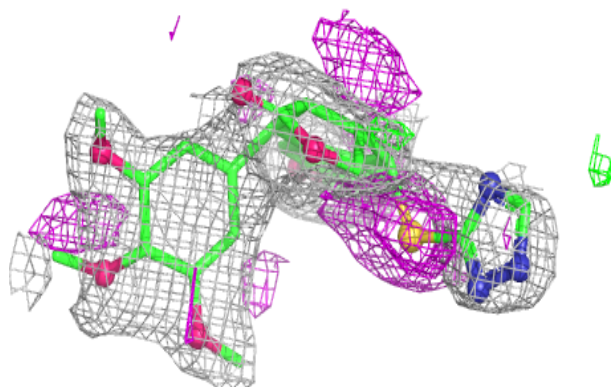
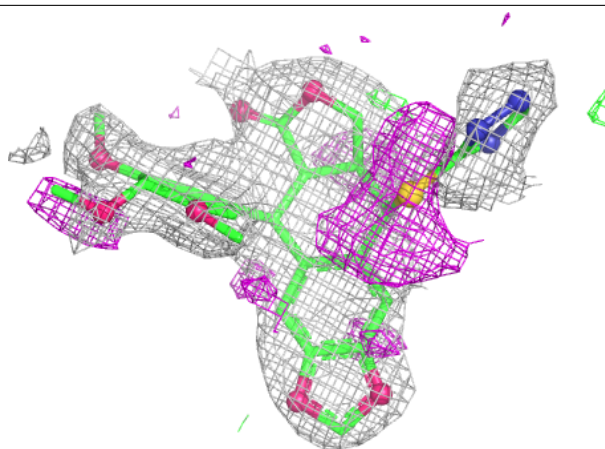
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	C	509	6/6	0.70	0.17	80,97,100,100	0
8	IMD	A	505	5/5	0.78	0.17	68,82,95,98	0
14	PEG	C	505	7/7	0.78	0.21	42,77,82,82	0
7	GOL	D	505	6/6	0.79	0.21	79,81,84,86	0
7	GOL	D	504	6/6	0.80	0.20	90,103,104,104	0
7	GOL	A	507	6/6	0.80	0.19	75,82,90,90	0
7	GOL	C	501	6/6	0.83	0.22	78,80,88,94	0
6	MG	A	502	1/1	0.83	0.10	40,40,40,40	0
9	CA	C	507	1/1	0.84	0.14	105,105,105,105	0
7	GOL	A	504	6/6	0.85	0.18	47,68,71,76	0
6	MG	D	502	1/1	0.86	0.14	52,52,52,52	0
7	GOL	C	504	6/6	0.86	0.16	67,70,83,84	0
13	NV4	D	507	35/35	0.87	0.16	41,64,88,100	0
8	IMD	C	508	5/5	0.87	0.16	38,48,56,56	0
15	ACP	F	402	31/31	0.88	0.12	51,78,113,122	0
7	GOL	D	506	6/6	0.89	0.15	54,62,67,68	0
6	MG	C	503	1/1	0.90	0.06	27,27,27,27	0
6	MG	F	401	1/1	0.91	0.11	75,75,75,75	0
11	NA	B	503	1/1	0.92	0.20	78,78,78,78	0
13	NV4	B	505	35/35	0.94	0.09	30,41,78,92	0
6	MG	D	503	1/1	0.95	0.17	60,60,60,60	0
6	MG	A	503	1/1	0.95	0.09	74,74,74,74	0
12	MES	B	504	12/12	0.96	0.08	35,41,56,59	0
6	MG	B	502	1/1	0.97	0.10	20,20,20,20	0
10	GDP	D	501	28/28	0.97	0.07	40,47,51,59	0
11	NA	C	506	1/1	0.98	0.10	27,27,27,27	0
5	GTP	A	501	32/32	0.98	0.06	23,31,45,46	0
5	GTP	C	502	32/32	0.99	0.04	21,24,32,36	0
10	GDP	B	501	28/28	0.99	0.04	17,28,33,35	0
9	CA	A	506	1/1	1.00	0.03	53,53,53,53	0

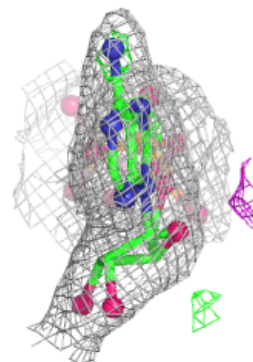
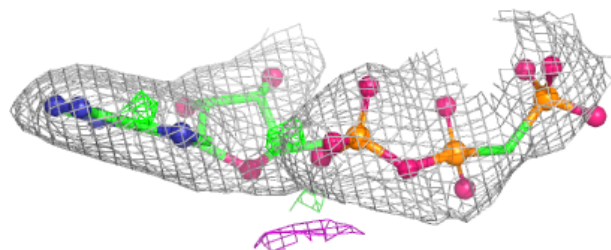
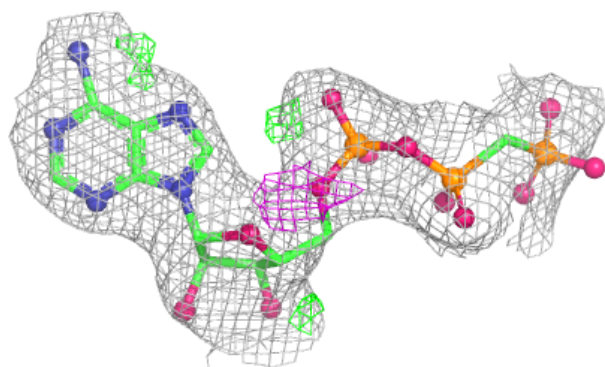
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NV4 D 507:

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

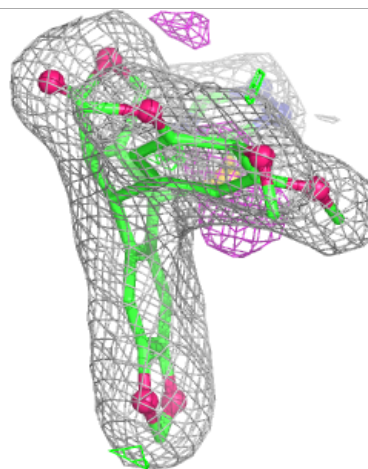
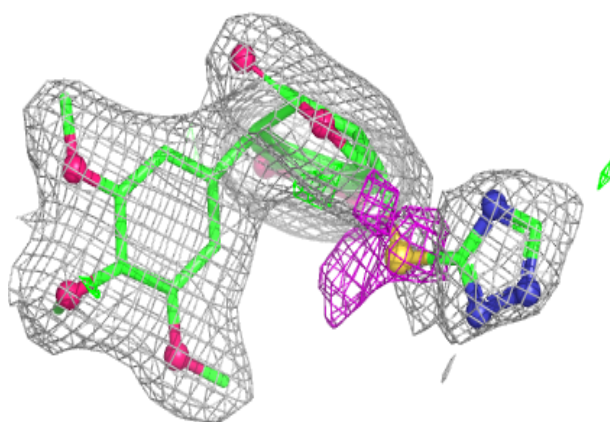
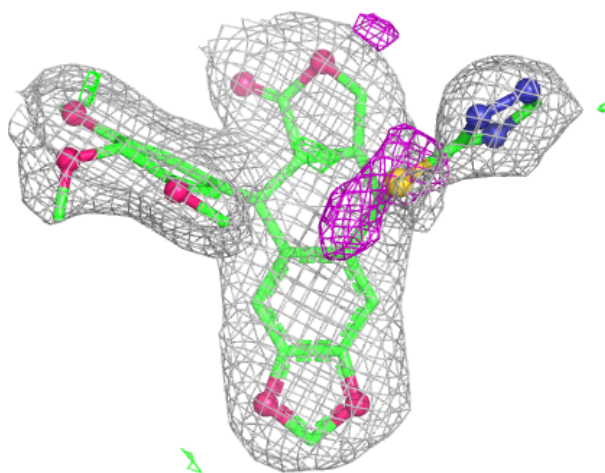
**Electron density around ACP F 402:**

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



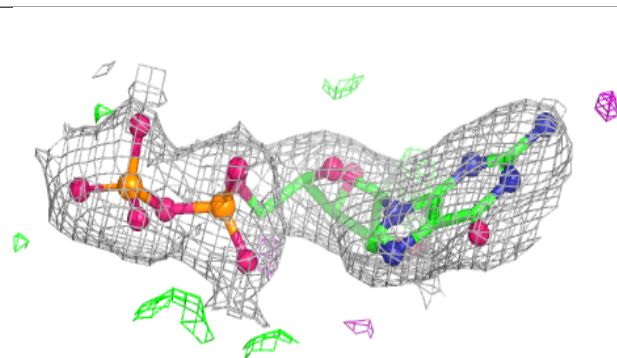
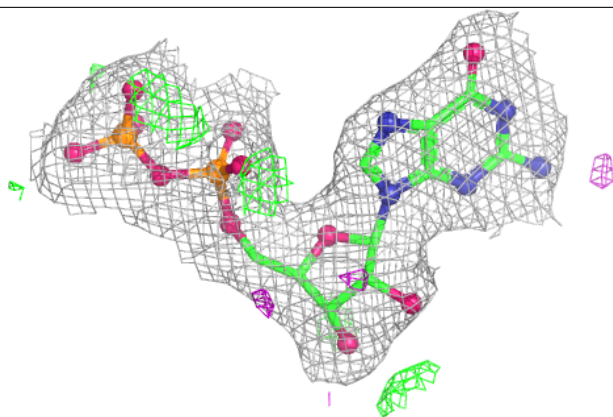
Electron density around NV4 B 505:

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

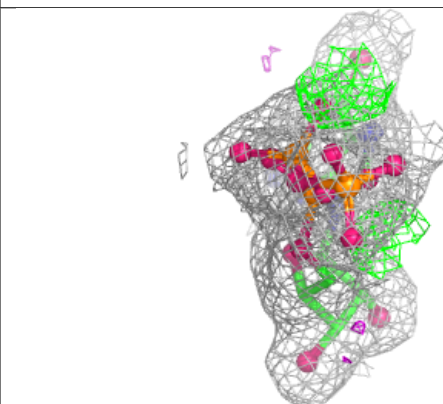
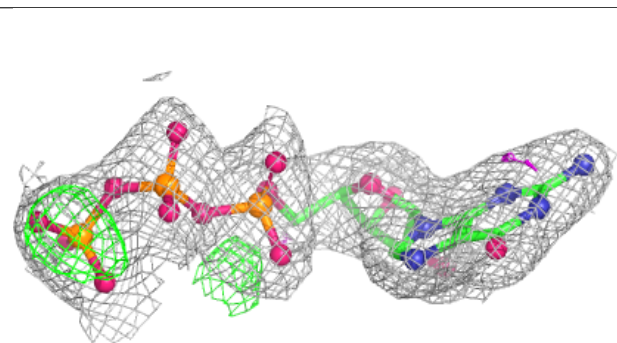
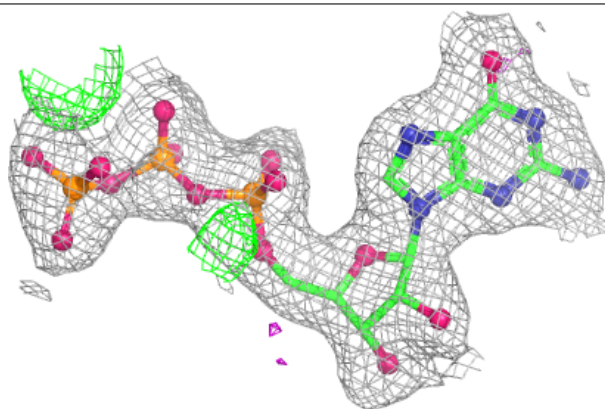


Electron density around GDP D 501:

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

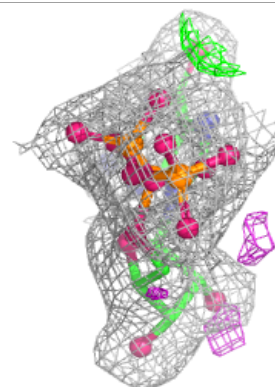
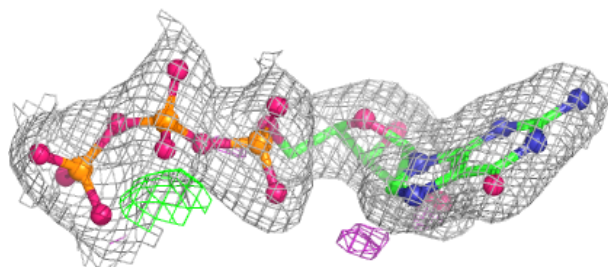
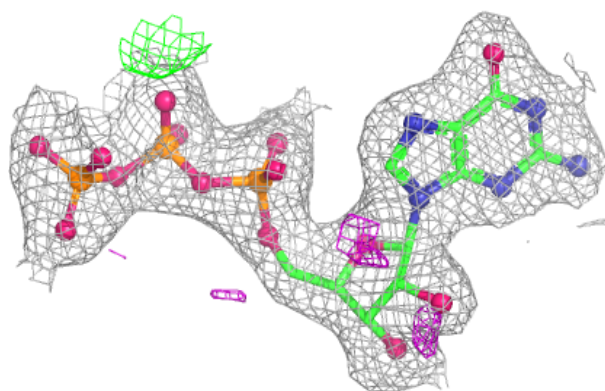
**Electron density around GTP A 501:**

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

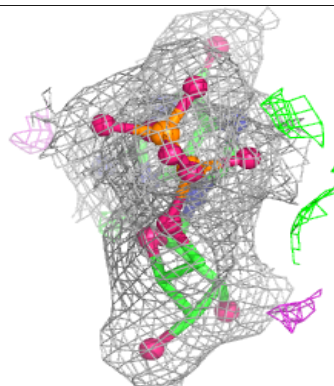
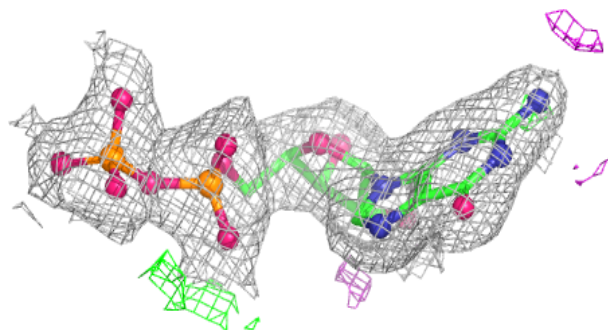
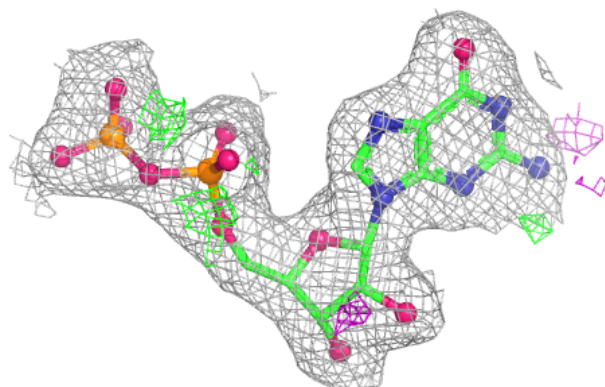


Electron density around GTP C 502:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.