



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:22 AM UTC

PDB ID : 8WMO / pdb_00008wmo
Title : Crystal structure analysis of tubulin and heterocyclic podophyllotoxins complex for anticancer agents
Authors : Zhao, W.; Bi, J.
Deposited on : 2023-10-04
Resolution : 2.89 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:

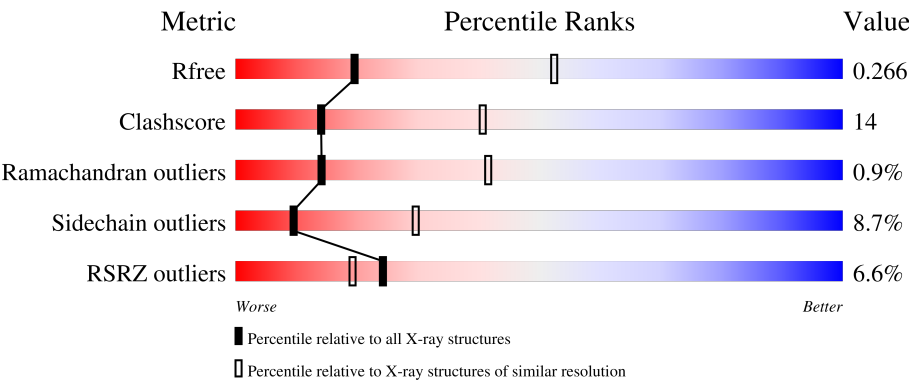
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	440	10% 66% 28% 5%
1	C	440	3% 68% 29%
2	B	445	4% 60% 32% 5%
2	D	445	10% 64% 27% 6%
3	E	138	2% 59% 27% 13%

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Mol	Chain	Length	Quality of chain
4	F	381	7% 54% 26% • 17%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 16707 atoms, of which 0 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3244	2061	540	622	21			
1	C	440	Total	C	N	O	S	0	0	0
			3363	2132	566	643	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3243	2040	543	636	24			
2	D	419	Total	C	N	O	S	0	0	0
			3162	1990	528	620	24			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			938	577	171	186	4			

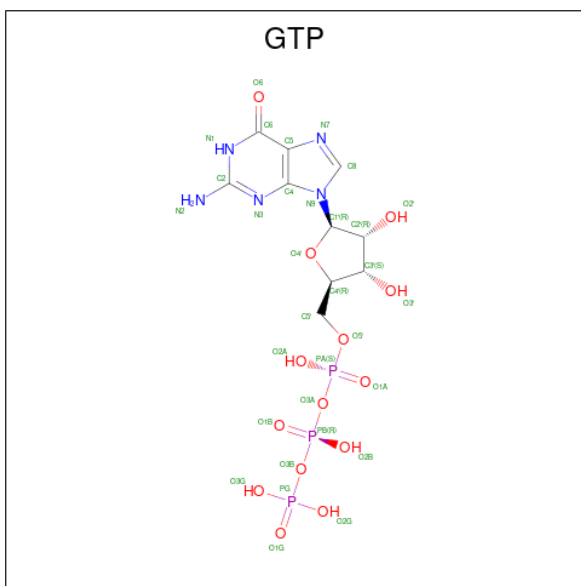
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	0	0
			2479	1589	418	458	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1
F	381	HIS	-	expression tag	UNP A0A8C9FGJ1

- 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		
5	D	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	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



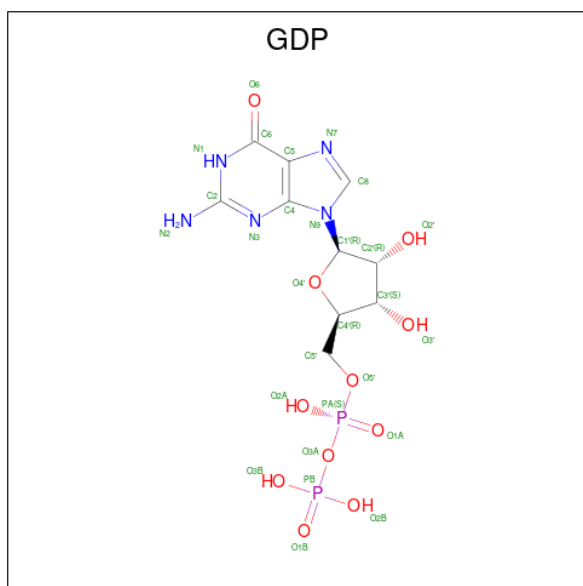
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



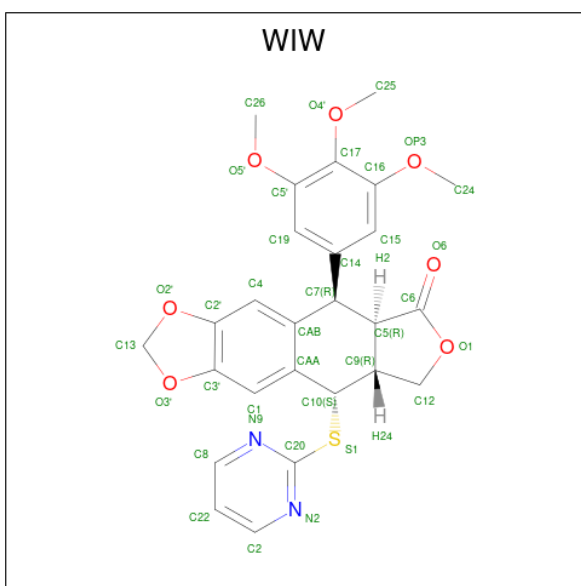
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



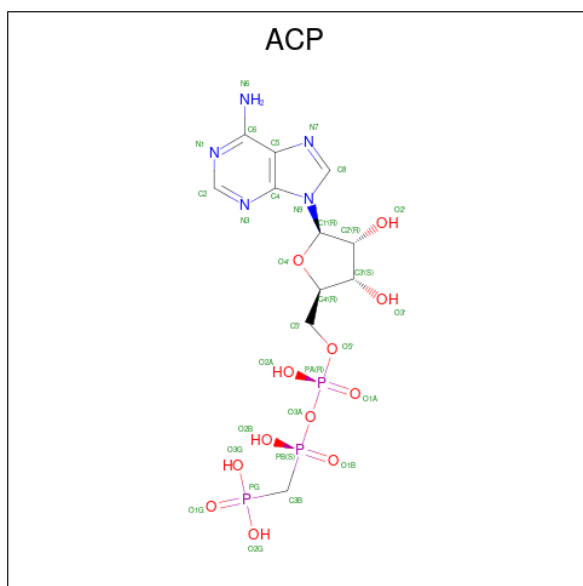
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (5 {S},5 {a} {R},8 {a} {R},9 {R})-5-pyrimidin-2-ylsulfanyl-9-(3,4,5-trimethoxyphenyl)-5 {a},6,8 {a},9-tetrahydro-5 {H}-[2]benzofuro[5,6-f][1,3]benzodioxol-8-one (CCD ID: WIW) (formula: C₂₆H₂₄N₂O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total Ca 1 1	0	0

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

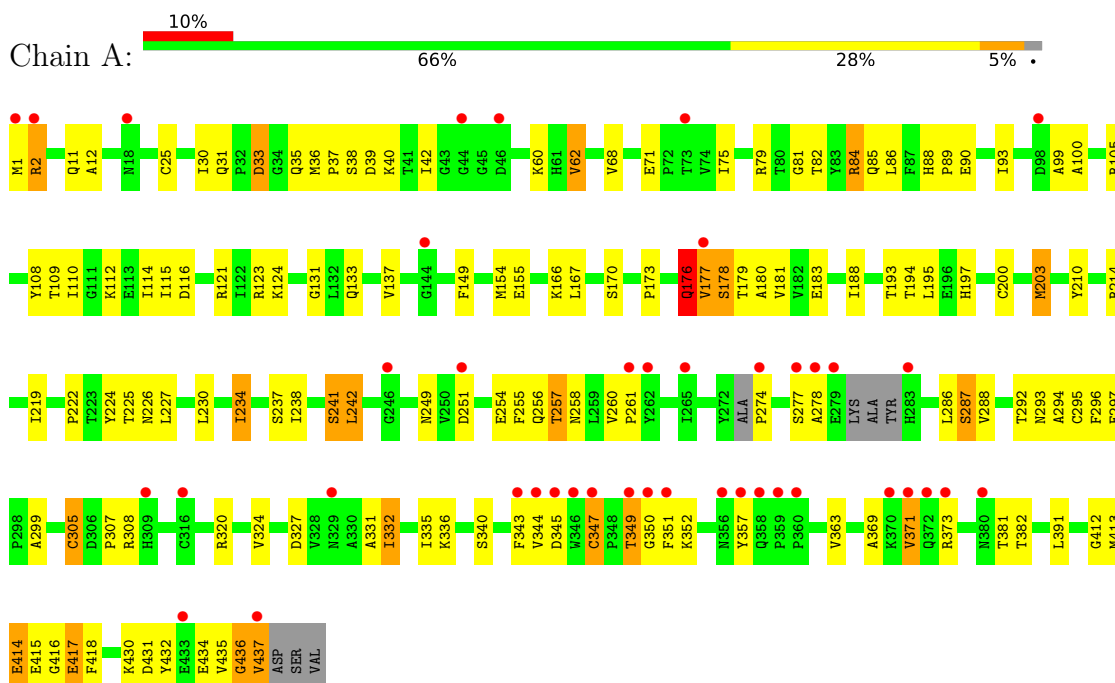
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	7	Total O 7 7	0	0
14	B	6	Total O 6 6	0	0
14	C	6	Total O 6 6	0	0
14	D	9	Total O 9 9	0	0
14	F	3	Total O 3 3	0	0

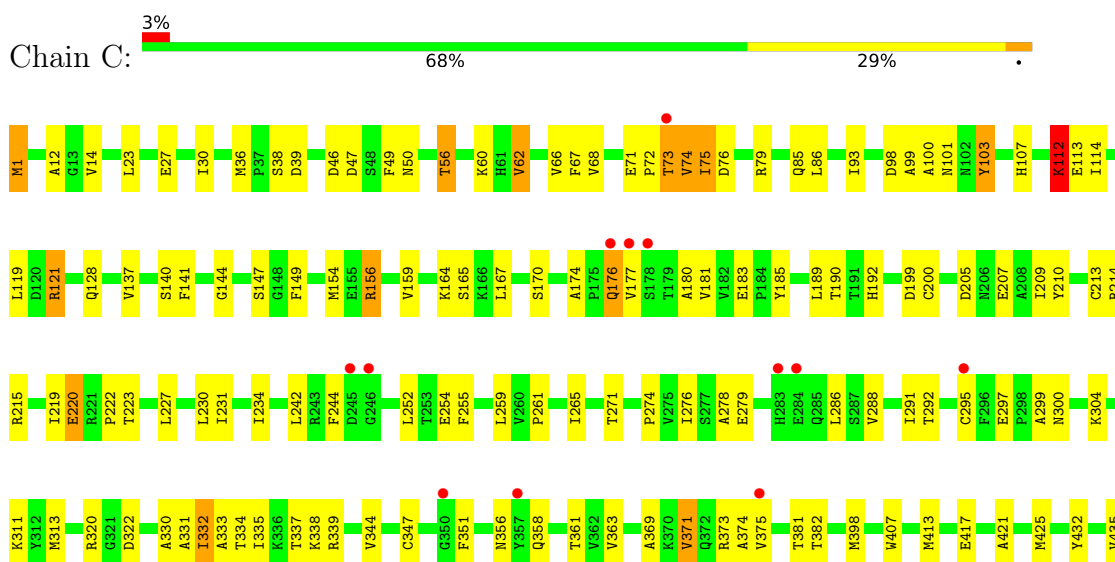
3 Residue-property plots

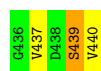
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Detyrosinated tubulin alpha-1B chain

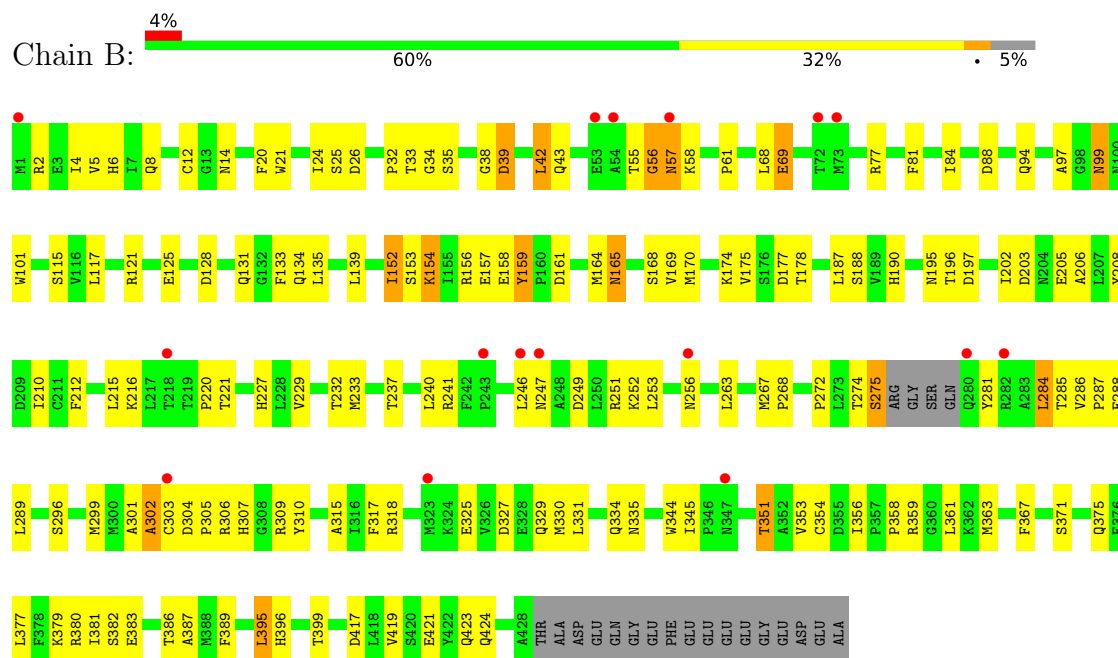


• Molecule 1: Detyrosinated tubulin alpha-1B chain

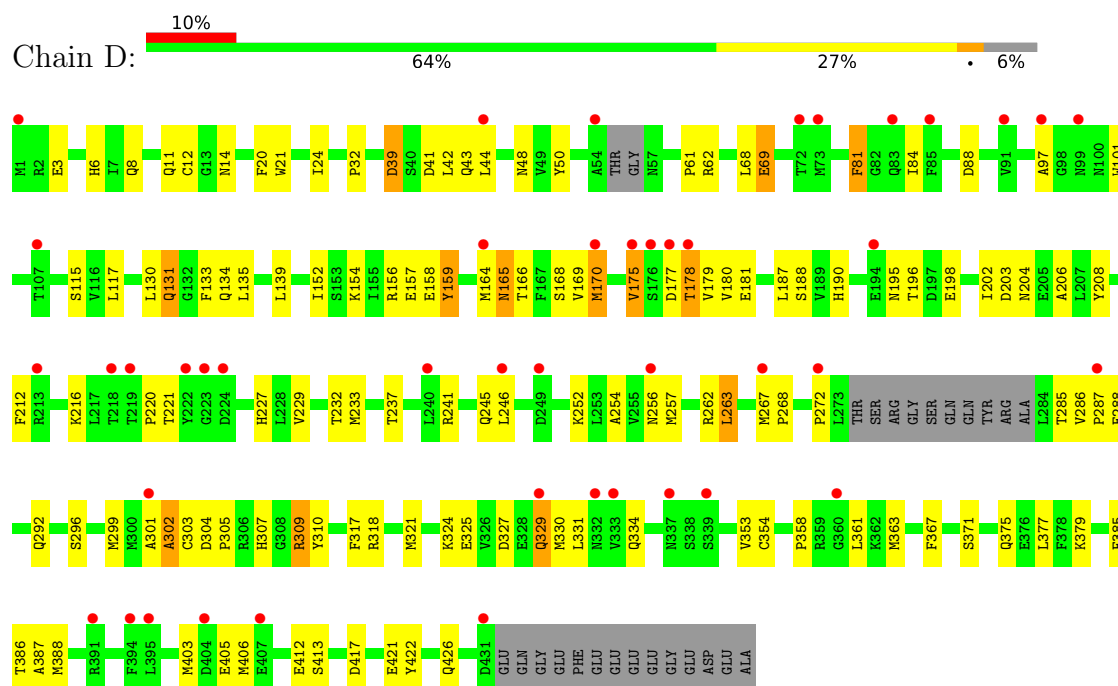




• Molecule 2: Tubulin beta chain

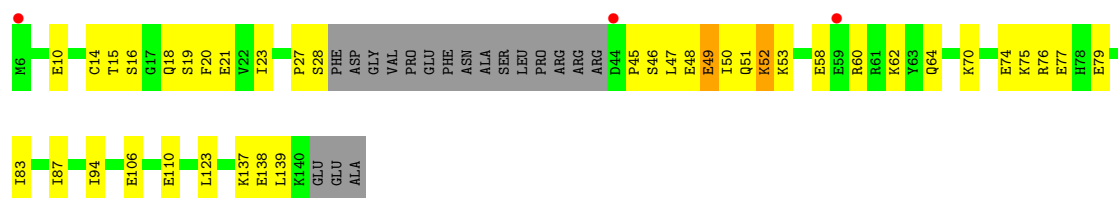


• Molecule 2: Tubulin beta chain

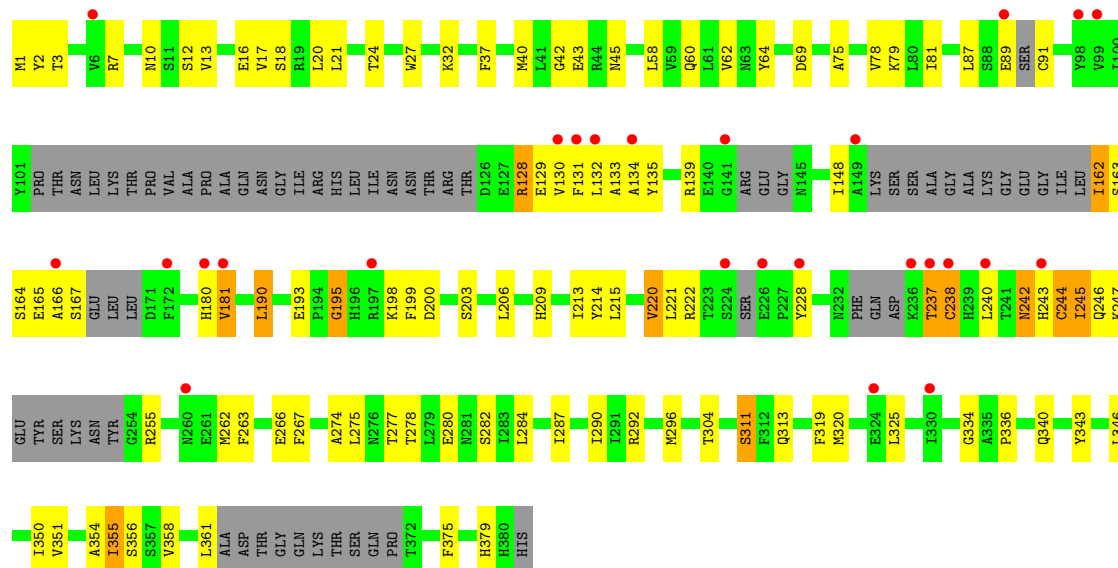


• Molecule 3: Stathmin-4





• Molecule 4: Tubulin-tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.82Å 156.45Å 179.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 2.89 49.86 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.86-2.89) 96.3 (49.86-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.224 , 0.266 0.224 , 0.266	Depositor DCC
R_{free} test set	3225 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16707	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, WIW, GTP, PEG, MES, GDP, EDO, ACP, 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	0.83	1/3318 (0.0%)	0.83	1/4528 (0.0%)
1	C	0.71	2/3440 (0.1%)	0.84	9/4686 (0.2%)
2	B	0.64	0/3316	0.80	3/4508 (0.1%)
2	D	0.53	0/3233	0.78	2/4403 (0.0%)
3	E	0.59	0/946	0.66	0/1266
4	F	0.42	0/2530	0.62	0/3430
All	All	0.65	3/16783 (0.0%)	0.78	15/22821 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	VAL	CA-C	-6.59	1.48	1.52
1	C	363	VAL	CA-C	6.50	1.59	1.53
1	A	363	VAL	CA-C	6.35	1.59	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	VAL	CA-C-O	6.54	123.57	119.51
2	B	281	TYR	N-CA-C	-6.53	105.61	113.97
1	A	62	VAL	N-CA-C	5.83	114.24	107.89
2	D	41	ASP	N-CA-C	-5.59	106.46	113.28
1	C	356	ASN	N-CA-C	-5.54	99.87	108.90
1	C	112	LYS	CA-C-N	-5.45	111.93	122.06
1	C	112	LYS	C-N-CA	-5.45	111.93	122.06
2	B	69	GLU	N-CA-C	-5.40	100.78	109.58
2	D	69	GLU	N-CA-C	-5.38	100.81	109.58
2	B	177	ASP	N-CA-C	-5.19	107.60	114.04
1	C	1	MET	CA-C-N	5.17	129.53	122.34
1	C	1	MET	C-N-CA	5.17	129.53	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	HIS	CA-C-N	-5.10	111.81	121.54
1	C	107	HIS	C-N-CA	-5.10	111.81	121.54
1	C	439	SER	N-CA-C	5.02	117.18	109.95

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	3244	0	3040	81	0
1	C	3363	0	3204	100	0
2	B	3243	0	3018	103	0
2	D	3162	0	2917	95	0
3	E	938	0	897	23	0
4	F	2479	0	2323	74	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	2	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	4	0	6	0	0
7	B	4	0	6	0	0
7	C	16	0	24	2	0
7	D	8	0	12	0	0
8	A	7	0	10	0	0
9	B	28	0	12	1	0
10	B	12	0	12	4	0
11	B	36	0	0	4	0
12	C	1	0	0	0	0
13	F	31	0	14	2	0
14	A	7	0	0	0	0
14	B	6	0	0	0	0
14	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	9	0	0	1	0
14	F	3	0	0	0	0
All	All	16707	0	15531	459	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (459) 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:36:MET:HE2	1:C:39:ASP:HB2	1.39	1.00
1:C:101:ASN:HD22	1:C:180:ALA:HB2	1.38	0.86
1:C:261:PRO:HG2	1:C:313:MET:HE2	1.61	0.83
3:E:14:CYS:SG	3:E:15:THR:N	2.56	0.79
4:F:304:THR:HG21	4:F:311:SER:HB2	1.65	0.77
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.66	0.75
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.52	0.75
2:B:8:GLN:HE21	2:B:14:ASN:HA	1.52	0.73
1:A:36:MET:HE2	1:A:39:ASP:HB2	1.70	0.73
2:B:249:ASP:HB2	2:B:252:LYS:HG3	1.72	0.71
1:C:137:VAL:HG21	1:C:154:MET:CE	2.21	0.71
1:C:332:ILE:HD12	7:C:505:EDO:H11	1.71	0.71
4:F:277:THR:HG22	4:F:278:THR:H	1.55	0.70
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.73	0.69
1:A:1:MET:O	1:A:2:ARG:C	2.35	0.69
1:C:101:ASN:ND2	1:C:180:ALA:HB2	2.08	0.69
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.76	0.68
1:C:137:VAL:HG21	1:C:154:MET:HE1	1.75	0.68
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.59	0.67
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.29	0.67
1:A:224:TYR:HA	1:A:227:LEU:HD12	1.77	0.66
2:B:272:PRO:HB3	2:B:284:LEU:HD21	1.77	0.66
4:F:190:LEU:HD23	4:F:199:PHE:HZ	1.59	0.66
2:B:32:PRO:HG3	2:B:81:PHE:CE1	2.31	0.66
2:B:284:LEU:HD12	2:B:284:LEU:H	1.62	0.65
2:D:203:ASP:HB3	2:D:301:ALA:O	1.97	0.65
2:B:156:ARG:CZ	10:B:503:MES:H21	2.27	0.64
1:C:180:ALA:HA	2:D:256:ASN:HD21	1.60	0.64
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.80	0.64
2:D:39:ASP:OD1	2:D:39:ASP:N	2.25	0.64
1:C:73:THR:O	1:C:74:VAL:C	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.80	0.63
2:B:203:ASP:HB3	2:B:301:ALA:O	1.97	0.63
1:C:100:ALA:HA	2:D:252:LYS:HG2	1.80	0.63
1:A:90:GLU:HB3	1:A:121:ARG:HD2	1.81	0.63
2:D:68:LEU:HD12	2:D:97:ALA:HB2	1.80	0.63
4:F:89:GLU:O	4:F:91:CYS:N	2.31	0.63
4:F:13:VAL:O	4:F:17:VAL:HG23	2.00	0.62
1:A:256:GLN:HG2	1:A:260:VAL:HB	1.81	0.62
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.65	0.62
1:C:101:ASN:OD1	2:D:252:LYS:HD3	2.00	0.61
4:F:16:GLU:O	4:F:20:LEU:HD12	2.00	0.61
1:A:241:SER:HB2	1:A:249:ASN:O	2.01	0.61
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.83	0.61
2:B:164:MET:HB3	2:B:196:THR:HA	1.81	0.61
2:B:335:ASN:ND2	4:F:58:LEU:HG	2.16	0.61
1:C:73:THR:O	1:C:75:ILE:N	2.33	0.61
1:C:252:LEU:HA	1:C:255:PHE:HD2	1.64	0.61
2:D:164:MET:HB3	2:D:196:THR:HA	1.81	0.61
2:D:164:MET:HG3	2:D:196:THR:HG22	1.83	0.61
2:D:179:VAL:O	2:D:388:MET:HE1	2.01	0.61
1:A:242:LEU:HD21	1:A:255:PHE:HE1	1.65	0.60
2:B:20:PHE:CD1	2:B:233:MET:HE2	2.37	0.60
2:B:164:MET:HG3	2:B:196:THR:HG22	1.83	0.60
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.84	0.60
1:C:36:MET:HE1	1:C:49:PHE:CZ	2.37	0.59
2:B:39:ASP:OD1	2:B:39:ASP:N	2.25	0.59
2:D:286:VAL:HG21	2:D:325:GLU:HB3	1.84	0.59
2:D:20:PHE:CD1	2:D:233:MET:HE2	2.37	0.59
2:D:329:GLN:HA	2:D:329:GLN:OE1	2.03	0.58
2:B:99:ASN:N	2:B:99:ASN:HD22	2.00	0.58
1:A:100:ALA:HA	2:B:252:LYS:HE3	1.84	0.58
2:B:42:LEU:HB3	2:B:356:ILE:HD11	1.85	0.58
1:C:220:GLU:OE1	2:D:324:LYS:HD3	2.04	0.58
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.85	0.58
2:B:6:HIS:HE2	2:B:8:GLN:HG3	1.69	0.57
1:C:103:TYR:C	1:C:103:TYR:CD1	2.81	0.57
4:F:40:MET:HG2	4:F:62:VAL:HG23	1.86	0.57
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.39	0.57
4:F:32:LYS:H	4:F:32:LYS:HD3	1.68	0.57
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.85	0.56
2:D:6:HIS:HE2	2:D:8:GLN:HG3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:75:ALA:O	4:F:79:LYS:HG3	2.04	0.56
1:A:176:GLN:O	1:A:177:VAL:C	2.45	0.56
1:C:230:LEU:O	1:C:234:ILE:HD12	2.05	0.56
1:C:121:ARG:CG	1:C:121:ARG:HH11	2.18	0.56
2:D:296:SER:HA	2:D:299:MET:HG2	1.87	0.56
4:F:148:ILE:HD12	4:F:162:ILE:HG12	1.86	0.56
2:D:375:GLN:HE21	2:D:379:LYS:HE3	1.71	0.56
1:C:295:CYS:SG	1:C:375:VAL:HG13	2.46	0.56
2:B:206:ALA:HB2	2:B:301:ALA:O	2.06	0.56
1:C:73:THR:O	1:C:76:ASP:N	2.35	0.56
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.88	0.56
1:A:292:THR:O	1:A:295:CYS:HB2	2.07	0.55
2:D:208:TYR:CE1	2:D:220:PRO:HG2	2.41	0.55
2:B:256:ASN:ND2	11:B:504:WIW:S1	2.79	0.55
1:C:192:HIS:CG	1:C:421:ALA:HA	2.41	0.55
2:D:417:ASP:O	2:D:421:GLU:HG3	2.05	0.55
2:B:358:PRO:HG2	2:B:361:LEU:HB2	1.88	0.55
1:A:297:GLU:HG3	1:A:299:ALA:H	1.71	0.55
2:B:386:THR:O	2:B:387:ALA:C	2.50	0.55
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.89	0.55
2:B:296:SER:HA	2:B:299:MET:HG2	1.87	0.55
2:D:309:ARG:NH1	14:D:601:HOH:O	2.39	0.55
1:A:133:GLN:NE2	1:A:251:ASP:HA	2.22	0.55
2:B:208:TYR:CE1	2:B:220:PRO:HG2	2.41	0.55
2:B:227:HIS:C	2:B:227:HIS:CD2	2.85	0.55
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.89	0.55
3:E:46:SER:O	3:E:47:LEU:C	2.50	0.54
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.89	0.54
2:D:206:ALA:HB2	2:D:301:ALA:O	2.06	0.54
2:D:227:HIS:C	2:D:227:HIS:CD2	2.85	0.54
1:C:159:VAL:HA	3:E:94:ILE:HG23	1.90	0.54
1:A:352:LYS:HG3	3:E:21:GLU:HG3	1.90	0.53
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.90	0.53
3:E:76:ARG:NH2	3:E:79:GLU:OE2	2.30	0.53
2:B:237:THR:O	2:B:241:ARG:HG3	2.09	0.53
2:D:321:MET:HB3	2:D:363:MET:SD	2.49	0.53
1:A:137:VAL:HG21	1:A:154:MET:CE	2.39	0.52
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.44	0.52
2:B:215:LEU:HD13	2:B:275:SER:HB2	1.90	0.52
1:C:292:THR:O	1:C:295:CYS:HB2	2.09	0.52
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:PRO:HD3	1:C:374:ALA:HA	1.91	0.52
2:D:288:GLU:O	2:D:292:GLN:HG3	2.09	0.52
2:D:309:ARG:HG3	2:D:426:GLN:HG3	1.92	0.52
4:F:346:LEU:O	4:F:350:ILE:HG13	2.09	0.52
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.91	0.52
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.39	0.52
1:C:121:ARG:HD3	1:C:121:ARG:N	2.24	0.52
2:D:330:MET:O	2:D:334:GLN:HG3	2.10	0.52
2:D:81:PHE:HD1	2:D:81:PHE:N	2.08	0.52
3:E:48:GLU:CD	3:E:48:GLU:H	2.17	0.52
1:A:154:MET:HE2	1:A:154:MET:HA	1.91	0.52
1:A:294:ALA:C	1:A:296:PHE:N	2.63	0.52
2:B:287:PRO:HA	2:B:329:GLN:HG3	1.91	0.52
1:A:350:GLY:HA3	3:E:23:ILE:HA	1.91	0.52
3:E:70:LYS:O	3:E:74:GLU:HG3	2.10	0.52
4:F:304:THR:CG2	4:F:311:SER:HB2	2.38	0.52
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.45	0.51
1:A:75:ILE:O	1:A:79:ARG:HG3	2.10	0.51
2:B:330:MET:O	2:B:334:GLN:HG3	2.10	0.51
1:A:68:VAL:HG22	1:A:93:ILE:HB	1.90	0.51
2:B:417:ASP:O	2:B:421:GLU:HG3	2.11	0.51
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.92	0.51
2:D:32:PRO:HG3	2:D:81:PHE:CE1	2.46	0.51
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.10	0.51
1:A:88:HIS:NE2	1:A:90:GLU:HB2	2.26	0.51
2:D:12:CYS:HB2	5:D:501:GTP:C8	2.45	0.51
2:D:157:GLU:HG3	3:E:123:LEU:HB3	1.92	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.28	0.51
1:C:103:TYR:C	1:C:103:TYR:HD1	2.17	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.28	0.51
4:F:356:SER:HB3	4:F:361:LEU:HD13	1.91	0.51
4:F:287:ILE:HG12	4:F:319:PHE:CD2	2.46	0.51
2:D:101:TRP:CE3	2:D:187:LEU:HD13	2.47	0.50
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.47	0.50
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.46	0.50
1:A:345:ASP:O	3:E:28:SER:HB3	2.11	0.50
2:B:288:GLU:O	2:B:289:LEU:C	2.55	0.50
1:A:296:PHE:HZ	1:A:351:PHE:HE2	1.60	0.50
1:A:343:PHE:CG	1:A:349:THR:HG22	2.46	0.50
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.93	0.50
1:C:407:TRP:CH2	2:D:254:ALA:HB1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ALA:O	1:C:334:THR:C	2.55	0.49
4:F:198:LYS:HD2	4:F:228:TYR:CE1	2.47	0.49
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.94	0.49
4:F:243:HIS:O	4:F:244:CYS:C	2.54	0.49
2:B:229:VAL:O	2:B:233:MET:HG3	2.13	0.49
4:F:203:SER:HB3	4:F:215:LEU:HD11	1.94	0.49
1:A:123:ARG:O	1:A:124:LYS:C	2.53	0.49
4:F:213:ILE:H	4:F:379:HIS:HB3	1.77	0.49
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.45	0.49
2:D:152:ILE:HG23	2:D:164:MET:HG2	1.94	0.49
4:F:134:ALA:O	4:F:135:TYR:C	2.55	0.49
4:F:163:SER:OG	4:F:164:SER:N	2.44	0.49
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.53	0.49
2:B:134:GLN:HA	2:B:165:ASN:O	2.13	0.49
2:B:274:THR:HG21	2:B:361:LEU:HD21	1.93	0.49
4:F:132:LEU:O	4:F:133:ALA:C	2.56	0.49
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.48	0.49
2:D:229:VAL:O	2:D:233:MET:HG3	2.12	0.49
2:B:57:ASN:O	2:B:58:LYS:C	2.55	0.49
2:B:94:GLN:HB3	1:C:1:MET:HE2	1.94	0.49
2:D:286:VAL:HB	2:D:287:PRO:HD3	1.95	0.48
4:F:20:LEU:O	4:F:24:THR:HG23	2.13	0.48
2:D:81:PHE:N	2:D:81:PHE:CD1	2.81	0.48
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.96	0.48
1:C:137:VAL:HG21	1:C:154:MET:HE3	1.95	0.48
2:D:169:VAL:HA	2:D:202:ILE:O	2.14	0.48
2:B:117:LEU:HD11	2:B:154:LYS:HB3	1.95	0.48
1:C:330:ALA:O	1:C:334:THR:HG23	2.12	0.48
1:A:214:ARG:HG2	1:A:219:ILE:O	2.14	0.48
2:D:175:VAL:HG21	2:D:204:ASN:HB3	1.95	0.48
3:E:83:ILE:O	3:E:87:ILE:HG13	2.14	0.48
4:F:242:ASN:OD1	4:F:242:ASN:N	2.44	0.48
2:B:272:PRO:HG3	2:B:284:LEU:HD11	1.95	0.48
2:D:152:ILE:HD12	2:D:164:MET:SD	2.54	0.48
1:A:176:GLN:O	1:A:178:SER:N	2.47	0.48
1:A:415:GLU:O	1:A:418:PHE:HB2	2.12	0.48
1:A:436:GLY:O	1:A:437:VAL:C	2.57	0.48
1:C:76:ASP:HA	1:C:79:ARG:HD2	1.95	0.48
1:C:147:SER:HB2	1:C:190:THR:HB	1.96	0.48
4:F:32:LYS:H	4:F:32:LYS:CD	2.26	0.48
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:HD21	2:B:168:SER:HB3	1.96	0.47
2:D:386:THR:O	2:D:387:ALA:C	2.57	0.47
1:A:173:PRO:HG2	1:A:391:LEU:HD21	1.97	0.47
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.49	0.47
2:D:130:LEU:HD21	2:D:133:PHE:CZ	2.49	0.47
4:F:64:TYR:HA	4:F:313:GLN:HG3	1.96	0.47
2:B:158:GLU:HB3	2:B:159:TYR:CD1	2.50	0.47
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.50	0.47
1:A:81:GLY:O	1:A:84:ARG:HB3	2.14	0.47
1:A:256:GLN:HE21	1:A:260:VAL:HB	1.79	0.47
1:A:416:GLY:O	1:A:417:GLU:C	2.57	0.47
2:B:212:PHE:O	2:B:216:LYS:HA	2.14	0.47
2:D:287:PRO:HG3	2:D:329:GLN:NE2	2.29	0.47
2:B:256:ASN:HB3	11:B:504:WIW:C2'	2.44	0.47
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.48	0.47
2:D:212:PHE:O	2:D:216:LYS:HA	2.14	0.47
4:F:1:MET:HE2	4:F:1:MET:HB2	1.85	0.47
2:B:56:GLY:C	2:B:58:LYS:H	2.22	0.47
1:C:351:PHE:H	7:C:505:EDO:H21	1.80	0.47
4:F:274:ALA:C	4:F:275:LEU:HD12	2.39	0.47
1:C:165:SER:HA	1:C:199:ASP:OD2	2.14	0.47
2:D:158:GLU:HB3	2:D:159:TYR:CD1	2.50	0.46
1:C:382:THR:HA	1:C:432:TYR:HD2	1.79	0.46
2:B:377:LEU:O	2:B:381:ILE:HG12	2.14	0.46
2:D:187:LEU:O	2:D:190:HIS:HB3	2.16	0.46
2:B:26:ASP:OD2	2:B:359:ARG:NE	2.48	0.46
2:B:32:PRO:HG3	2:B:81:PHE:CD1	2.50	0.46
2:B:81:PHE:HD1	2:B:81:PHE:N	2.13	0.46
2:D:134:GLN:HA	2:D:165:ASN:O	2.15	0.46
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.97	0.46
2:D:237:THR:O	2:D:241:ARG:HG3	2.15	0.46
4:F:3:THR:OG1	4:F:37:PHE:HA	2.15	0.46
4:F:284:LEU:HD23	4:F:284:LEU:HA	1.65	0.46
1:A:60:LYS:HG2	1:A:62:VAL:HG22	1.98	0.46
2:B:187:LEU:O	2:B:190:HIS:HB3	2.16	0.46
4:F:135:TYR:OH	4:F:165:GLU:HA	2.16	0.46
2:B:197:ASP:OD1	10:B:503:MES:H32	2.15	0.46
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.98	0.46
1:C:207:GLU:CD	1:C:304:LYS:HD2	2.41	0.46
3:E:106:GLU:O	3:E:110:GLU:HG3	2.16	0.46
2:D:159:TYR:CD1	2:D:159:TYR:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:129:GLU:O	4:F:130:VAL:C	2.58	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45
2:B:38:GLY:HA3	2:B:43:GLN:OE1	2.16	0.45
2:B:159:TYR:CD1	2:B:159:TYR:N	2.84	0.45
2:D:405:GLU:O	2:D:406:MET:C	2.58	0.45
3:E:48:GLU:O	3:E:49:GLU:C	2.58	0.45
1:C:278:ALA:O	1:C:279:GLU:C	2.59	0.45
2:D:61:PRO:HD2	2:D:84:ILE:O	2.16	0.45
3:E:138:GLU:O	3:E:139:LEU:HD23	2.15	0.45
4:F:237:THR:O	4:F:238:CYS:C	2.60	0.45
1:A:413:MET:HE2	1:A:413:MET:HB3	1.79	0.45
2:B:169:VAL:HA	2:B:202:ILE:O	2.16	0.45
4:F:351:VAL:HA	4:F:355:ILE:HG13	1.99	0.45
2:B:310:TYR:CD1	2:B:371:SER:HB2	2.52	0.45
1:C:223:THR:O	1:C:227:LEU:HG	2.17	0.45
4:F:209:HIS:CE1	4:F:358:VAL:HG22	2.50	0.45
1:C:1:MET:HE3	1:C:1:MET:HB3	1.91	0.45
2:D:177:ASP:O	2:D:178:THR:C	2.58	0.45
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.98	0.45
4:F:275:LEU:HD23	4:F:325:LEU:HD11	1.99	0.45
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.52	0.45
2:B:335:ASN:HD21	4:F:58:LEU:HG	1.82	0.45
2:D:11:GLN:HB3	5:D:501:GTP:O2A	2.16	0.45
3:E:50:ILE:O	3:E:51:GLN:C	2.59	0.45
3:E:52:LYS:O	3:E:53:LYS:C	2.60	0.45
4:F:351:VAL:O	4:F:356:SER:OG	2.32	0.45
1:A:99:ALA:O	1:A:100:ALA:C	2.58	0.45
1:C:100:ALA:HA	2:D:252:LYS:CG	2.47	0.45
2:D:299:MET:HE3	2:D:305:PRO:HG3	1.98	0.45
1:A:36:MET:O	1:A:37:PRO:C	2.60	0.44
2:B:379:LYS:O	2:B:383:GLU:HG3	2.17	0.44
1:C:432:TYR:O	1:C:435:VAL:HG22	2.17	0.44
2:D:385:PHE:CE1	2:D:412:GLU:HB2	2.52	0.44
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.52	0.44
2:D:285:THR:H	2:D:288:GLU:HB2	1.81	0.44
2:D:310:TYR:CD1	2:D:371:SER:HB2	2.52	0.44
4:F:292:ARG:HB3	4:F:296:MET:HE2	1.98	0.44
1:A:287:SER:O	1:A:288:VAL:C	2.59	0.44
2:B:81:PHE:CD1	2:B:81:PHE:N	2.85	0.44
1:C:205:ASP:OD2	1:C:304:LYS:HG3	2.16	0.44
2:D:6:HIS:NE2	2:D:8:GLN:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:THR:HB	2:D:181:GLU:HG3	1.99	0.44
1:A:114:ILE:HG23	1:A:149:PHE:CE1	2.53	0.44
2:B:272:PRO:HD2	2:B:361:LEU:HD13	2.00	0.44
1:C:60:LYS:HG2	1:C:62:VAL:HG22	1.98	0.44
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.82	0.44
1:C:288:VAL:O	1:C:291:ILE:HG12	2.16	0.44
1:C:333:ALA:O	1:C:337:THR:HG23	2.16	0.44
4:F:128:ARG:O	4:F:129:GLU:C	2.57	0.44
2:B:389:PHE:HE1	2:B:395:LEU:HD21	1.81	0.44
1:A:307:PRO:O	1:A:308:ARG:C	2.60	0.44
2:D:245:GLN:O	2:D:246:LEU:C	2.61	0.44
4:F:190:LEU:HD23	4:F:199:PHE:CZ	2.46	0.44
1:A:320:ARG:O	1:A:373:ARG:HA	2.18	0.44
1:A:382:THR:HA	1:A:432:TYR:HD1	1.82	0.44
2:B:256:ASN:HB3	11:B:504:WIW:C4	2.47	0.44
1:C:174:ALA:HB1	1:C:176:GLN:HE21	1.82	0.44
4:F:334:GLY:C	4:F:336:PRO:HD3	2.43	0.44
2:B:237:THR:HA	2:B:240:LEU:HD12	1.99	0.44
2:B:267:MET:HE3	2:B:301:ALA:HB3	2.00	0.44
1:C:30:ILE:HG12	1:C:36:MET:HG3	2.00	0.44
1:C:219:ILE:O	1:C:220:GLU:C	2.61	0.44
1:A:2:ARG:HA	1:A:131:GLY:O	2.18	0.44
2:B:34:GLY:O	2:B:58:LYS:HA	2.17	0.44
1:C:72:PRO:O	1:C:73:THR:O	2.36	0.44
2:D:156:ARG:HB3	3:E:123:LEU:HD11	1.99	0.44
4:F:274:ALA:O	4:F:275:LEU:HD12	2.18	0.44
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.53	0.43
1:C:185:TYR:OH	1:C:398:MET:HB3	2.17	0.43
1:A:254:GLU:O	1:A:255:PHE:C	2.61	0.43
2:B:327:ASP:O	2:B:331:LEU:HD12	2.18	0.43
2:B:375:GLN:HE22	2:B:423:GLN:HE21	1.66	0.43
2:D:158:GLU:HB3	2:D:159:TYR:CE1	2.53	0.43
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.81	0.43
2:B:35:SER:HA	2:B:57:ASN:HD21	1.82	0.43
2:B:135:LEU:HD22	2:B:152:ILE:HD11	2.01	0.43
2:B:299:MET:HE3	2:B:305:PRO:HG3	1.98	0.43
2:B:423:GLN:O	2:B:424:GLN:C	2.61	0.43
4:F:37:PHE:O	4:F:60:GLN:NE2	2.47	0.43
2:B:158:GLU:C	2:B:159:TYR:CD1	2.96	0.43
2:B:301:ALA:O	2:B:302:ALA:HB2	2.19	0.43
2:B:304:ASP:HB3	2:B:307:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:GLN:HB2	2:B:419:VAL:HG13	1.99	0.43
1:C:344:VAL:HG23	1:C:347:CYS:HB3	2.00	0.43
1:C:413:MET:HE3	1:C:417:GLU:HB2	1.99	0.43
2:D:158:GLU:C	2:D:159:TYR:CD1	2.96	0.43
1:A:203:MET:HE2	1:A:203:MET:HB2	1.87	0.43
1:A:357:TYR:OH	3:E:18:GLN:HG3	2.18	0.43
2:D:267:MET:HE3	2:D:301:ALA:HB3	2.00	0.43
2:D:327:ASP:O	2:D:331:LEU:HD12	2.18	0.43
1:C:56:THR:OG1	1:C:60:LYS:HB3	2.19	0.43
1:C:331:ALA:O	1:C:335:ILE:HG13	2.19	0.43
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.53	0.43
2:B:6:HIS:NE2	2:B:8:GLN:HG3	2.32	0.43
3:E:52:LYS:HA	3:E:52:LYS:HD3	1.68	0.43
4:F:165:GLU:O	4:F:167:SER:N	2.52	0.43
4:F:193:GLU:C	4:F:195:GLY:H	2.25	0.43
2:B:152:ILE:HG22	2:B:195:ASN:HB3	2.01	0.43
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.53	0.43
2:B:161:ASP:O	2:B:251:ARG:NH2	2.51	0.43
2:B:253:LEU:HD13	11:B:504:WIW:C15	2.48	0.43
1:C:75:ILE:O	1:C:79:ARG:HG3	2.19	0.43
2:D:3:GLU:O	2:D:131:GLN:HG3	2.18	0.43
2:D:245:GLN:HE21	2:D:245:GLN:HB2	1.62	0.43
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.59	0.43
1:C:66:VAL:HG12	1:C:68:VAL:HG23	1.99	0.43
1:C:330:ALA:O	1:C:331:ALA:C	2.62	0.43
1:A:305:CYS:O	1:A:307:PRO:HD3	2.19	0.42
2:B:286:VAL:O	2:B:287:PRO:C	2.59	0.42
1:C:156:ARG:HH11	1:C:156:ARG:HD3	1.73	0.42
2:B:359:ARG:HD3	2:B:359:ARG:HA	1.66	0.42
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.53	0.42
4:F:10:ASN:OD1	4:F:10:ASN:N	2.51	0.42
4:F:220:VAL:HG23	4:F:263:PHE:CE1	2.53	0.42
4:F:221:LEU:HB2	4:F:262:MET:O	2.19	0.42
4:F:287:ILE:HG12	4:F:319:PHE:CE2	2.54	0.42
1:A:40:LYS:HA	1:A:40:LYS:HD3	1.74	0.42
1:A:430:LYS:O	1:A:431:ASP:C	2.61	0.42
2:B:158:GLU:HB3	2:B:159:TYR:CE1	2.53	0.42
1:C:297:GLU:HG3	1:C:299:ALA:H	1.85	0.42
1:C:46:ASP:OD1	1:C:46:ASP:N	2.53	0.42
1:C:154:MET:HE2	1:C:154:MET:HA	2.01	0.42
2:D:48:ASN:O	2:D:62:ARG:NH2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:THR:O	2:D:286:VAL:C	2.63	0.42
1:A:256:GLN:O	1:A:257:THR:C	2.63	0.42
2:B:88:ASP:OD1	2:B:88:ASP:N	2.52	0.42
1:A:331:ALA:O	1:A:332:ILE:C	2.62	0.42
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.01	0.42
1:C:271:THR:HG23	1:C:300:ASN:O	2.19	0.42
2:D:135:LEU:HB3	2:D:166:THR:HG22	2.02	0.42
2:D:170:MET:HE3	2:D:170:MET:HB3	1.84	0.42
2:D:304:ASP:HB3	2:D:307:HIS:CE1	2.54	0.42
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.00	0.42
2:B:170:MET:HG3	2:B:377:LEU:HD11	2.01	0.42
2:D:20:PHE:CG	2:D:233:MET:HE2	2.54	0.42
4:F:266:GLU:HA	4:F:266:GLU:OE1	2.19	0.42
1:A:431:ASP:O	1:A:435:VAL:HG22	2.19	0.42
2:B:227:HIS:C	2:B:227:HIS:HD2	2.27	0.42
3:E:10:GLU:O	3:E:20:PHE:HA	2.20	0.42
4:F:135:TYR:O	4:F:139:ARG:N	2.51	0.42
1:C:68:VAL:HG11	1:C:149:PHE:CE2	2.55	0.42
1:C:214:ARG:HG2	1:C:219:ILE:O	2.20	0.42
1:A:115:ILE:HG23	1:A:116:ASP:N	2.34	0.42
1:C:23:LEU:O	1:C:27:GLU:HG3	2.20	0.42
2:D:301:ALA:O	2:D:302:ALA:HB2	2.19	0.42
4:F:43:GLU:HG3	4:F:45:ASN:O	2.20	0.42
1:A:234:ILE:O	1:A:238:ILE:HG13	2.20	0.41
1:A:412:GLY:O	3:E:60:ARG:NH2	2.53	0.41
2:B:61:PRO:HD2	2:B:84:ILE:O	2.20	0.41
1:C:265:ILE:HG21	1:C:313:MET:HE1	2.02	0.41
2:D:88:ASP:OD1	2:D:88:ASP:N	2.52	0.41
2:D:152:ILE:HG22	2:D:195:ASN:HB3	2.02	0.41
4:F:18:SER:HA	4:F:21:LEU:HD12	2.01	0.41
1:A:108:TYR:O	1:A:109:THR:C	2.62	0.41
1:A:230:LEU:O	1:A:234:ILE:HD12	2.20	0.41
1:C:99:ALA:HB3	1:C:144:GLY:HA3	2.01	0.41
1:C:425:MET:HE3	1:C:425:MET:HB3	1.85	0.41
2:D:180:VAL:O	2:D:181:GLU:C	2.61	0.41
2:D:304:ASP:HB3	2:D:307:HIS:ND1	2.35	0.41
1:A:11:GLN:O	1:A:12:ALA:C	2.64	0.41
1:A:434:GLU:O	1:A:435:VAL:C	2.62	0.41
2:B:121:ARG:O	2:B:125:GLU:HG3	2.20	0.41
2:B:246:LEU:O	2:B:247:ASN:C	2.63	0.41
2:D:50:TYR:CD2	2:D:241:ARG:HG2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:320:MET:HE1	13:F:401:ACP:C2	2.51	0.41
1:A:31:GLN:HG3	1:A:35:GLN:O	2.20	0.41
2:B:5:VAL:HB	2:B:133:PHE:CD1	2.55	0.41
2:B:20:PHE:CG	2:B:233:MET:HE2	2.54	0.41
2:B:197:ASP:OD2	10:B:503:MES:H52	2.20	0.41
2:B:232:THR:HG21	2:B:268:PRO:HB2	2.02	0.41
2:D:318:ARG:HA	2:D:354:CYS:O	2.21	0.41
1:C:121:ARG:HD2	1:C:121:ARG:HA	1.76	0.41
1:C:413:MET:HE2	1:C:413:MET:HB3	1.79	0.41
4:F:242:ASN:ND2	13:F:401:ACP:H5'2	2.35	0.41
1:A:81:GLY:O	1:A:82:THR:C	2.60	0.41
1:C:322:ASP:HB3	1:C:373:ARG:HH21	1.86	0.41
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.35	0.41
10:B:503:MES:H51	10:B:503:MES:H82	1.64	0.41
2:D:263:LEU:HD12	2:D:422:TYR:CE2	2.56	0.41
1:A:154:MET:O	1:A:155:GLU:C	2.63	0.41
1:A:294:ALA:C	1:A:296:PHE:H	2.28	0.41
2:D:227:HIS:C	2:D:227:HIS:HD2	2.27	0.41
4:F:130:VAL:O	4:F:131:PHE:C	2.61	0.41
1:A:88:HIS:O	1:A:89:PRO:C	2.64	0.41
2:B:286:VAL:HB	2:B:287:PRO:HD3	2.03	0.41
2:B:315:ALA:HB3	2:B:351:THR:HG23	2.03	0.41
2:B:317:PHE:HB2	2:B:353:VAL:HG22	2.03	0.41
2:B:344:TRP:CE3	2:B:345:ILE:HG13	2.56	0.41
2:B:396:HIS:HA	2:B:399:THR:OG1	2.20	0.41
1:C:62:VAL:HG13	1:C:86:LEU:O	2.21	0.41
2:D:358:PRO:HG2	2:D:361:LEU:HD12	2.03	0.41
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.03	0.41
1:C:180:ALA:O	1:C:183:GLU:HG3	2.20	0.41
1:C:335:ILE:O	1:C:339:ARG:N	2.51	0.41
1:A:180:ALA:HB3	1:A:183:GLU:HG2	2.04	0.40
1:A:414:GLU:O	1:A:415:GLU:C	2.64	0.40
1:C:213:CYS:HB3	1:C:219:ILE:HD12	2.03	0.40
2:D:272:PRO:HD2	2:D:361:LEU:HD13	2.03	0.40
2:D:285:THR:O	2:D:288:GLU:N	2.54	0.40
2:D:403:MET:HE2	2:D:403:MET:HB3	1.79	0.40
3:E:137:LYS:C	3:E:139:LEU:H	2.28	0.40
2:B:25:SER:HB2	2:B:81:PHE:HE2	1.86	0.40
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.91	0.40
1:C:337:THR:OG1	1:C:338:LYS:N	2.54	0.40
1:C:369:ALA:O	1:C:371:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:32:LYS:HD3	4:F:32:LYS:N	2.33	0.40
4:F:244:CYS:SG	4:F:245:ILE:N	2.94	0.40
4:F:290:ILE:HG21	4:F:319:PHE:HE1	1.86	0.40
1:C:259:LEU:O	1:C:261:PRO:HD3	2.20	0.40
1:A:105:ARG:HG2	1:A:110:ILE:CG1	2.51	0.40
1:A:335:ILE:O	1:A:336:LYS:C	2.62	0.40
2:B:4:ILE:HG13	2:B:131:GLN:OE1	2.21	0.40
2:B:285:THR:O	2:B:286:VAL:C	2.64	0.40
2:B:318:ARG:HA	2:B:354:CYS:O	2.21	0.40
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.03	0.40
1:C:47:ASP:O	1:C:50:ASN:HB2	2.21	0.40
1:C:167:LEU:HA	1:C:200:CYS:O	2.22	0.40
2:D:317:PHE:HB2	2:D:353:VAL:HG22	2.03	0.40
1:A:194:THR:O	1:A:195:LEU:C	2.62	0.40
1:A:225:THR:O	1:A:226:ASN:C	2.63	0.40
1:A:417:GLU:O	1:A:418:PHE:C	2.65	0.40
2:D:232:THR:HG21	2:D:268:PRO:HB2	2.02	0.40
2:D:377:LEU:HD23	2:D:377:LEU:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/440 (97%)	394 (92%)	28 (7%)	5 (1%)	10	34
1	C	438/440 (100%)	414 (94%)	20 (5%)	4 (1%)	14	41
2	B	420/445 (94%)	390 (93%)	26 (6%)	4 (1%)	12	39
2	D	413/445 (93%)	387 (94%)	25 (6%)	1 (0%)	43	72
3	E	116/138 (84%)	109 (94%)	5 (4%)	2 (2%)	7	26
4	F	297/381 (78%)	260 (88%)	35 (12%)	2 (1%)	18	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2111/2289 (92%)	1954 (93%)	139 (7%)	18 (1%)	14 41

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	42	LEU
2	B	302	ALA
1	C	73	THR
1	C	74	VAL
2	D	302	ALA
4	F	166	ALA
1	A	2	ARG
1	A	178	SER
1	A	261	PRO
1	A	176	GLN
2	B	56	GLY
1	C	220	GLU
3	E	27	PRO
3	E	45	PRO
2	B	55	THR
1	C	112	LYS
4	F	195	GLY
1	A	436	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	333/371 (90%)	294 (88%)	39 (12%)	5 17
1	C	352/371 (95%)	325 (92%)	27 (8%)	12 35
2	B	342/383 (89%)	309 (90%)	33 (10%)	8 26
2	D	331/383 (86%)	307 (93%)	24 (7%)	13 38
3	E	94/123 (76%)	87 (93%)	7 (7%)	13 38
4	F	256/339 (76%)	237 (93%)	19 (7%)	13 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1708/1970 (87%)	1559 (91%)	149 (9%)	9 30

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	33	ASP
1	A	38	SER
1	A	42	ILE
1	A	71	GLU
1	A	84	ARG
1	A	85	GLN
1	A	112	LYS
1	A	166	LYS
1	A	170	SER
1	A	176	GLN
1	A	177	VAL
1	A	179	THR
1	A	181	VAL
1	A	188	ILE
1	A	193	THR
1	A	203	MET
1	A	234	ILE
1	A	237	SER
1	A	241	SER
1	A	242	LEU
1	A	257	THR
1	A	258	ASN
1	A	277	SER
1	A	286	LEU
1	A	287	SER
1	A	293	ASN
1	A	305	CYS
1	A	324	VAL
1	A	327	ASP
1	A	332	ILE
1	A	340	SER
1	A	347	CYS
1	A	349	THR
1	A	371	VAL
1	A	381	THR
1	A	414	GLU

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Mol	Chain	Res	Type
1	A	417	GLU
1	A	437	VAL
2	B	2	ARG
2	B	33	THR
2	B	39	ASP
2	B	57	ASN
2	B	69	GLU
2	B	77	ARG
2	B	99	ASN
2	B	115	SER
2	B	128	ASP
2	B	152	ILE
2	B	153	SER
2	B	154	LYS
2	B	157	GLU
2	B	159	TYR
2	B	165	ASN
2	B	175	VAL
2	B	178	THR
2	B	188	SER
2	B	210	ILE
2	B	221	THR
2	B	263	LEU
2	B	275	SER
2	B	284	LEU
2	B	303	CYS
2	B	306	ARG
2	B	309	ARG
2	B	325	GLU
2	B	351	THR
2	B	363	MET
2	B	367	PHE
2	B	380	ARG
2	B	382	SER
2	B	395	LEU
1	C	38	SER
1	C	56	THR
1	C	75	ILE
1	C	85	GLN
1	C	103	TYR
1	C	121	ARG
1	C	128	GLN

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Mol	Chain	Res	Type
1	C	156	ARG
1	C	164	LYS
1	C	176	GLN
1	C	177	VAL
1	C	181	VAL
1	C	189	LEU
1	C	215	ARG
1	C	242	LEU
1	C	254	GLU
1	C	276	ILE
1	C	286	LEU
1	C	311	LYS
1	C	320	ARG
1	C	332	ILE
1	C	361	THR
1	C	371	VAL
1	C	381	THR
1	C	437	VAL
1	C	439	SER
1	C	440	VAL
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	44	LEU
2	D	69	GLU
2	D	81	PHE
2	D	115	SER
2	D	131	GLN
2	D	159	TYR
2	D	165	ASN
2	D	170	MET
2	D	175	VAL
2	D	178	THR
2	D	188	SER
2	D	198	GLU
2	D	221	THR
2	D	257	MET
2	D	262	ARG
2	D	263	LEU
2	D	303	CYS
2	D	309	ARG
2	D	329	GLN

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Mol	Chain	Res	Type
2	D	367	PHE
2	D	413	SER
3	E	16	SER
3	E	19	SER
3	E	49	GLU
3	E	52	LYS
3	E	64	GLN
3	E	75	LYS
3	E	77	GLU
4	F	12	SER
4	F	69	ASP
4	F	128	ARG
4	F	162	ILE
4	F	180	HIS
4	F	181	VAL
4	F	190	LEU
4	F	220	VAL
4	F	237	THR
4	F	238	CYS
4	F	240	LEU
4	F	242	ASN
4	F	244	CYS
4	F	245	ILE
4	F	246	GLN
4	F	247	LYS
4	F	255	ARG
4	F	311	SER
4	F	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	176	GLN
1	A	256	GLN
1	A	358	GLN
1	A	406	HIS
2	B	8	GLN
2	B	99	ASN
2	B	134	GLN
2	B	227	HIS
2	B	329	GLN

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Mol	Chain	Res	Type
2	B	423	GLN
1	C	11	GLN
1	C	28	HIS
1	C	176	GLN
1	C	256	GLN
1	C	285	GLN
1	C	358	GLN
1	C	372	GLN
2	D	8	GLN
2	D	99	ASN
2	D	131	GLN
2	D	134	GLN
2	D	165	ASN
2	D	227	HIS
2	D	245	GLN
2	D	375	GLN
2	D	384	GLN
2	D	396	HIS
2	D	423	GLN
3	E	64	GLN
3	E	71	HIS
3	E	108	ASN
4	F	145	ASN
4	F	232	ASN
4	F	379	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	501	6	33,34,34	1.58	5 (15%)	50,54,54	1.86	12 (24%)
7	EDO	A	503	-	3,3,3	0.61	0	2,2,2	0.19	0
10	MES	B	503	-	12,12,12	2.36	1 (8%)	15,16,16	2.16	3 (20%)
11	WIW	B	504	-	39,41,41	1.78	7 (17%)	55,60,60	1.68	13 (23%)
7	EDO	C	507	-	3,3,3	0.41	0	2,2,2	0.39	0
5	GTP	D	501	6	33,34,34	0.86	1 (3%)	50,54,54	1.51	10 (20%)
7	EDO	D	503	-	3,3,3	0.48	0	2,2,2	0.47	0
7	EDO	C	505	-	3,3,3	0.49	0	2,2,2	0.61	0
13	ACP	F	401	-	31,33,33	1.14	2 (6%)	47,52,52	0.77	1 (2%)
7	EDO	B	505	-	3,3,3	0.37	0	2,2,2	0.41	0
7	EDO	C	506	-	3,3,3	0.54	0	2,2,2	0.31	0
9	GDP	B	501	6	29,30,30	1.28	2 (6%)	45,47,47	1.97	11 (24%)
5	GTP	A	501	6	33,34,34	1.04	2 (6%)	50,54,54	1.59	12 (24%)
8	PEG	A	504	-	6,6,6	0.37	0	5,5,5	0.33	0
7	EDO	D	504	-	3,3,3	1.58	0	2,2,2	0.87	0
7	EDO	C	504	-	3,3,3	0.61	0	2,2,2	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
7	EDO	A	503	-	-	0/1/1/1	-
10	MES	B	503	-	-	2/6/14/14	0/1/1/1
11	WIW	B	504	-	-	2/14/49/49	0/6/6/6
7	EDO	C	507	-	-	0/1/1/1	-
5	GTP	D	501	6	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	503	-	-	1/1/1/1	-
7	EDO	C	505	-	-	0/1/1/1	-
13	ACP	F	401	-	-	0/19/38/38	0/3/3/3
7	EDO	B	505	-	-	0/1/1/1	-
7	EDO	C	506	-	-	0/1/1/1	-
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
8	PEG	A	504	-	-	2/4/4/4	-
7	EDO	D	504	-	-	0/1/1/1	-
7	EDO	C	504	-	-	1/1/1/1	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.91	1.66	1.77
11	B	504	WIW	CAB-C7	5.63	1.59	1.51
5	C	501	GTP	PB-O3A	5.03	1.64	1.59
13	F	401	ACP	PB-O3A	4.93	1.63	1.58
11	B	504	WIW	C20-S1	4.25	1.82	1.76
13	F	401	ACP	PA-O3A	3.79	1.63	1.59
5	C	501	GTP	PA-O3A	3.79	1.63	1.59
11	B	504	WIW	C10-S1	3.73	1.89	1.84
5	C	501	GTP	C5-N7	-3.62	1.31	1.39
9	B	501	GDP	C6-N1	-3.46	1.32	1.38
9	B	501	GDP	C5-C4	3.04	1.47	1.38
5	A	501	GTP	PA-O3A	2.83	1.62	1.59
5	C	501	GTP	C5-C6	-2.79	1.34	1.44
5	C	501	GTP	O4'-C4'	-2.58	1.39	1.45
11	B	504	WIW	C19-C14	2.53	1.42	1.39
5	D	501	GTP	C2-N3	2.49	1.39	1.33
5	A	501	GTP	PB-O3B	2.25	1.61	1.59
11	B	504	WIW	CAB-CAA	2.25	1.44	1.40
11	B	504	WIW	C4-CAB	2.06	1.42	1.39
11	B	504	WIW	C1-CAA	2.01	1.42	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	C5-N4-C3	6.35	122.51	108.84
9	B	501	GDP	C5-C4-N3	-6.08	118.71	128.39
9	B	501	GDP	C2-N3-C4	5.12	121.11	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C5-C4-N3	-4.87	120.64	128.39
13	F	401	ACP	PB-O3A-PA	-4.67	117.13	132.37
5	C	501	GTP	O6-C6-C5	-4.63	114.31	126.53
5	C	501	GTP	C2-N3-C4	4.49	120.04	112.30
11	B	504	WIW	OP3-C16-C17	4.47	122.79	115.14
9	B	501	GDP	N9-C4-N3	4.41	134.76	125.95
5	D	501	GTP	C5-C4-N3	-4.35	121.47	128.39
11	B	504	WIW	OP3-C16-C15	-4.11	116.99	124.08
9	B	501	GDP	C6-C5-N7	3.91	137.40	130.29
5	C	501	GTP	C2-N1-C6	-3.68	118.44	125.11
5	D	501	GTP	C2-N1-C6	-3.59	118.59	125.11
5	A	501	GTP	C5-C4-N3	-3.56	122.72	128.39
11	B	504	WIW	O5'-C5'-C17	3.28	120.77	115.14
5	D	501	GTP	C2-N3-C4	3.28	117.94	112.30
11	B	504	WIW	C13-O3'-C3'	3.27	109.69	105.32
5	C	501	GTP	N2-C2-N1	3.22	123.56	116.76
5	C	501	GTP	N9-C4-N3	3.19	132.34	125.95
11	B	504	WIW	C13-O2'-C2'	3.18	109.58	105.32
10	B	503	MES	O2S-S-C8	3.17	111.51	106.73
9	B	501	GDP	O4'-C1'-N9	-3.14	101.25	108.36
5	A	501	GTP	C2-N3-C4	3.06	117.57	112.30
11	B	504	WIW	O2'-C2'-C4	3.05	131.91	127.86
9	B	501	GDP	O2A-PA-O3A	2.99	115.35	107.27
11	B	504	WIW	O6-C6-C5	-2.97	125.60	129.38
11	B	504	WIW	O5'-C5'-C19	-2.96	118.97	124.08
5	C	501	GTP	O2A-PA-O3A	2.94	115.23	107.27
5	C	501	GTP	C5-C6-N1	2.91	120.66	113.25
9	B	501	GDP	C4-C5-N7	-2.83	106.18	110.67
5	C	501	GTP	N9-C8-N7	-2.80	108.21	113.40
5	A	501	GTP	O2B-PB-O3A	2.79	114.82	107.27
11	B	504	WIW	O3'-C13-O2'	-2.77	103.75	108.09
5	A	501	GTP	O2A-PA-O3A	2.74	114.69	107.27
11	B	504	WIW	O3'-C3'-C1	2.69	131.44	127.86
5	C	501	GTP	O6-C6-N1	2.61	125.03	120.11
5	A	501	GTP	N9-C8-N7	-2.57	108.64	113.40
5	D	501	GTP	N9-C4-N3	2.56	131.07	125.95
5	A	501	GTP	O4'-C1'-N9	-2.52	102.65	108.36
5	C	501	GTP	C8-N7-C5	2.47	108.66	104.26
5	D	501	GTP	N9-C8-N7	-2.45	108.87	113.40
5	A	501	GTP	N2-C2-N1	2.44	121.90	116.76
5	D	501	GTP	C2'-C1'-N9	2.43	120.02	113.25
10	B	503	MES	O1S-S-C8	2.41	110.37	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N1-C6	-2.40	120.77	125.11
5	D	501	GTP	O6-C6-C5	-2.34	120.35	126.53
5	A	501	GTP	C8-N7-C5	2.34	108.42	104.26
11	B	504	WIW	CAA-CAB-C7	2.34	120.46	114.39
5	A	501	GTP	C4-C5-N7	-2.33	106.97	110.67
9	B	501	GDP	O3'-C3'-C4'	-2.32	104.42	111.08
5	D	501	GTP	O2A-PA-O3A	2.25	113.36	107.27
5	D	501	GTP	C5-C6-N1	2.25	118.97	113.25
5	A	501	GTP	C2'-C3'-C4'	2.19	106.85	102.61
9	B	501	GDP	C5-C6-N1	2.12	118.64	113.25
11	B	504	WIW	O3'-C3'-C2'	-2.11	107.24	109.79
9	B	501	GDP	O3B-PB-O2B	-2.10	99.93	107.80
5	D	501	GTP	C8-N7-C5	2.05	107.92	104.26
5	C	501	GTP	O3A-PB-O1B	2.05	116.86	110.70
11	B	504	WIW	C8-N9-C20	2.01	117.93	114.96
5	A	501	GTP	O3A-PB-O1B	2.01	116.76	110.70
9	B	501	GDP	O6-C6-C5	-2.01	121.22	126.53

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
11	B	504	WIW	C15-C16-OP3-C24
7	C	504	EDO	O1-C1-C2-O2
11	B	504	WIW	C17-C16-OP3-C24
8	A	504	PEG	O1-C1-C2-O2
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
8	A	504	PEG	C1-C2-O2-C3

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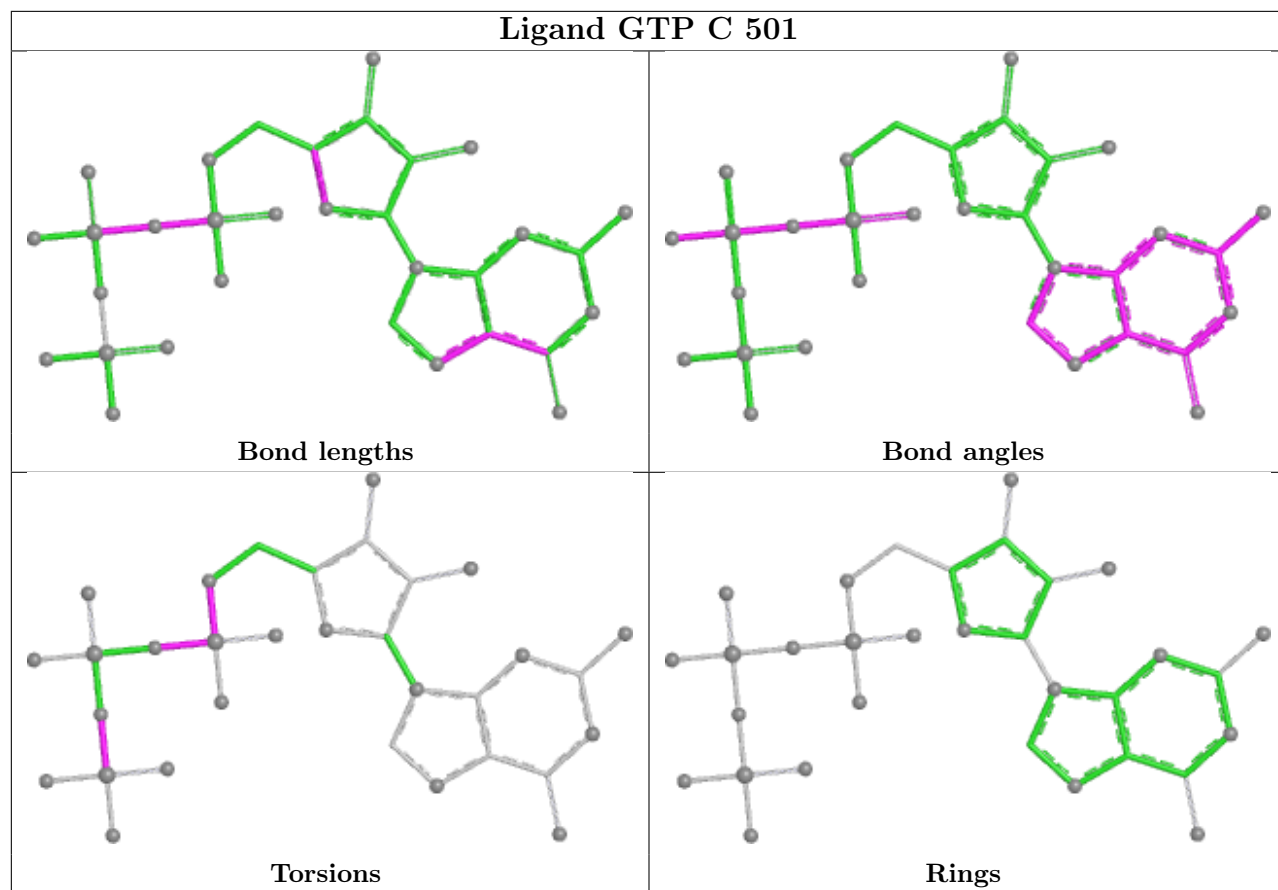
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	O4'-C4'-C5'-O5'
7	D	503	EDO	O1-C1-C2-O2
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O1A

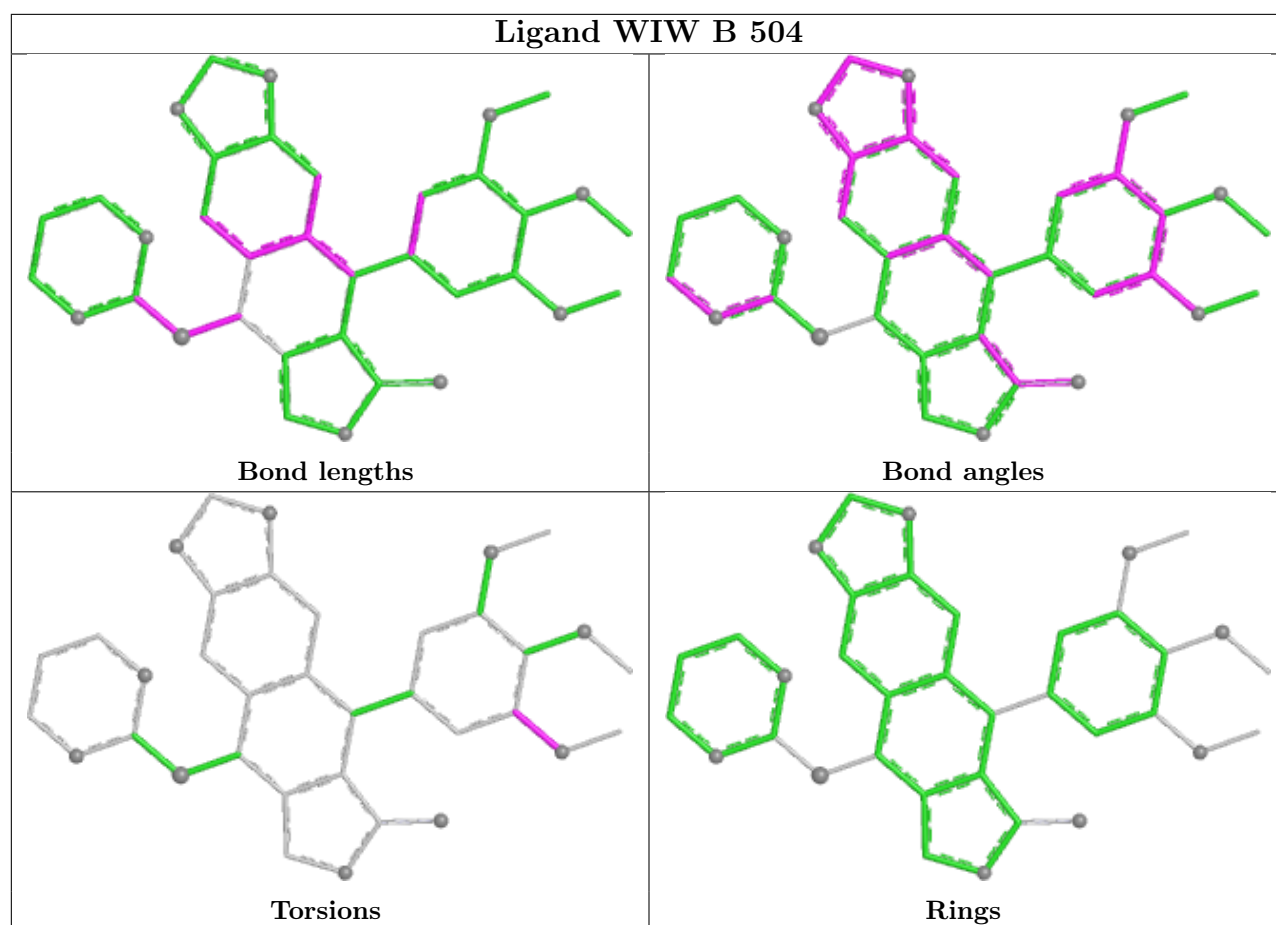
There are no ring outliers.

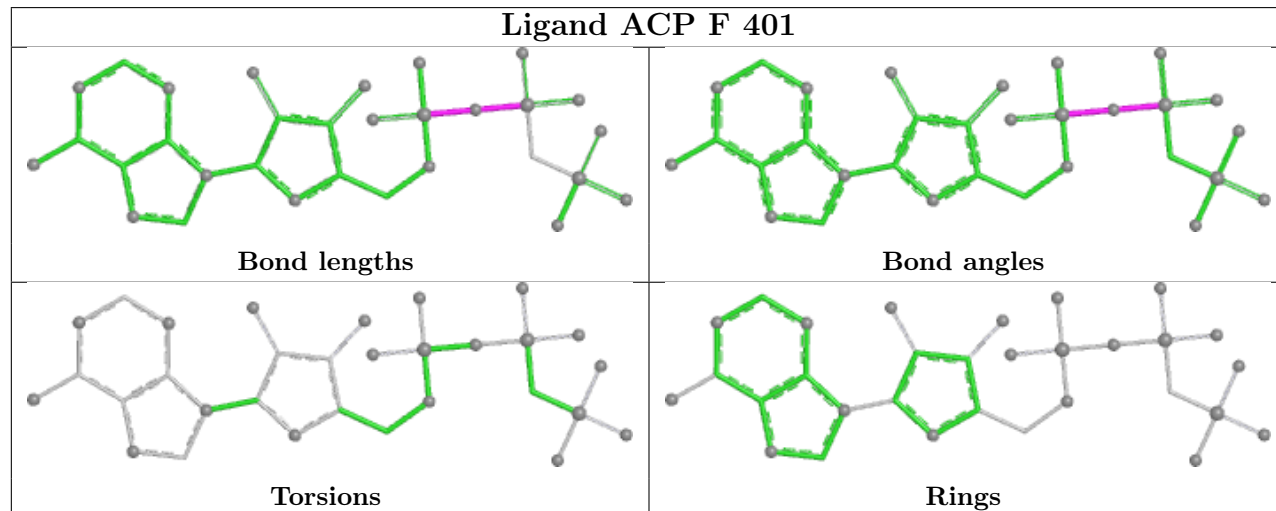
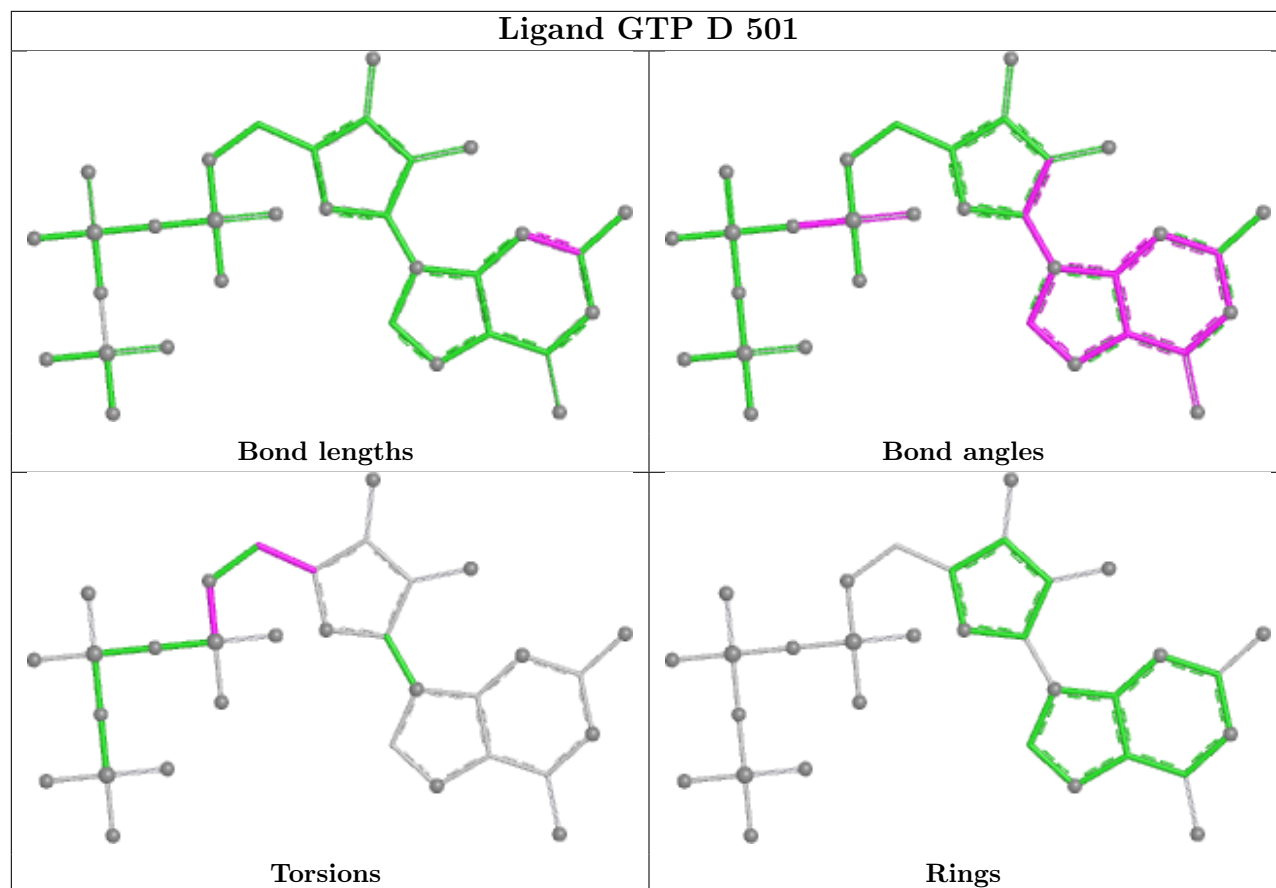
6 monomers are involved in 15 short contacts:

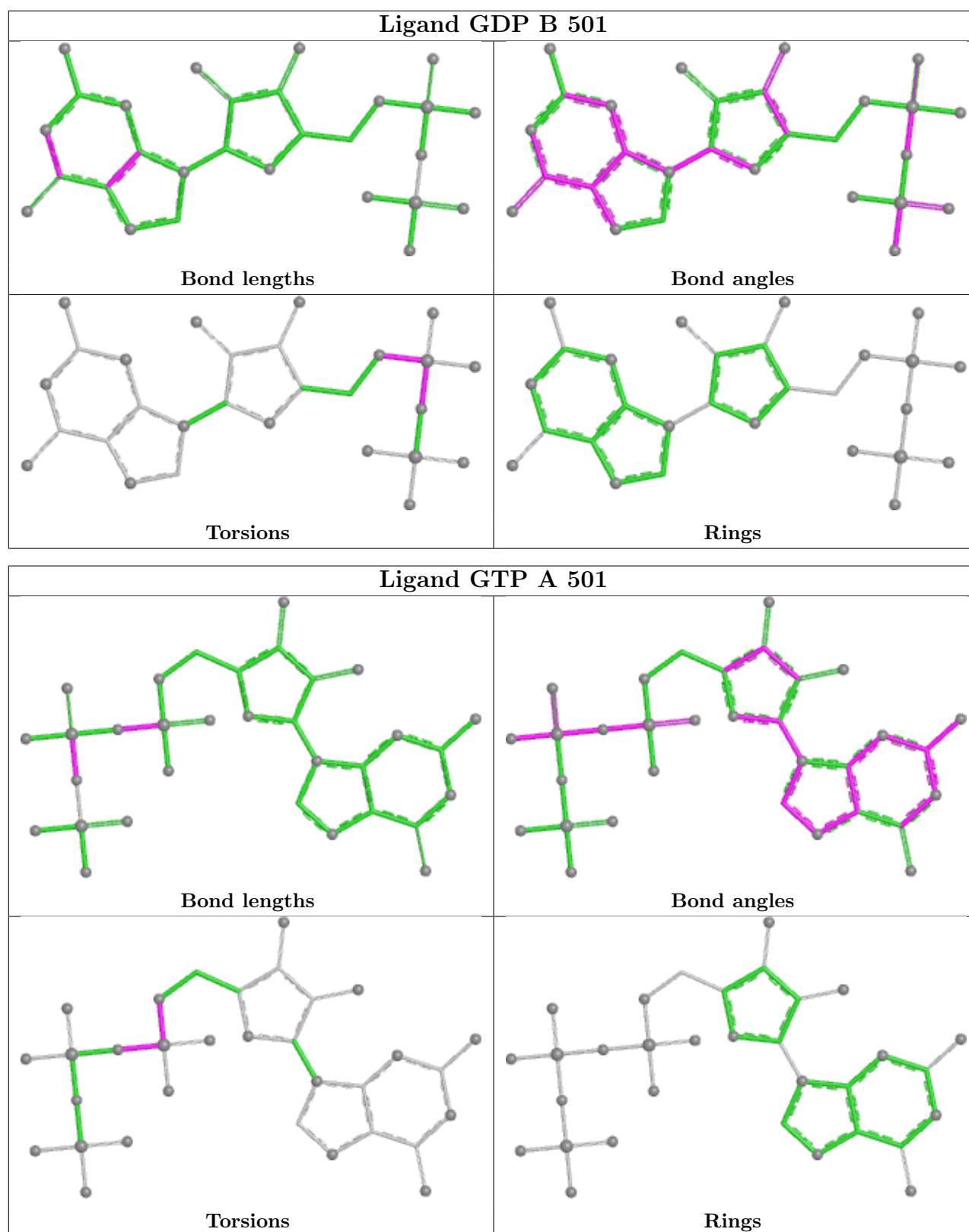
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	4	0
11	B	504	WIW	4	0
5	D	501	GTP	2	0
7	C	505	EDO	2	0
13	F	401	ACP	2	0
9	B	501	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	433/440 (98%)	0.76	42 (9%) 13 11	47, 68, 94, 118	0
1	C	440/440 (100%)	0.24	12 (2%) 56 47	40, 56, 81, 107	0
2	B	424/445 (95%)	0.41	16 (3%) 44 36	43, 64, 90, 108	0
2	D	419/445 (94%)	0.83	44 (10%) 11 10	47, 76, 99, 116	0
3	E	120/138 (86%)	0.43	3 (2%) 58 48	51, 73, 97, 106	0
4	F	317/381 (83%)	0.67	26 (8%) 17 14	58, 84, 122, 135	0
All	All	2153/2289 (94%)	0.57	143 (6%) 24 19	40, 69, 102, 135	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.7
2	D	339	SER	5.7
1	A	277	SER	5.3
1	C	178	SER	4.6
1	A	278	ALA	4.5
1	C	283	HIS	4.4
1	A	347	CYS	4.3
4	F	226	GLU	4.3
1	A	283	HIS	4.2
4	F	131	PHE	4.1
3	E	44	ASP	4.0
2	D	97	ALA	4.0
2	B	57	ASN	3.8
2	D	73	MET	3.8
2	D	99	ASN	3.7
4	F	134	ALA	3.6
2	D	176	SER	3.5
2	B	247	ASN	3.5
1	A	261	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	172	PHE	3.5
4	F	236	LYS	3.4
1	A	359	PRO	3.3
1	A	437	VAL	3.3
4	F	99	VAL	3.3
1	A	329	ASN	3.3
2	D	333	VAL	3.3
1	A	372	GLN	3.2
1	A	356	ASN	3.2
1	C	176	GLN	3.1
2	D	170	MET	3.1
1	C	73	THR	3.1
2	D	360	GLY	3.1
4	F	98	TYR	3.0
2	D	72	THR	3.0
2	D	329	GLN	3.0
1	A	274	PRO	3.0
4	F	330	ILE	3.0
1	A	46	ASP	3.0
2	B	246	LEU	3.0
1	A	371	VAL	3.0
2	D	91	VAL	2.9
2	B	1	MET	2.9
4	F	141	GLY	2.9
1	A	345	ASP	2.9
2	D	177	ASP	2.9
1	A	357	TYR	2.8
2	D	178	THR	2.8
2	D	332	ASN	2.8
4	F	237	THR	2.8
2	D	272	PRO	2.8
2	D	54	ALA	2.8
2	B	347	ASN	2.8
1	A	246	GLY	2.8
1	C	246	GLY	2.8
2	D	175	VAL	2.7
2	D	1	MET	2.7
1	C	177	VAL	2.7
3	E	6	MET	2.7
4	F	224	SER	2.7
1	A	358	GLN	2.7
1	A	343	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	260	ASN	2.7
1	C	245	ASP	2.7
2	D	164	MET	2.7
1	C	350	GLY	2.7
3	E	59	GLU	2.6
4	F	238	CYS	2.6
2	D	267	MET	2.6
2	D	391	ARG	2.6
1	A	44	GLY	2.6
2	B	280	GLN	2.6
2	B	218	THR	2.5
2	D	218	THR	2.5
2	D	240	LEU	2.5
4	F	149	ALA	2.5
1	A	370	LYS	2.5
2	D	249	ASP	2.5
4	F	324	GLU	2.5
1	A	144	GLY	2.4
2	D	301	ALA	2.4
2	D	44	LEU	2.4
2	D	404	ASP	2.4
2	D	83	GLN	2.4
1	A	349	THR	2.4
1	A	309	HIS	2.4
4	F	243	HIS	2.4
1	A	265	ILE	2.4
1	A	316	CYS	2.4
1	A	373	ARG	2.4
2	D	213	ARG	2.4
2	D	85	PHE	2.4
1	A	18	ASN	2.4
4	F	228	TYR	2.4
1	A	344	VAL	2.3
2	D	394	PHE	2.3
2	B	303	CYS	2.3
1	A	73	THR	2.3
1	A	360	PRO	2.3
4	F	197	ARG	2.3
1	A	433	GLU	2.3
1	C	284	GLU	2.3
4	F	89	GLU	2.3
1	C	357	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	380	ASN	2.3
2	D	407	GLU	2.3
2	D	224	ASP	2.3
2	D	222	TYR	2.2
1	A	350	GLY	2.2
4	F	166	ALA	2.2
1	A	98	ASP	2.2
2	B	282	ARG	2.2
1	C	375	VAL	2.2
2	D	219	THR	2.2
2	B	53	GLU	2.2
1	A	2	ARG	2.2
4	F	180	HIS	2.2
2	B	243	PRO	2.2
4	F	6	VAL	2.2
2	B	72	THR	2.2
1	A	351	PHE	2.2
4	F	240	LEU	2.2
2	B	73	MET	2.1
1	A	346	TRP	2.1
2	B	256	ASN	2.1
2	D	256	ASN	2.1
4	F	181	VAL	2.1
2	D	223	GLY	2.1
2	D	194	GLU	2.1
1	A	177	VAL	2.1
4	F	130	VAL	2.1
1	A	251	ASP	2.1
2	B	54	ALA	2.1
1	A	279	GLU	2.1
2	D	246	LEU	2.0
2	B	323	MET	2.0
1	C	295	CYS	2.0
2	D	287	PRO	2.0
2	D	395	LEU	2.0
4	F	132	LEU	2.0
2	D	337	ASN	2.0
2	D	107	THR	2.0
2	D	431	ASP	2.0
1	A	262	TYR	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](#)

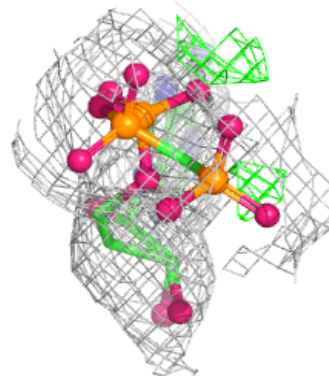
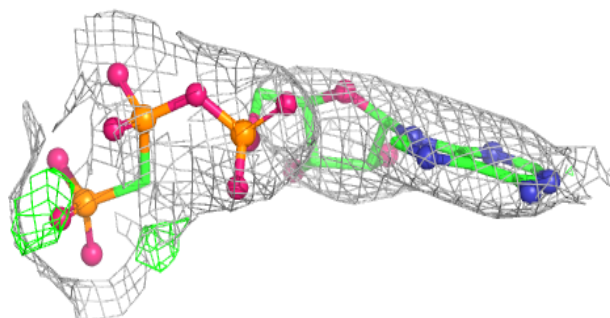
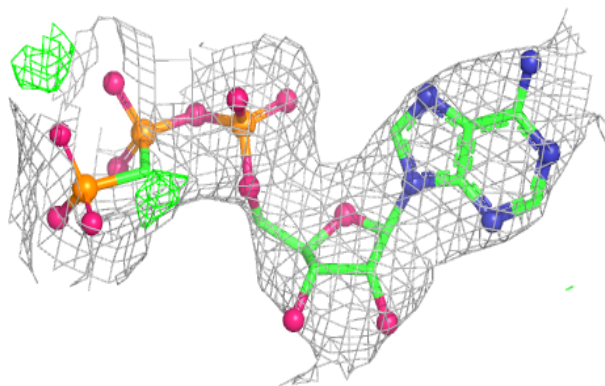
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	502	1/1	0.39	0.22	88,88,88,88	0
7	EDO	C	507	4/4	0.53	0.19	86,86,93,94	0
6	MG	C	502	1/1	0.80	0.28	55,55,55,55	0
7	EDO	D	504	4/4	0.81	0.15	87,89,90,90	0
7	EDO	A	503	4/4	0.82	0.20	67,72,80,80	0
7	EDO	B	505	4/4	0.82	0.19	65,68,71,71	0
8	PEG	A	504	7/7	0.82	0.15	72,79,87,92	0
7	EDO	C	506	4/4	0.83	0.18	68,69,71,76	0
13	ACP	F	401	31/31	0.86	0.11	88,95,112,123	0
11	WIW	B	504	36/36	0.87	0.19	48,59,69,84	36
6	MG	B	502	1/1	0.87	0.29	58,58,58,58	0
12	CA	C	503	1/1	0.88	0.08	76,76,76,76	1
7	EDO	D	503	4/4	0.88	0.13	71,74,74,86	0
7	EDO	C	505	4/4	0.89	0.11	61,67,67,70	0
6	MG	A	502	1/1	0.89	0.28	52,52,52,52	0
5	GTP	D	501	32/32	0.89	0.11	62,75,94,120	0
7	EDO	C	504	4/4	0.94	0.11	57,61,63,66	0
10	MES	B	503	12/12	0.95	0.09	57,69,75,78	0
5	GTP	C	501	32/32	0.96	0.10	43,55,67,364	0
9	GDP	B	501	28/28	0.96	0.08	41,53,59,86	0
5	GTP	A	501	32/32	0.96	0.07	43,52,57,61	0

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

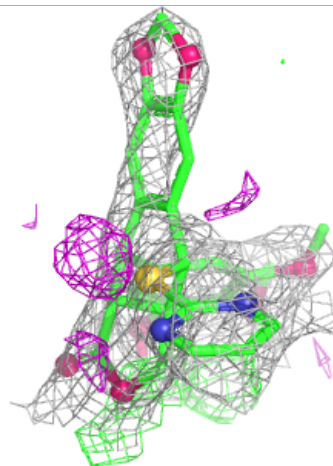
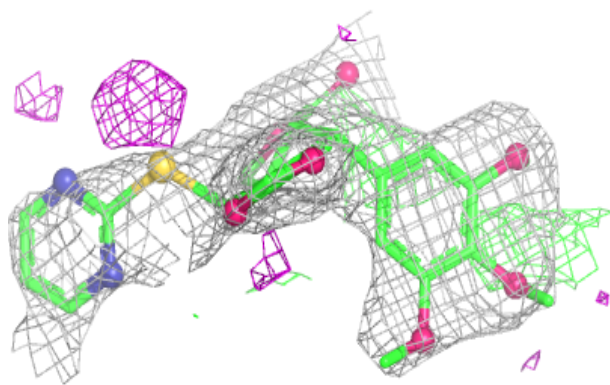
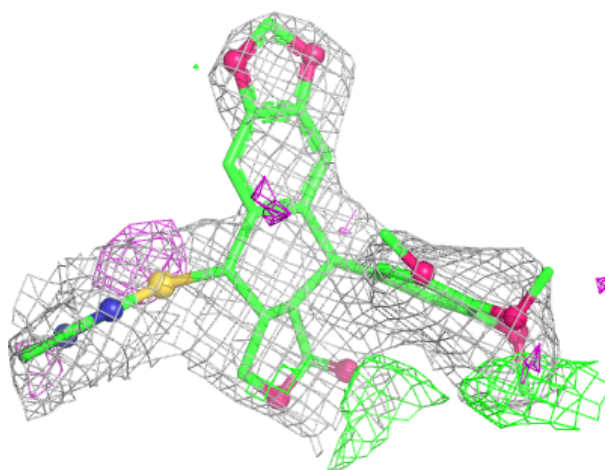
Electron density around ACP F 401:

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



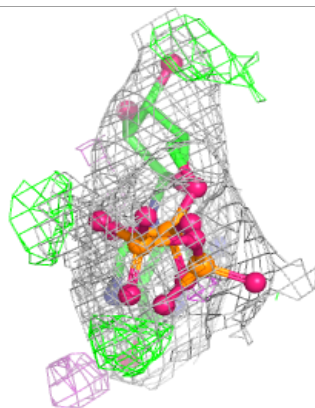
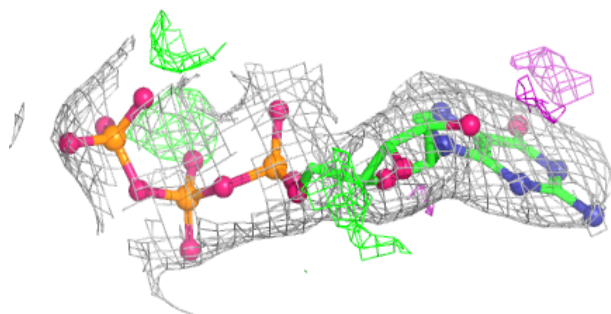
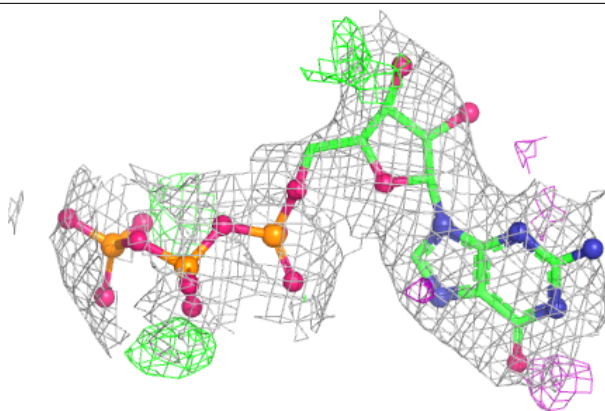
Electron density around WIW B 504:

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

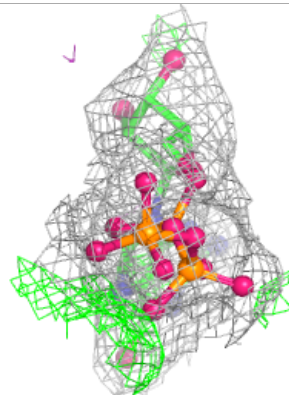
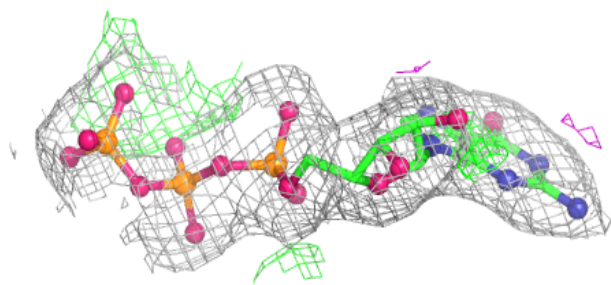
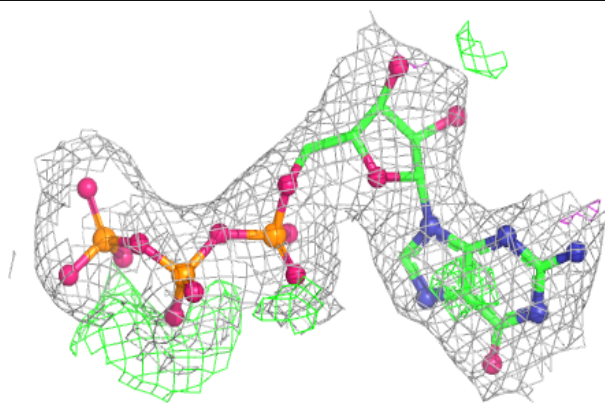


Electron density around GTP D 501:

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

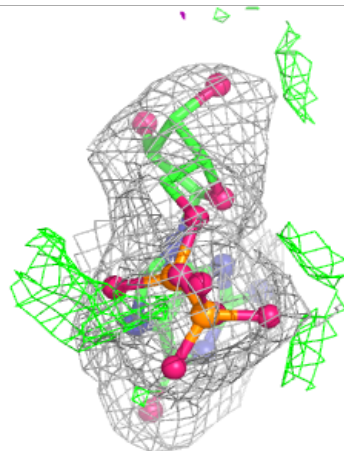
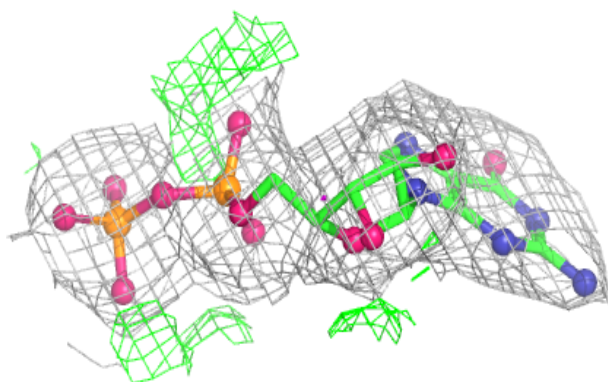
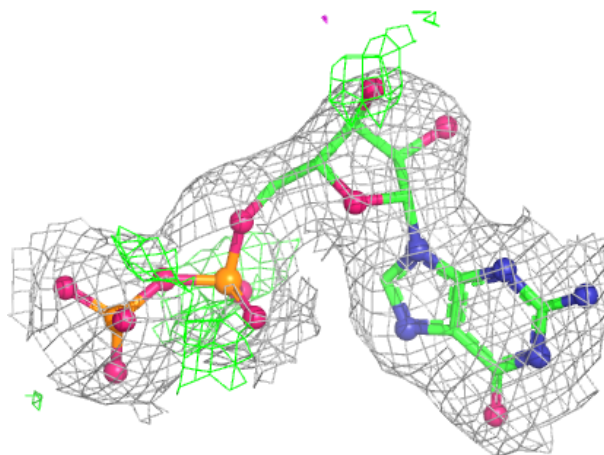
**Electron density around GTP C 501:**

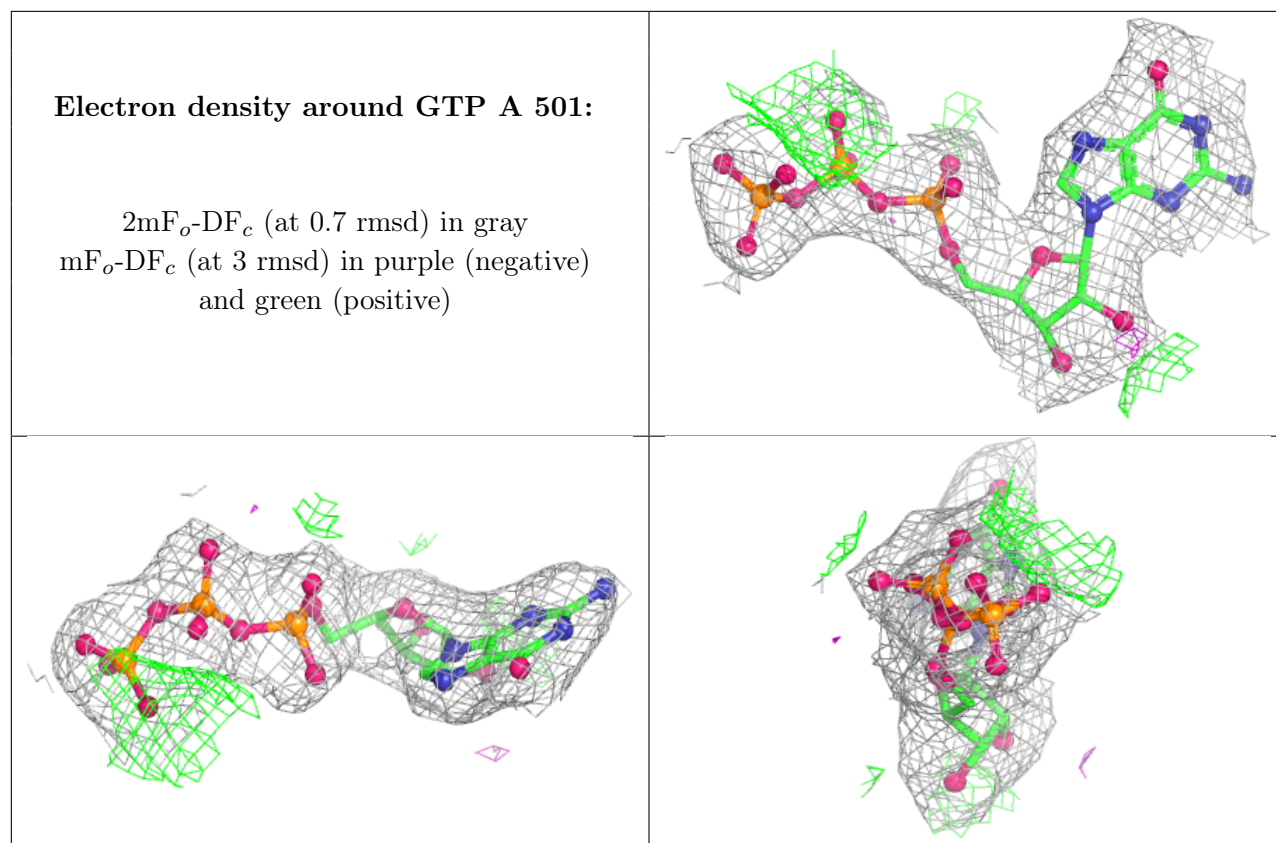
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.