



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:28 AM UTC

PDB ID : 4X1Y / pdb_00004x1y
Title : Discovery of cytotoxic Dolastatin 10 analogs with N-terminal modifications
Authors : Parris, K.D.
Deposited on : 2014-11-25
Resolution : 3.19 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

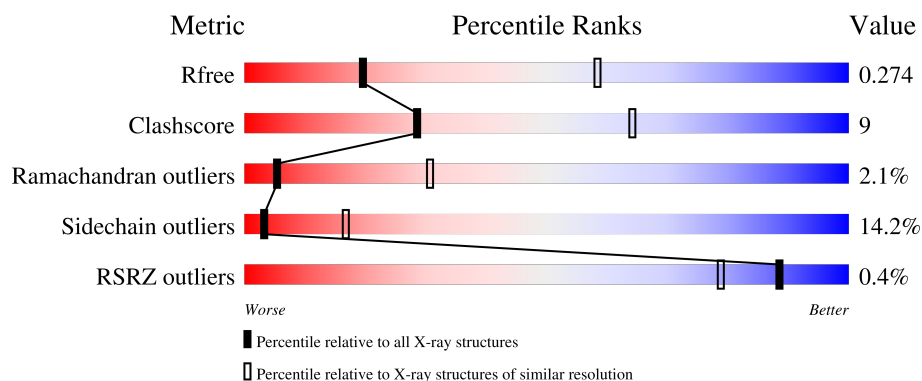
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	 63% 26% 5% • 5%
1	C	451	 67% 24% • • 5%
2	B	445	 59% 31% 5% • •
2	D	445	 66% 26% • •
3	E	142	 59% 22% 5% • 13%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14715 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3363	2132	572	638	21			
1	C	430	Total	C	N	O	S	0	2	0
			3351	2124	569	635	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3342	2100	568	649	25			
2	D	430	Total	C	N	O	S	0	1	0
			3369	2112	578	655	24			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1008	626	184	195	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

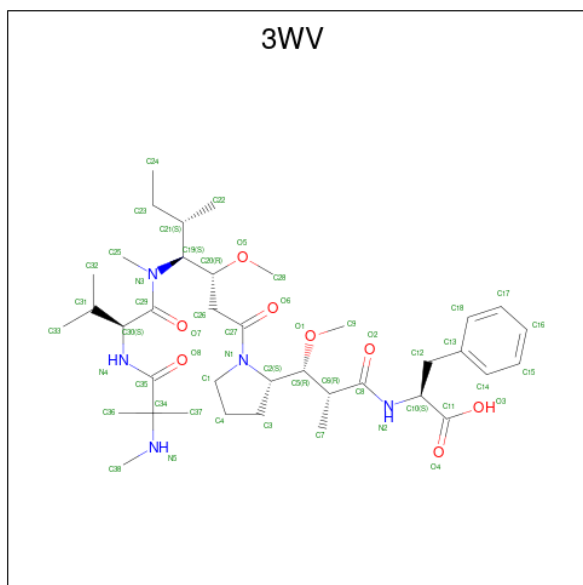
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 8 is N,2-dimethyl-L-alanyl-N-[(3R,4S,5S)-1-{(2S)-2-[(1R,2R)-3-{[(1S)-1-carboxy-2-phenylethyl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (CCD ID: 3WV) (formula: C₃₈H₆₃N₅O₈).

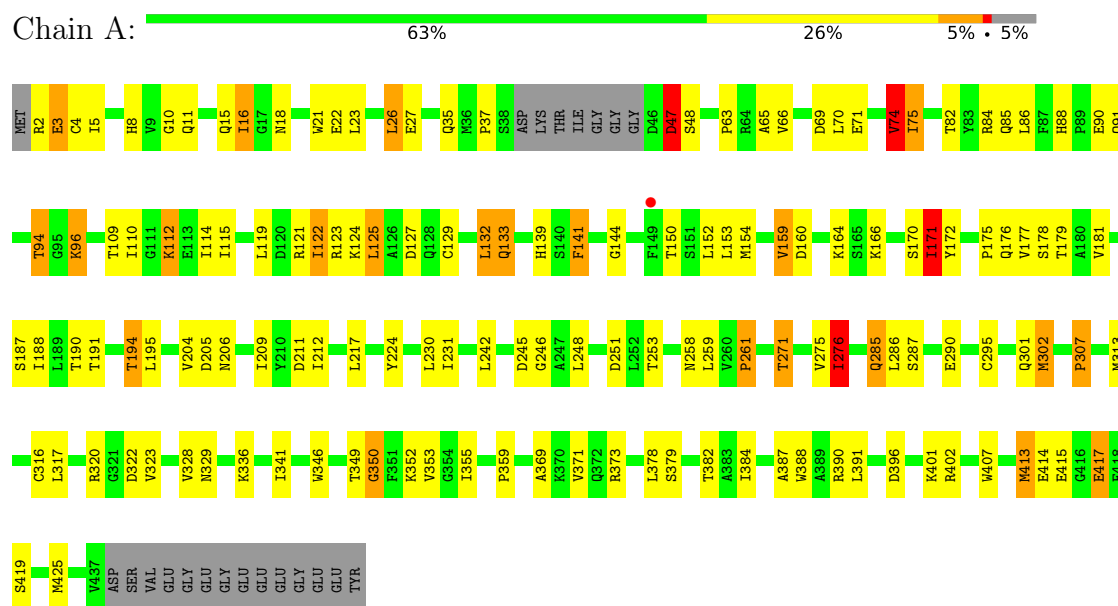


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			51	38	5	8		
8	D	1	Total	C	N	O	0	0
			51	38	5	8		

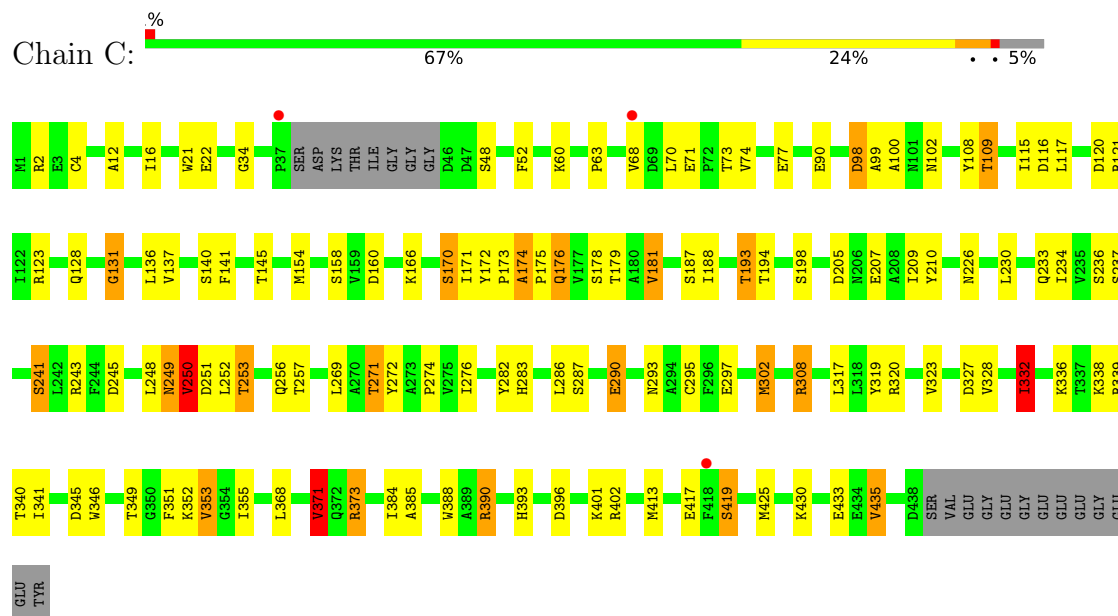
3 Residue-property plots [i](#)

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.

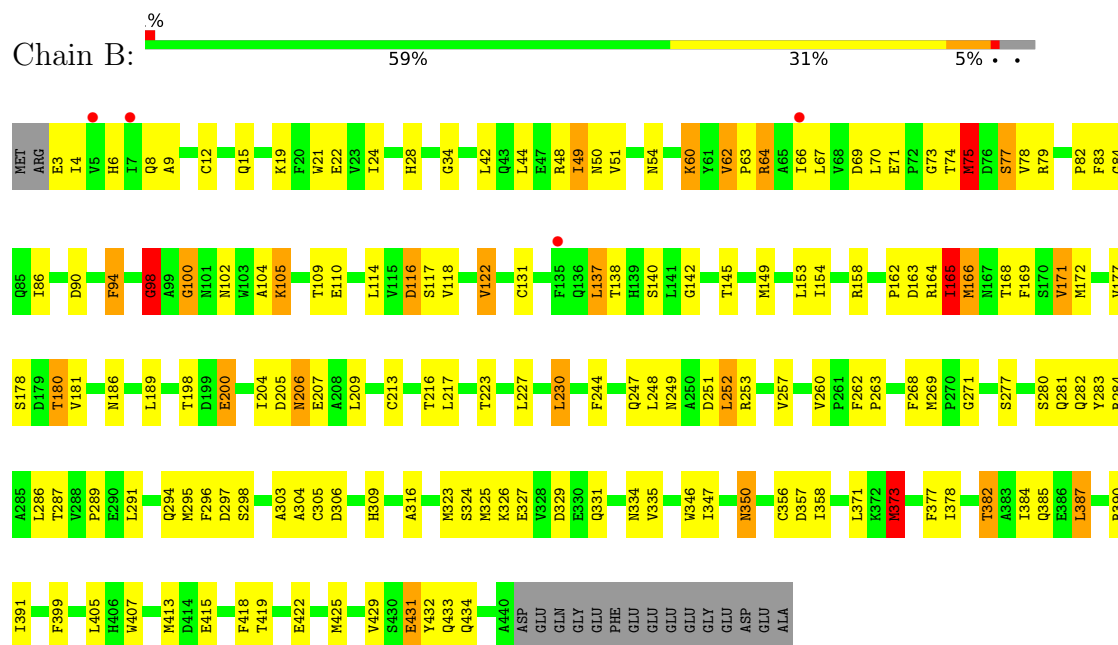
• Molecule 1: Tubulin alpha chain



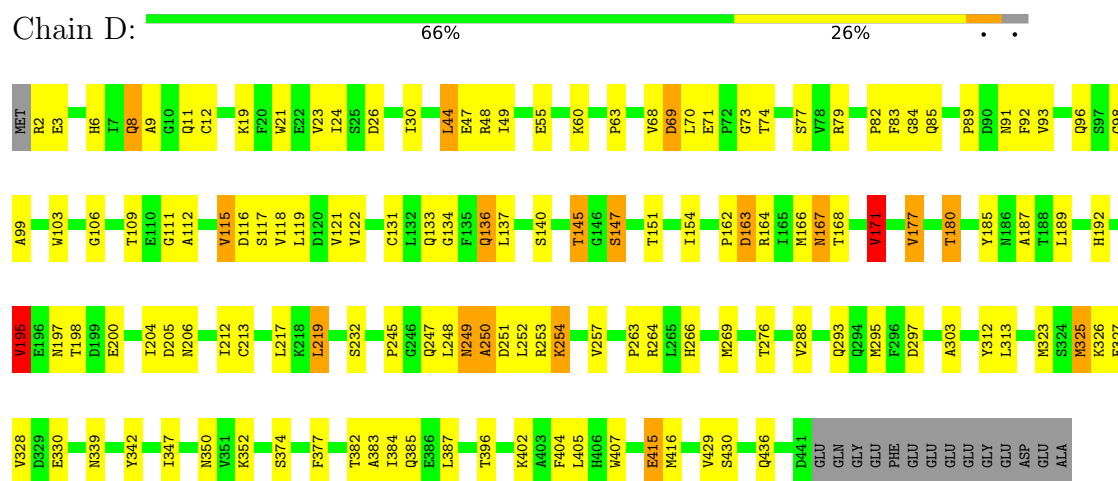
• Molecule 1: Tubulin alpha chain



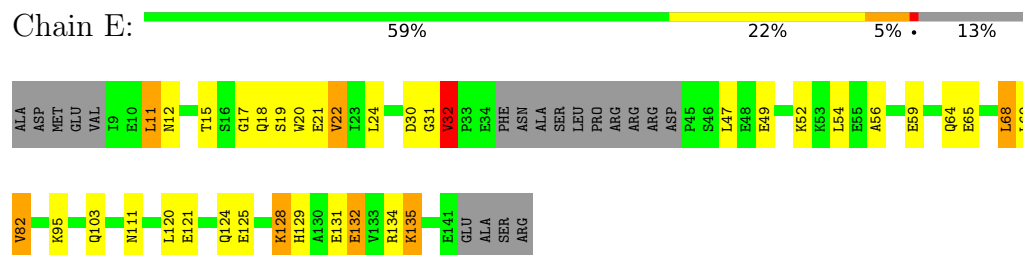
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.61Å 127.86Å 255.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.59 – 3.19 30.59 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.59-3.19) 98.9 (30.59-3.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.188 , 0.273 0.207 , 0.274	Depositor DCC
R_{free} test set	2285 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	95.4	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14715	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: LOC, MG, GTP, 3WV, GDP

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	0.89	0/3440	1.51	44/4671 (0.9%)
1	C	0.90	1/3432 (0.0%)	1.52	34/4662 (0.7%)
2	B	0.93	1/3417 (0.0%)	1.61	52/4634 (1.1%)
2	D	0.88	0/3446	1.48	27/4670 (0.6%)
3	E	0.90	1/1019 (0.1%)	1.63	5/1355 (0.4%)
All	All	0.90	3/14754 (0.0%)	1.54	162/19992 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	75	MET	SD-CE	-6.43	1.63	1.79
3	E	32	VAL	CA-C	5.72	1.58	1.52
1	C	174	ALA	CA-C	5.39	1.57	1.52

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	VAL	CA-C-N	8.85	127.67	121.65
1	C	353	VAL	C-N-CA	8.85	127.67	121.65
2	D	248	LEU	CA-C-N	8.48	136.96	121.70
2	D	248	LEU	C-N-CA	8.48	136.96	121.70
1	C	308	ARG	N-CA-C	-8.12	103.16	113.23
2	D	249	ASN	CA-C-N	7.81	135.76	121.70
2	D	249	ASN	C-N-CA	7.81	135.76	121.70
2	D	288	VAL	N-CA-CB	7.44	115.19	110.50
2	B	171	VAL	N-CA-CB	7.29	118.48	110.53
2	D	69	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	276	ILE	N-CA-C	6.93	118.79	108.46
3	E	82	VAL	N-CA-CB	6.88	118.60	110.55
2	D	9	ALA	N-CA-C	6.86	119.59	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	PHE	CA-CB-CG	6.83	120.63	113.80
1	C	98	ASP	CA-CB-CG	6.72	119.32	112.60
1	C	433	GLU	CA-C-N	6.66	129.50	120.38
1	C	433	GLU	C-N-CA	6.66	129.50	120.38
2	D	197	ASN	CA-CB-CG	6.64	119.24	112.60
2	D	163	ASP	CA-CB-CG	6.43	119.03	112.60
2	D	171	VAL	CA-C-N	6.37	129.20	120.67
2	D	171	VAL	C-N-CA	6.37	129.20	120.67
2	B	251	ASP	CA-C-N	6.33	129.59	120.79
2	B	251	ASP	C-N-CA	6.33	129.59	120.79
1	A	415	GLU	N-CA-C	-6.31	104.46	111.71
1	A	115	ILE	N-CA-C	6.25	116.74	110.23
1	A	382	THR	CA-C-N	6.25	129.28	120.28
1	A	382	THR	C-N-CA	6.25	129.28	120.28
2	D	297	ASP	CA-CB-CG	6.24	118.84	112.60
2	B	122	VAL	N-CA-CB	6.23	119.01	110.54
2	B	248	LEU	CA-C-N	6.19	132.84	121.70
2	B	248	LEU	C-N-CA	6.19	132.84	121.70
2	B	15	GLN	CA-C-N	6.17	128.56	120.60
2	B	15	GLN	C-N-CA	6.17	128.56	120.60
1	C	175	PRO	CA-C-N	6.14	128.51	120.28
1	C	175	PRO	C-N-CA	6.14	128.51	120.28
2	B	98	GLY	N-CA-C	6.13	127.72	113.18
2	B	263	PRO	CA-C-N	6.12	129.09	120.28
2	B	263	PRO	C-N-CA	6.12	129.09	120.28
1	A	350	GLY	N-CA-C	6.07	119.36	110.38
1	A	112	LYS	CA-C-N	6.07	129.23	120.79
1	A	112	LYS	C-N-CA	6.07	129.23	120.79
2	D	407	TRP	N-CA-C	-6.04	104.62	112.23
1	A	74	VAL	N-CA-C	6.03	116.21	110.42
1	A	322	ASP	CA-CB-CG	6.00	118.61	112.60
1	C	102	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	85	GLN	CA-C-N	5.94	128.52	120.38
1	A	85	GLN	C-N-CA	5.94	128.52	120.38
1	A	224	TYR	CA-C-N	5.92	128.53	120.54
1	A	224	TYR	C-N-CA	5.92	128.53	120.54
1	C	419	SER	CA-C-N	5.90	128.50	120.54
1	C	419	SER	C-N-CA	5.90	128.50	120.54
3	E	68	LEU	CA-C-N	5.90	128.18	120.28
3	E	68	LEU	C-N-CA	5.90	128.18	120.28
1	A	22	GLU	N-CA-C	-5.89	104.78	111.14
1	C	345	ASP	CA-CB-CG	5.88	118.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	ASP	N-CA-C	5.83	115.80	108.45
2	B	77	SER	CA-C-N	5.78	127.93	120.70
2	B	77	SER	C-N-CA	5.78	127.93	120.70
1	C	137	VAL	N-CA-C	5.77	116.11	107.51
2	B	390	ARG	CA-C-N	5.76	128.03	120.60
2	B	390	ARG	C-N-CA	5.76	128.03	120.60
1	C	250	VAL	N-CA-CB	5.70	120.63	111.23
1	A	359	PRO	N-CA-C	5.69	117.64	110.70
1	C	371	VAL	N-CA-CB	5.67	118.39	110.56
2	B	207	GLU	N-CA-C	-5.66	104.80	110.97
2	B	334	ASN	CA-C-N	5.64	127.67	120.56
2	B	334	ASN	C-N-CA	5.64	127.67	120.56
2	B	181	VAL	CA-C-N	5.64	129.89	120.64
2	B	181	VAL	C-N-CA	5.64	129.89	120.64
2	B	382	THR	CA-C-N	5.63	128.10	120.38
2	B	382	THR	C-N-CA	5.63	128.10	120.38
1	A	10	GLY	CA-C-N	5.63	128.09	120.38
1	A	10	GLY	C-N-CA	5.63	128.09	120.38
2	B	399	PHE	N-CA-C	5.62	117.40	111.28
2	B	116	ASP	CA-C-N	5.60	127.78	120.28
2	B	116	ASP	C-N-CA	5.60	127.78	120.28
1	C	131	GLY	CA-C-N	5.59	128.70	120.82
1	C	131	GLY	C-N-CA	5.59	128.70	120.82
2	B	304	ALA	CA-C-N	5.58	131.74	121.85
2	B	304	ALA	C-N-CA	5.58	131.74	121.85
2	B	297	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	307	PRO	CA-C-N	5.57	128.31	120.28
1	A	307	PRO	C-N-CA	5.57	128.31	120.28
2	B	418	PHE	CA-C-N	5.52	127.67	120.28
2	B	418	PHE	C-N-CA	5.52	127.67	120.28
1	A	159	VAL	CA-C-N	5.49	128.39	120.38
1	A	159	VAL	C-N-CA	5.49	128.39	120.38
1	A	285	GLN	CA-C-N	5.46	128.61	120.90
1	A	285	GLN	C-N-CA	5.46	128.61	120.90
2	B	189	LEU	CA-C-N	5.45	127.85	120.44
2	B	189	LEU	C-N-CA	5.45	127.85	120.44
2	B	244	PHE	N-CA-C	5.44	118.95	108.45
2	D	162	PRO	CA-C-N	5.43	128.57	120.31
2	D	162	PRO	C-N-CA	5.43	128.57	120.31
2	B	9	ALA	N-CA-C	5.43	117.75	108.90
2	B	357	ASP	N-CA-C	5.41	118.98	112.38
1	C	396	ASP	CA-C-N	5.39	127.45	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	396	ASP	C-N-CA	5.39	127.45	120.44
2	D	297	ASP	CA-C-N	5.39	127.77	120.38
2	D	297	ASP	C-N-CA	5.39	127.77	120.38
1	C	226	ASN	CA-CB-CG	5.38	117.98	112.60
2	D	3	GLU	N-CA-C	5.37	118.86	110.32
2	D	313	LEU	N-CA-C	-5.36	104.86	111.40
2	D	327	GLU	N-CA-C	-5.35	105.36	111.14
1	C	390	ARG	CA-C-N	5.35	127.39	120.44
1	C	390	ARG	C-N-CA	5.35	127.39	120.44
2	B	207	GLU	CA-C-N	5.32	127.36	120.44
2	B	207	GLU	C-N-CA	5.32	127.36	120.44
2	B	297	ASP	CA-C-N	5.32	128.15	120.38
2	B	297	ASP	C-N-CA	5.32	128.15	120.38
1	C	181	VAL	N-CA-CB	5.30	117.75	110.54
1	A	211	ASP	CA-C-N	5.29	127.70	120.46
1	A	211	ASP	C-N-CA	5.29	127.70	120.46
2	B	294	GLN	CA-C-N	5.28	127.61	120.38
2	B	294	GLN	C-N-CA	5.28	127.61	120.38
1	A	26	LEU	CA-C-N	5.28	127.88	120.28
1	A	26	LEU	C-N-CA	5.28	127.88	120.28
2	B	326	LYS	CA-C-N	5.26	127.64	120.54
2	B	326	LYS	C-N-CA	5.26	127.64	120.54
1	C	332	ILE	CA-C-N	5.25	127.58	120.44
1	C	332	ILE	C-N-CA	5.25	127.58	120.44
3	E	111	ASN	CA-CB-CG	5.24	117.84	112.60
2	D	167	ASN	CA-CB-CG	5.24	117.84	112.60
3	E	128	LYS	N-CA-C	-5.21	105.25	111.03
1	A	127	ASP	N-CA-C	-5.20	106.78	113.01
2	B	94	PHE	N-CA-C	5.19	117.14	108.99
2	B	171	VAL	CB-CA-C	5.18	117.89	111.15
1	A	47	ASP	CA-CB-CG	5.18	117.78	112.60
2	B	180	THR	CA-C-N	5.17	127.54	120.46
2	B	180	THR	C-N-CA	5.17	127.54	120.46
2	B	162	PRO	CA-C-N	5.16	128.16	120.31
2	B	162	PRO	C-N-CA	5.16	128.16	120.31
1	C	193	THR	N-CA-C	5.16	116.91	111.28
1	C	22	GLU	N-CA-C	-5.13	105.34	111.03
2	D	187	ALA	CA-C-N	5.09	127.42	120.54
2	D	187	ALA	C-N-CA	5.09	127.42	120.54
1	C	393	HIS	CA-C-N	5.09	127.41	120.54
1	C	393	HIS	C-N-CA	5.09	127.41	120.54
1	A	415	GLU	CA-C-N	5.09	125.73	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	GLU	C-N-CA	5.09	125.73	120.03
1	A	144	GLY	CA-C-N	5.08	129.11	120.88
1	A	144	GLY	C-N-CA	5.08	129.11	120.88
1	A	176	GLN	CA-C-N	5.07	129.75	122.45
1	A	176	GLN	C-N-CA	5.07	129.75	122.45
2	B	165	ILE	N-CA-C	5.06	116.09	109.21
2	D	330	GLU	CA-C-N	5.06	127.02	120.44
2	D	330	GLU	C-N-CA	5.06	127.02	120.44
1	A	171	ILE	CB-CA-C	5.06	118.10	111.53
1	A	122	ILE	N-CA-C	-5.05	105.92	110.82
2	B	165	ILE	CB-CA-C	5.05	118.51	111.34
1	C	373	ARG	N-CA-C	5.04	117.61	108.69
1	A	4	CYS	N-CA-C	5.03	116.50	107.80
1	C	272	TYR	N-CA-C	5.03	117.33	110.24
1	C	282	TYR	CA-C-N	5.03	131.15	121.54
1	C	282	TYR	C-N-CA	5.03	131.15	121.54
2	D	180	THR	CA-C-N	5.01	127.33	120.46
2	D	180	THR	C-N-CA	5.01	127.33	120.46
1	A	396	ASP	N-CA-C	5.01	117.64	111.82
1	A	84	ARG	CA-C-N	5.01	127.41	120.29
1	A	84	ARG	C-N-CA	5.01	127.41	120.29
1	A	152	LEU	CA-C-N	5.01	126.95	120.44
1	A	152	LEU	C-N-CA	5.01	126.95	120.44

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	3363	0	3274	61	0
1	C	3351	0	3258	54	0
2	B	3342	0	3198	68	0
2	D	3369	0	3237	64	0
3	E	1008	0	1022	14	0
4	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	1	0
7	B	29	0	25	0	0
7	D	29	0	25	0	0
8	B	51	0	61	2	0
8	D	51	0	61	4	0
All	All	14715	0	14209	255	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 9.

All (255) 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:252:LEU:HD23	1:C:253:THR:H	1.23	1.00
2:D:133:GLN:HE21	2:D:252:LEU:H	1.18	0.88
1:C:308:ARG:NE	1:C:340:THR:HG21	1.89	0.87
2:B:306:ASP:HB3	2:B:309:HIS:HD2	1.42	0.83
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.64	0.80
2:D:69:ASP:HA	2:D:145:THR:HG21	1.64	0.79
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.67	0.77
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.66	0.76
1:A:301:GLN:HE22	1:A:307:PRO:HG3	1.52	0.74
2:B:48:ARG:HH12	2:B:249:ASN:H	1.35	0.74
1:A:171:ILE:HG23	1:A:206:ASN:HD21	1.54	0.72
2:B:253:ARG:O	2:B:257:VAL:HG23	1.90	0.71
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.73	0.70
1:C:338:LYS:HD3	1:C:340:THR:HB	1.74	0.69
1:C:308:ARG:CD	1:C:340:THR:HG21	2.22	0.68
1:A:259:LEU:O	1:A:261:PRO:HD3	1.93	0.68
2:D:106:GLY:O	2:D:111:GLY:HA3	1.92	0.68
1:A:276:ILE:HG23	1:A:369:ALA:HB3	1.75	0.68
1:C:302:MET:HE3	1:C:302:MET:HA	1.75	0.68
2:D:249:ASN:H	2:D:250:ALA:HB2	1.58	0.67
8:D:503:3WV:C25	8:D:503:3WV:H5	2.24	0.67
1:C:252:LEU:HD23	1:C:253:THR:N	2.04	0.66
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.36	0.66
2:D:19:LYS:O	2:D:23:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.78	0.66
2:B:324:SER:HB3	2:B:327:GLU:HB2	1.78	0.66
1:A:387:ALA:HA	1:A:390:ARG:HE	1.61	0.66
1:C:287:SER:HA	1:C:373:ARG:HH21	1.61	0.66
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.78	0.65
1:C:308:ARG:CZ	1:C:340:THR:HG21	2.26	0.65
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.78	0.65
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.77	0.65
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.79	0.65
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.78	0.65
1:C:241:SER:HA	1:C:250:VAL:HB	1.79	0.64
2:D:249:ASN:N	2:D:250:ALA:HB2	2.12	0.64
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.78	0.64
2:D:195:VAL:HG22	2:D:264:ARG:HG2	1.80	0.64
2:B:431:GLU:HA	2:B:434:GLN:HE21	1.63	0.63
2:D:192:HIS:O	2:D:195:VAL:HG12	1.99	0.63
8:D:503:3WV:H5	8:D:503:3WV:H51	1.80	0.62
3:E:11:LEU:HB2	3:E:20:TRP:HA	1.82	0.62
3:E:11:LEU:HD23	3:E:21:GLU:HB2	1.80	0.62
1:C:308:ARG:HD2	1:C:340:THR:HG21	1.82	0.61
2:B:331:GLN:O	2:B:335:VAL:HG23	2.01	0.61
2:B:206:ASN:HD21	6:B:501:GDP:HN22	1.48	0.61
3:E:129:HIS:O	3:E:132:GLU:HG3	2.02	0.60
1:A:246:GLY:HA2	3:E:17:GLY:HA3	1.83	0.59
2:B:271:GLY:HA3	2:B:377:PHE:HB3	1.84	0.59
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.83	0.59
1:C:308:ARG:HD2	1:C:340:THR:CG2	2.33	0.59
1:C:141:PHE:CE1	1:C:170:SER:HB2	2.37	0.59
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.84	0.59
2:B:44:LEU:HD23	2:B:49:ILE:HD13	1.84	0.58
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.51	0.58
1:C:385:ALA:HA	1:C:388:TRP:HD1	1.68	0.58
2:B:50:ASN:O	2:B:64:ARG:NH2	2.36	0.58
2:D:253:ARG:O	2:D:257:VAL:HG23	2.01	0.58
1:C:302:MET:HA	1:C:302:MET:CE	2.34	0.57
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.85	0.57
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.86	0.57
2:B:382:THR:HA	2:B:432:TYR:HD2	1.68	0.57
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.40	0.57
1:C:346:TRP:HZ2	1:C:435:VAL:HG22	1.70	0.57
2:D:206:ASN:HD21	6:D:501:GDP:HN22	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.87	0.56
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.87	0.56
2:D:249:ASN:HA	2:D:250:ALA:CB	2.36	0.56
2:D:44:LEU:HA	2:D:49:ILE:HB	1.88	0.56
2:D:415:GLU:H	2:D:415:GLU:CD	2.14	0.56
1:A:69:ASP:HB3	1:A:75:ILE:HD12	1.87	0.55
2:B:83:PHE:O	2:B:86:ILE:HG22	2.06	0.55
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.87	0.55
1:A:5:ILE:HG12	1:A:132:LEU:HD11	1.88	0.55
1:A:204:VAL:HG22	1:A:302:MET:HE1	1.88	0.55
1:A:3:GLU:HG3	1:A:129:CYS:HB3	1.89	0.55
2:B:142:GLY:O	2:B:186:ASN:ND2	2.41	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.54
2:D:136:GLN:HA	2:D:167:ASN:O	2.07	0.54
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.90	0.54
1:C:286:LEU:HD23	1:C:290:GLU:HB3	1.88	0.54
1:C:237:SER:HA	1:C:320:ARG:HH11	1.72	0.54
2:D:133:GLN:HE21	2:D:252:LEU:N	1.97	0.54
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.44	0.53
2:B:79:ARG:HH22	2:B:94:PHE:HE2	1.57	0.53
2:B:407:TRP:CZ2	1:C:257:THR:HA	2.43	0.53
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.90	0.53
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.90	0.53
2:D:116:ASP:HA	2:D:119:LEU:HD12	1.90	0.53
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.90	0.53
1:A:154:MET:HG3	1:A:194:THR:HG23	1.90	0.53
1:C:70:LEU:HG	1:C:145:THR:HG23	1.91	0.53
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.44	0.53
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.73	0.52
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.90	0.52
2:D:71:GLU:HG2	2:D:98:GLY:HA2	1.91	0.52
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.91	0.52
1:A:286:LEU:HD23	1:A:290:GLU:HB3	1.92	0.52
2:D:133:GLN:NE2	2:D:252:LEU:H	1.98	0.52
2:B:323:MET:HE3	2:B:373:MET:HE3	1.91	0.52
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.91	0.52
1:A:23:LEU:HA	1:A:26:LEU:HD12	1.92	0.51
2:D:382:THR:OG1	2:D:436:GLN:HG3	2.10	0.51
2:B:346:TRP:CD1	2:B:346:TRP:H	2.28	0.51
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.76	0.51
2:B:217:LEU:HD11	2:B:230:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:THR:HA	2:D:154:ILE:HD12	1.93	0.50
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.46	0.50
1:A:70:LEU:HD21	1:A:114:ILE:HG21	1.94	0.50
1:A:328:VAL:HG21	1:A:355:ILE:HD11	1.92	0.50
1:C:269:LEU:HB2	1:C:384:ILE:HD13	1.93	0.50
2:D:166:MET:HG3	2:D:198:THR:HG22	1.93	0.50
1:C:174:ALA:HB1	1:C:176:GLN:HE22	1.76	0.50
2:D:83:PHE:O	2:D:85:GLN:N	2.45	0.50
2:D:103:TRP:HD1	2:D:147:SER:HB2	1.77	0.50
2:D:89:PRO:HA	2:D:92:PHE:CD1	2.48	0.49
2:D:249:ASN:HA	2:D:250:ALA:HB3	1.93	0.49
2:D:68:VAL:HG22	2:D:93:VAL:HB	1.95	0.49
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.94	0.49
2:B:164:ARG:NH1	2:B:253:ARG:HH22	2.11	0.49
1:A:191:THR:O	1:A:195:LEU:HB2	2.12	0.49
2:B:137:LEU:HD22	2:B:154:ILE:HD11	1.94	0.49
1:A:11:GLN:HG2	1:A:15:GLN:HE21	1.78	0.49
1:A:346:TRP:HE3	3:E:32:VAL:HG13	1.77	0.49
2:D:325:MET:HA	2:D:328:VAL:HB	1.94	0.49
2:B:34:GLY:O	2:B:60:LYS:HA	2.13	0.48
2:D:263:PRO:O	2:D:266:HIS:HD2	1.96	0.48
1:C:176:GLN:H	1:C:176:GLN:NE2	2.11	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.13	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.48
1:A:175:PRO:HA	1:A:179:THR:HG21	1.95	0.48
1:C:252:LEU:CD2	1:C:253:THR:H	2.11	0.48
1:A:96:LYS:HG2	2:B:131:CYS:HB2	1.95	0.48
1:A:329:ASN:ND2	3:E:22:VAL:HG11	2.28	0.48
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.48	0.48
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.30	0.48
1:C:141:PHE:HB2	1:C:173:PRO:HD3	1.94	0.48
1:A:407:TRP:CE2	2:B:257:VAL:HA	2.48	0.48
2:D:134:GLY:HA2	2:D:164:ARG:HB3	1.96	0.48
1:A:258:ASN:HA	1:A:352:LYS:HZ2	1.79	0.48
1:C:34:GLY:HA3	1:C:60:LYS:HG2	1.95	0.48
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.96	0.48
1:C:317:LEU:HD13	1:C:332:ILE:HD11	1.96	0.48
2:D:177:VAL:HA	8:D:503:3WV:H43	1.95	0.48
2:B:382:THR:HA	2:B:432:TYR:CD2	2.48	0.47
2:D:213:CYS:HA	2:D:217:LEU:HD12	1.95	0.47
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ASP:HB3	2:D:254:LYS:HB2	1.96	0.47
2:D:119:LEU:HA	2:D:122:VAL:HG22	1.95	0.47
1:A:212:ILE:HG23	1:A:275:VAL:HG11	1.95	0.47
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.33	0.47
2:B:260:VAL:HG12	2:B:262:PHE:O	2.15	0.47
2:B:425:MET:O	2:B:429:VAL:HG23	2.14	0.47
1:C:176:GLN:H	1:C:176:GLN:CD	2.22	0.47
2:B:28:HIS:HB3	2:B:49:ILE:HD11	1.96	0.47
1:A:261:PRO:HG2	1:A:313:MET:HG3	1.97	0.47
1:A:5:ILE:HD12	1:A:125:LEU:HD22	1.97	0.46
1:C:271:THR:HG21	1:C:295:CYS:O	2.14	0.46
4:A:600:GTP:O2A	4:A:600:GTP:H8	1.98	0.46
2:B:78:VAL:O	2:B:84:GLY:HA3	2.15	0.46
2:D:249:ASN:CA	2:D:250:ALA:CB	2.93	0.46
1:A:16:ILE:HG12	1:A:231:ILE:HG21	1.97	0.46
1:A:329:ASN:HD21	3:E:22:VAL:HG11	1.79	0.46
2:B:371:LEU:H	2:B:371:LEU:HD23	1.81	0.46
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.98	0.46
1:A:287:SER:HA	1:A:373:ARG:HH11	1.81	0.46
2:B:350:ASN:H	2:B:350:ASN:HD22	1.63	0.46
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.33	0.46
1:A:123:ARG:HH22	1:A:160:ASP:HB3	1.80	0.46
2:B:166:MET:HB3	2:B:198:THR:HA	1.97	0.46
1:A:248:LEU:HB2	3:E:19:SER:HB3	1.98	0.46
3:E:125:GLU:HA	3:E:128:LYS:HE3	1.98	0.46
1:A:133:GLN:HE22	1:A:251:ASP:HA	1.81	0.45
2:B:385:GLN:HE22	2:B:433:GLN:NE2	2.15	0.45
1:A:75:ILE:HB	1:A:94:THR:HG23	1.99	0.45
1:A:90:GLU:O	1:A:121:ARG:HG2	2.16	0.45
2:B:98:GLY:C	2:B:100:GLY:H	2.24	0.45
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.52	0.45
1:C:249:ASN:CB	1:C:355:ILE:H	2.29	0.45
8:B:503:3WV:H24	8:B:503:3WV:H38	1.99	0.45
2:D:339:ASN:HB3	2:D:342:TYR:HD2	1.82	0.45
1:A:141:PHE:HD1	1:A:172:TYR:HA	1.81	0.45
2:D:2:ARG:HB3	2:D:131:CYS:HB3	1.99	0.45
2:B:204:ILE:HG22	2:B:209:LEU:HD11	1.99	0.44
3:E:56:ALA:HA	3:E:59:GLU:CD	2.43	0.44
8:B:503:3WV:H46	8:B:503:3WV:H31	1.99	0.44
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.99	0.44
1:C:249:ASN:HB2	1:C:355:ILE:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:TRP:CE3	1:C:425:MET:HE1	2.53	0.44
2:B:165:ILE:HG22	2:B:252:LEU:HD23	2.00	0.44
2:B:28:HIS:HD1	2:B:49:ILE:HD12	1.82	0.44
2:B:114:LEU:O	2:B:118:VAL:HG23	2.17	0.43
2:B:280:SER:HA	2:B:281:GLN:HA	1.73	0.43
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.64	0.43
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.83	0.43
1:C:207:GLU:O	1:C:210:TYR:HB3	2.17	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.17	0.43
1:C:346:TRP:CZ2	1:C:435:VAL:HG22	2.53	0.43
1:A:75:ILE:HB	1:A:94:THR:CG2	2.48	0.43
2:B:172:MET:O	2:B:206:ASN:HB2	2.19	0.43
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.00	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.43
2:D:68:VAL:HG21	2:D:118:VAL:HG13	2.01	0.43
3:E:132:GLU:HA	3:E:135:LYS:HB3	1.99	0.43
1:C:52:PHE:CD1	1:C:243:ARG:HG2	2.54	0.43
8:D:503:3WV:H5	8:D:503:3WV:H50	1.99	0.43
2:D:6:HIS:HD2	2:D:136:GLN:OE1	2.01	0.43
1:A:350:GLY:HA2	3:E:24:LEU:HD12	2.01	0.43
1:C:158:SER:OG	1:C:166:LYS:HE3	2.18	0.43
2:D:30:ILE:HD11	2:D:49:ILE:HD11	2.00	0.43
1:A:316:CYS:HB2	1:A:378:LEU:HB2	2.02	0.42
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.01	0.42
1:A:175:PRO:HA	1:A:179:THR:CG2	2.49	0.42
2:B:387:LEU:O	2:B:391:ILE:HG12	2.19	0.42
2:D:185:TYR:O	2:D:189:LEU:HG	2.19	0.42
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.34	0.42
1:C:174:ALA:HB1	1:C:176:GLN:NE2	2.33	0.42
2:B:54:ASN:HB2	2:B:62:VAL:HG13	2.01	0.42
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.01	0.42
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.01	0.42
1:A:317:LEU:HD12	1:A:353:VAL:HG22	2.00	0.42
2:D:198:THR:OG1	2:D:266:HIS:CE1	2.73	0.42
2:D:112:ALA:O	2:D:115:VAL:HG12	2.19	0.42
2:D:295:MET:HE2	2:D:295:MET:HB3	1.73	0.42
2:D:213:CYS:HB3	2:D:219:LEU:HD12	2.02	0.42
1:A:112:LYS:HE3	3:E:54:LEU:HB3	2.02	0.41
1:A:119:LEU:HA	1:A:122:ILE:HD12	2.02	0.41
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.19	0.41
2:B:154:ILE:HG23	2:B:166:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:LEU:HD23	2:B:149:MET:HE1	2.02	0.41
2:D:79:ARG:HH21	2:D:89:PRO:HB3	1.85	0.41
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.41
2:B:22:GLU:HB2	2:B:83:PHE:CD2	2.56	0.41
2:D:12:CYS:CB	2:D:140:SER:HB3	2.45	0.41
2:D:47:GLU:HB3	2:D:245:PRO:HG3	2.03	0.41
2:D:249:ASN:CA	2:D:250:ALA:HB2	2.51	0.41
2:B:12:CYS:CB	2:B:140:SER:HB3	2.51	0.41
2:B:305:CYS:SG	2:B:384:ILE:HA	2.61	0.41
1:C:70:LEU:HD12	1:C:99:ALA:HB2	2.02	0.41
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.39	0.41
2:D:91:ASN:HA	2:D:121:VAL:HG11	2.03	0.41
2:D:269:MET:HE1	2:D:383:ALA:HB3	2.02	0.41
1:C:154:MET:HG3	1:C:194:THR:HG23	2.02	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.56	0.41
1:A:346:TRP:H	1:A:346:TRP:CD1	2.39	0.40
1:C:302:MET:HE3	1:C:302:MET:CA	2.48	0.40
1:A:21:TRP:CE2	1:A:65:ALA:HB2	2.56	0.40
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.03	0.40
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.57	0.40
1:A:271:THR:HG23	1:A:301:GLN:HA	2.02	0.40
2:B:69:ASP:HA	2:B:145:THR:HG21	2.04	0.40
2:B:74:THR:O	2:B:77:SER:HB3	2.21	0.40
1:C:413:MET:HE3	1:C:417:GLU:HB2	2.04	0.40
2:B:205:ASP:O	2:B:209:LEU:HG	2.22	0.40
1:C:413:MET:HE2	1:C:413:MET:HB3	1.86	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	425/451 (94%)	378 (89%)	40 (9%)	7 (2%)	7	36
1	C	428/451 (95%)	377 (88%)	41 (10%)	10 (2%)	5	29
2	B	426/445 (96%)	384 (90%)	31 (7%)	11 (3%)	4	26
2	D	429/445 (96%)	396 (92%)	25 (6%)	8 (2%)	6	33
3	E	119/142 (84%)	112 (94%)	4 (3%)	3 (2%)	4	27
All	All	1827/1934 (94%)	1647 (90%)	141 (8%)	39 (2%)	5	31

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	LYS
2	B	98	GLY
1	C	249	ASN
1	C	283	HIS
2	D	84	GLY
2	D	250	ALA
3	E	32	VAL
1	A	178	SER
2	B	109	THR
2	B	282	GLN
2	B	283	TYR
2	B	373	MET
1	C	73	THR
2	D	73	GLY
2	D	109	THR
3	E	31	GLY
2	B	100	GLY
1	C	109	THR
2	D	180	THR
2	D	404	PHE
3	E	15	THR
2	B	284	ARG
1	C	108	TYR
1	C	250	VAL
2	D	82	PRO
1	A	261	PRO
1	A	413	MET
2	B	73	GLY
1	C	241	SER
1	C	336	LYS
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	349	THR
2	B	82	PRO
2	B	178	SER
1	A	341	ILE
1	C	131	GLY
1	A	37	PRO
1	C	115	ILE
2	D	195	VAL

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	362/378 (96%)	308 (85%)	54 (15%)	3	15
1	C	359/378 (95%)	307 (86%)	52 (14%)	3	16
2	B	364/383 (95%)	310 (85%)	54 (15%)	3	15
2	D	369/383 (96%)	331 (90%)	38 (10%)	7	28
3	E	107/125 (86%)	84 (78%)	23 (22%)	1	6
All	All	1561/1647 (95%)	1340 (86%)	221 (14%)	3	17

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	GLU
1	A	16	ILE
1	A	27	GLU
1	A	35	GLN
1	A	47	ASP
1	A	48	SER
1	A	66	VAL
1	A	71	GLU
1	A	74	VAL
1	A	75	ILE

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Mol	Chain	Res	Type
1	A	82	THR
1	A	86	LEU
1	A	94	THR
1	A	96	LYS
1	A	109	THR
1	A	124	LYS
1	A	125	LEU
1	A	132	LEU
1	A	133	GLN
1	A	141	PHE
1	A	153	LEU
1	A	164	LYS
1	A	166	LYS
1	A	170	SER
1	A	171	ILE
1	A	181	VAL
1	A	187	SER
1	A	188	ILE
1	A	190	THR
1	A	194	THR
1	A	209	ILE
1	A	217	LEU
1	A	230	LEU
1	A	242	LEU
1	A	245	ASP
1	A	253	THR
1	A	271	THR
1	A	276	ILE
1	A	285	GLN
1	A	295	CYS
1	A	302	MET
1	A	320	ARG
1	A	323	VAL
1	A	336	LYS
1	A	371	VAL
1	A	379	SER
1	A	384	ILE
1	A	391	LEU
1	A	401	LYS
1	A	402	ARG
1	A	414	GLU
1	A	417	GLU

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Mol	Chain	Res	Type
1	A	419	SER
2	B	3	GLU
2	B	4	ILE
2	B	19	LYS
2	B	24	ILE
2	B	42	LEU
2	B	49	ILE
2	B	51	VAL
2	B	62	VAL
2	B	64	ARG
2	B	66	ILE
2	B	67	LEU
2	B	70	LEU
2	B	71	GLU
2	B	75	MET
2	B	90	ASP
2	B	105	LYS
2	B	110	GLU
2	B	116	ASP
2	B	117	SER
2	B	122	VAL
2	B	137	LEU
2	B	153	LEU
2	B	158	ARG
2	B	163	ASP
2	B	165	ILE
2	B	166	MET
2	B	171	VAL
2	B	177	VAL
2	B	180	THR
2	B	200	GLU
2	B	206	ASN
2	B	216	THR
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	247	GLN
2	B	252	LEU
2	B	277	SER
2	B	286	LEU
2	B	291	LEU
2	B	296	PHE

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Mol	Chain	Res	Type
2	B	298	SER
2	B	325	MET
2	B	329	ASP
2	B	350	ASN
2	B	356	CYS
2	B	358	ILE
2	B	373	MET
2	B	387	LEU
2	B	405	LEU
2	B	415	GLU
2	B	419	THR
2	B	422	GLU
2	B	431	GLU
1	C	2	ARG
1	C	16	ILE
1	C	48	SER
1	C	68	VAL
1	C	74	VAL
1	C	77	GLU
1	C	90	GLU
1	C	109	THR
1	C	116	ASP
1	C	117	LEU
1	C	120	ASP
1	C	121	ARG
1	C	123	ARG
1	C	128	GLN
1	C	160	ASP
1	C	170	SER
1	C	171	ILE
1	C	176	GLN
1	C	178	SER
1	C	179	THR
1	C	181	VAL
1	C	187	SER
1	C	188	ILE
1	C	193	THR
1	C	198	SER
1	C	233	GLN
1	C	236	SER
1	C	245	ASP
1	C	248	LEU

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Mol	Chain	Res	Type
1	C	251	ASP
1	C	253	THR
1	C	256	GLN
1	C	271	THR
1	C	276	ILE
1	C	290	GLU
1	C	293	ASN
1	C	297	GLU
1	C	302	MET
1	C	327	ASP
1	C	332	ILE
1	C	339	ARG
1	C	341	ILE
1	C	349	THR
1	C	352	LYS
1	C	368	LEU
1	C	371	VAL
1	C	390	ARG
1	C	401	LYS
1	C	402	ARG
1	C	419	SER
1	C	430	LYS
1	C	435	VAL
2	D	8	GLN
2	D	24	ILE
2	D	26	ASP
2	D	44	LEU
2	D	48	ARG
2	D	55	GLU
2	D	60	LYS
2	D	77	SER
2	D	96	GLN
2	D	115	VAL
2	D	117	SER
2	D	136	GLN
2	D	145	THR
2	D	147	SER
2	D	163	ASP
2	D	171	VAL
2	D	177	VAL
2	D	195	VAL
2	D	200	GLU

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Mol	Chain	Res	Type
2	D	212	ILE
2	D	219	LEU
2	D	247	GLN
2	D	254	LYS
2	D	276	THR
2	D	293	GLN
2	D	323	MET
2	D	325	MET
2	D	326	LYS
2	D	352	LYS
2	D	374	SER
2	D	384	ILE
2	D	387	LEU
2	D	396	THR
2	D	402	LYS
2	D	405	LEU
2	D	415	GLU
2	D	416	MET
2	D	430	SER
3	E	11	LEU
3	E	12	ASN
3	E	18	GLN
3	E	22	VAL
3	E	30	ASP
3	E	49	GLU
3	E	52	LYS
3	E	64	GLN
3	E	65	GLU
3	E	68	LEU
3	E	69	LEU
3	E	72	LEU
3	E	80	ARG
3	E	82	VAL
3	E	95	LYS
3	E	103	GLN
3	E	120	LEU
3	E	121	GLU
3	E	124	GLN
3	E	131	GLU
3	E	132	GLU
3	E	134	ARG
3	E	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	28	HIS
1	A	91	GLN
1	A	128	GLN
1	A	139	HIS
1	A	192	HIS
1	A	206	ASN
1	A	258	ASN
1	A	301	GLN
1	A	372	GLN
1	A	406	HIS
2	B	8	GLN
2	B	14	ASN
2	B	91	ASN
2	B	96	GLN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	309	HIS
2	B	350	ASN
2	B	385	GLN
2	B	424	ASN
2	B	434	GLN
2	B	436	GLN
1	C	8	HIS
1	C	18	ASN
1	C	35	GLN
1	C	50	ASN
1	C	128	GLN
1	C	176	GLN
1	C	249	ASN
1	C	293	ASN
1	C	393	HIS
2	D	6	HIS
2	D	91	ASN
2	D	133	GLN
2	D	139	HIS
2	D	193	GLN
2	D	197	ASN

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Mol	Chain	Res	Type
2	D	206	ASN
2	D	249	ASN
2	D	266	HIS
2	D	300	ASN
2	D	331	GLN
2	D	339	ASN
2	D	424	ASN
2	D	426	ASN
2	D	433	GLN
3	E	12	ASN
3	E	18	GLN
3	E	90	ASN
3	E	111	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
8	3WV	B	503	-	51,52,52	1.16	6 (11%)	58,73,73	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LOC	B	502	-	31,31,31	0.71	1 (3%)	44,44,44	0.89	1 (2%)
4	GTP	C	600	5	33,34,34	2.22	2 (6%)	50,54,54	0.55	0
7	LOC	D	502	-	31,31,31	0.52	0	44,44,44	0.78	3 (6%)
4	GTP	A	600	5	33,34,34	2.29	2 (6%)	50,54,54	0.53	0
6	GDP	D	501	-	29,30,30	0.55	0	45,47,47	0.55	0
6	GDP	B	501	-	29,30,30	0.49	0	45,47,47	0.60	0
8	3WV	D	503	-	51,52,52	1.19	6 (11%)	58,73,73	1.79	12 (20%)

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
8	3WV	B	503	-	-	18/74/85/85	0/2/2/2
7	LOC	B	502	-	-	0/12/25/25	0/3/3/3
4	GTP	C	600	5	-	6/22/38/38	0/3/3/3
7	LOC	D	502	-	-	0/12/25/25	0/3/3/3
4	GTP	A	600	5	-	8/22/38/38	0/3/3/3
6	GDP	D	501	-	-	5/16/32/32	0/3/3/3
6	GDP	B	501	-	-	7/16/32/32	0/3/3/3
8	3WV	D	503	-	-	13/74/85/85	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	PA-O3A	-9.16	1.49	1.59
4	A	600	GTP	PB-O3B	-8.97	1.49	1.59
4	C	600	GTP	PB-O3B	-8.81	1.50	1.59
4	C	600	GTP	PA-O3A	-8.68	1.50	1.59
8	D	503	3WV	C19-N3	5.24	1.58	1.47
8	B	503	3WV	C19-N3	4.67	1.57	1.47
7	B	502	LOC	C11-C14	3.44	1.58	1.53
8	B	503	3WV	C20-C19	3.42	1.60	1.52
8	B	503	3WV	O4-C11	3.24	1.31	1.22
8	D	503	3WV	C6-C8	3.16	1.57	1.52
8	D	503	3WV	O4-C11	3.15	1.31	1.22
8	B	503	3WV	C21-C19	2.78	1.60	1.54
8	B	503	3WV	C6-C8	2.74	1.56	1.52
8	D	503	3WV	O3-C11	-2.69	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	3WV	C20-C19	2.58	1.58	1.52
8	B	503	3WV	O3-C11	-2.40	1.23	1.30
8	D	503	3WV	C21-C19	2.25	1.59	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	3WV	C25-N3-C19	-5.44	108.73	119.48
7	B	502	LOC	C14-C11-N1	5.28	118.48	114.31
8	B	503	3WV	C25-N3-C19	-4.83	109.94	119.48
8	B	503	3WV	C19-N3-C29	4.79	134.05	120.34
8	B	503	3WV	C22-C21-C19	4.65	123.78	111.38
8	D	503	3WV	C31-C30-C29	4.46	119.43	110.71
8	D	503	3WV	C30-C29-N3	4.33	127.36	118.80
8	D	503	3WV	O1-C5-C6	4.07	115.48	105.83
8	D	503	3WV	O7-C29-C30	-3.71	112.97	119.96
8	D	503	3WV	C25-N3-C29	3.50	133.51	122.24
8	D	503	3WV	C31-C30-N4	3.34	119.51	111.44
8	B	503	3WV	C6-C8-N2	-3.04	111.86	116.35
8	B	503	3WV	O1-C5-C6	2.98	112.90	105.83
8	D	503	3WV	C35-C34-N5	-2.97	105.78	110.53
8	B	503	3WV	O4-C11-C10	-2.94	112.78	122.26
8	B	503	3WV	O3-C11-C10	2.80	122.99	113.51
8	B	503	3WV	C35-C34-N5	-2.70	106.22	110.53
8	D	503	3WV	O3-C11-C10	2.65	122.48	113.51
8	D	503	3WV	O4-C11-C10	-2.60	113.86	122.26
7	D	502	LOC	C11-C14-C15	-2.18	115.14	117.06
8	D	503	3WV	C7-C6-C8	-2.15	104.51	108.77
8	D	503	3WV	C30-N4-C35	2.10	125.93	121.29
8	B	503	3WV	C25-N3-C29	-2.07	115.58	122.24
7	D	502	LOC	C10-C11-N1	2.05	113.51	109.76
7	D	502	LOC	C10-C11-C14	2.02	113.26	110.71

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
6	D	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O1A
6	D	501	GDP	C5'-O5'-PA-O2A
8	B	503	3WV	C30-C29-N3-C25
8	B	503	3WV	O7-C29-N3-C25
8	B	503	3WV	C21-C19-C20-C26
8	B	503	3WV	N3-C19-C20-O5
8	B	503	3WV	C21-C19-C20-O5
8	B	503	3WV	C20-C19-C21-C23
8	B	503	3WV	N3-C19-C21-C22
8	B	503	3WV	C6-C5-O1-C9
8	D	503	3WV	C36-C34-N5-C38
8	D	503	3WV	C37-C34-N5-C38
8	D	503	3WV	O7-C29-C30-C31
8	D	503	3WV	N3-C29-C30-C31
8	D	503	3WV	N3-C19-C20-C26
8	D	503	3WV	C26-C20-O5-C28
8	B	503	3WV	C36-C34-C35-O8
8	B	503	3WV	C36-C34-C35-N4
8	B	503	3WV	N5-C34-C35-N4
8	B	503	3WV	N5-C34-C35-O8
8	B	503	3WV	C22-C21-C23-C24
8	D	503	3WV	C22-C21-C23-C24
8	D	503	3WV	C19-C21-C23-C24
8	D	503	3WV	C29-C30-C31-C33
8	D	503	3WV	C31-C30-N4-C35
8	D	503	3WV	C6-C5-O1-C9
8	B	503	3WV	N3-C19-C21-C23
4	C	600	GTP	PB-O3A-PA-O1A
6	B	501	GDP	C3'-C4'-C5'-O5'
8	B	503	3WV	C19-C21-C23-C24
4	A	600	GTP	C5'-O5'-PA-O1A
8	B	503	3WV	N3-C19-C20-C26
8	D	503	3WV	C12-C10-C11-O4
8	D	503	3WV	C12-C10-C11-O3
6	B	501	GDP	O4'-C4'-C5'-O5'
6	D	501	GDP	O4'-C4'-C5'-O5'
6	D	501	GDP	C3'-C4'-C5'-O5'
4	A	600	GTP	C4'-C5'-O5'-PA

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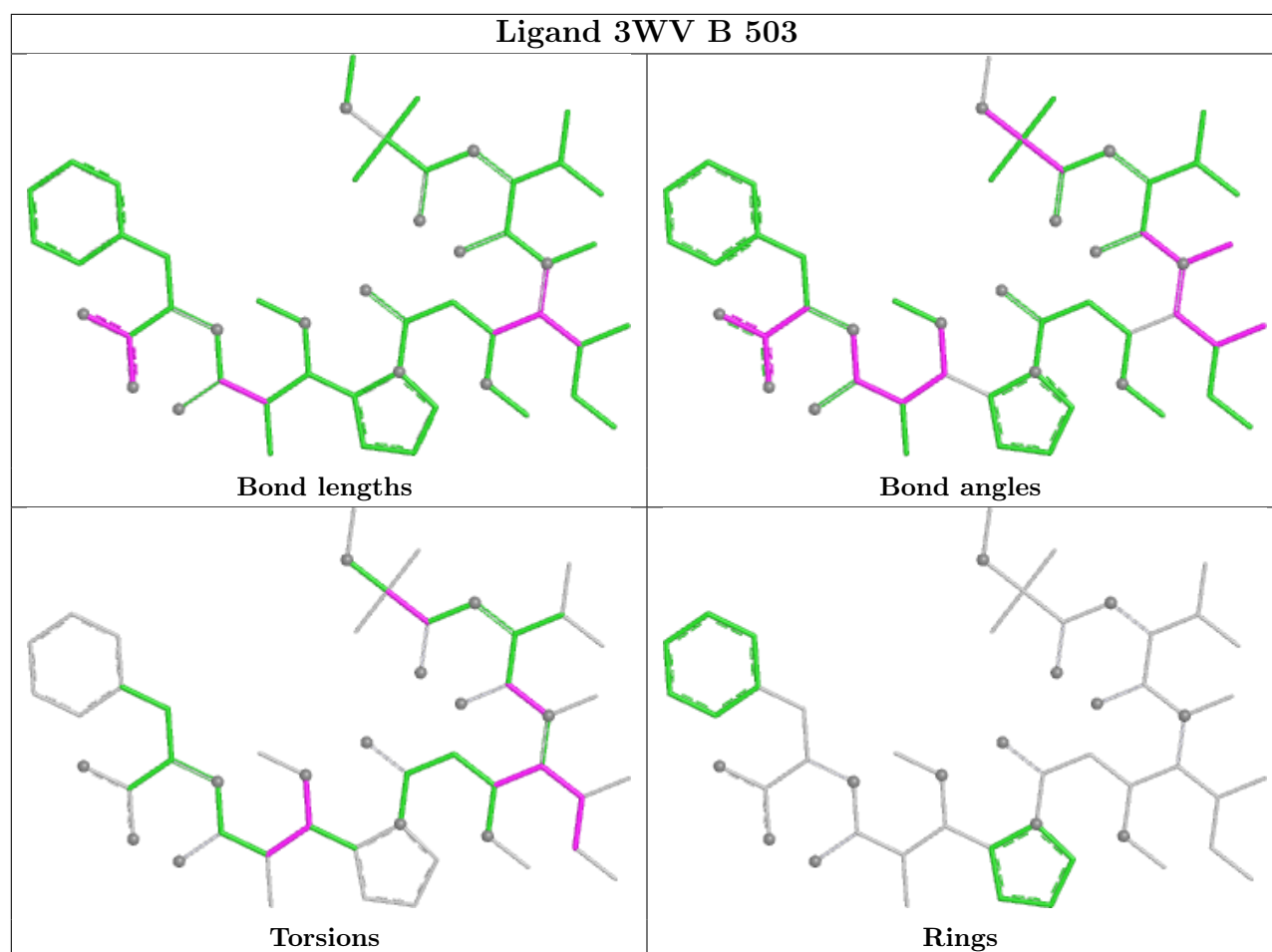
Mol	Chain	Res	Type	Atoms
8	B	503	3WV	C2-C5-C6-C8
4	A	600	GTP	PA-O3A-PB-O2B
6	B	501	GDP	PB-O3A-PA-O1A
4	A	600	GTP	C3'-C4'-C5'-O5'
6	B	501	GDP	C4'-C5'-O5'-PA
8	B	503	3WV	O7-C29-N3-C19
4	A	600	GTP	O4'-C4'-C5'-O5'
4	C	600	GTP	C4'-C5'-O5'-PA
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A

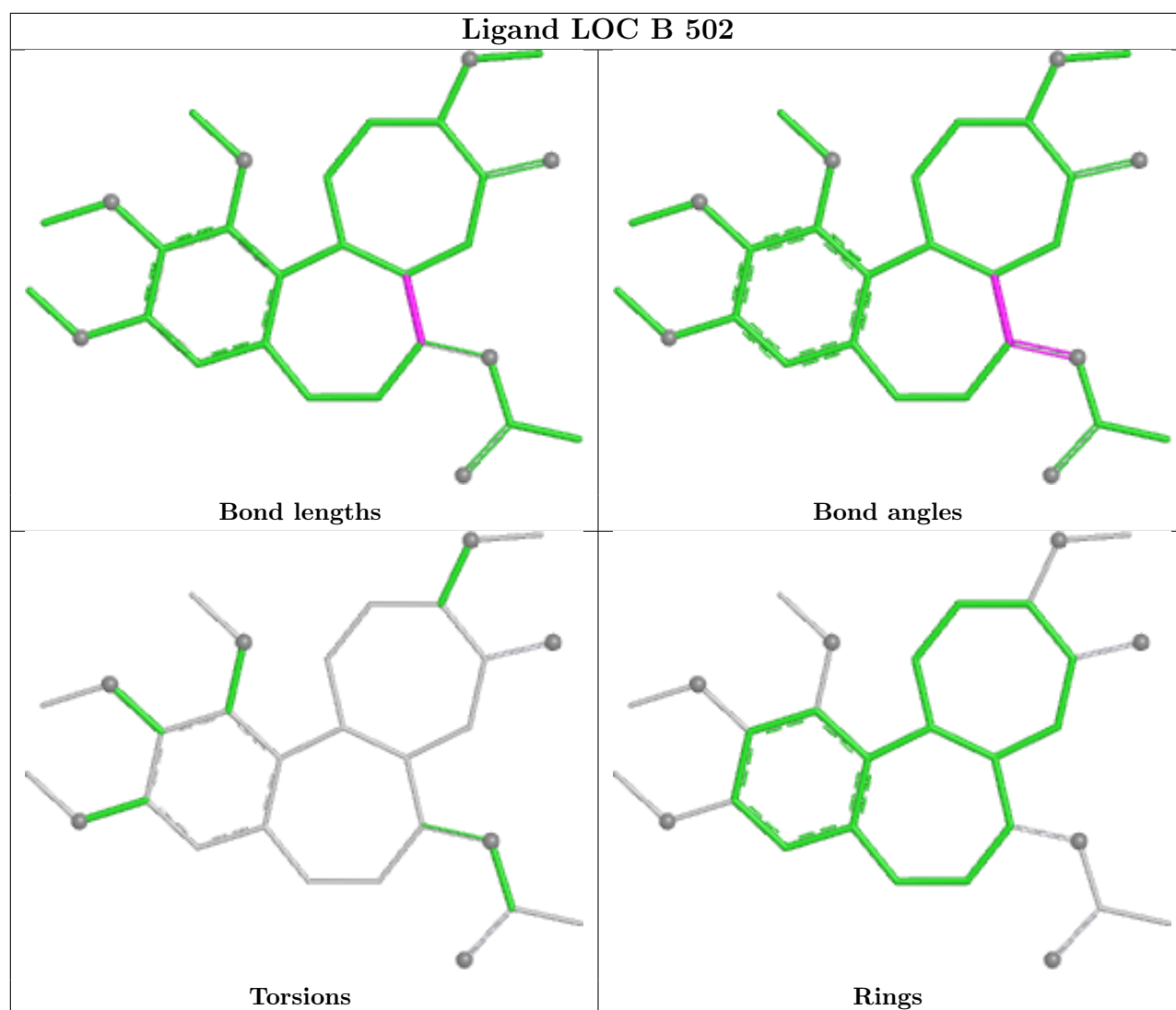
There are no ring outliers.

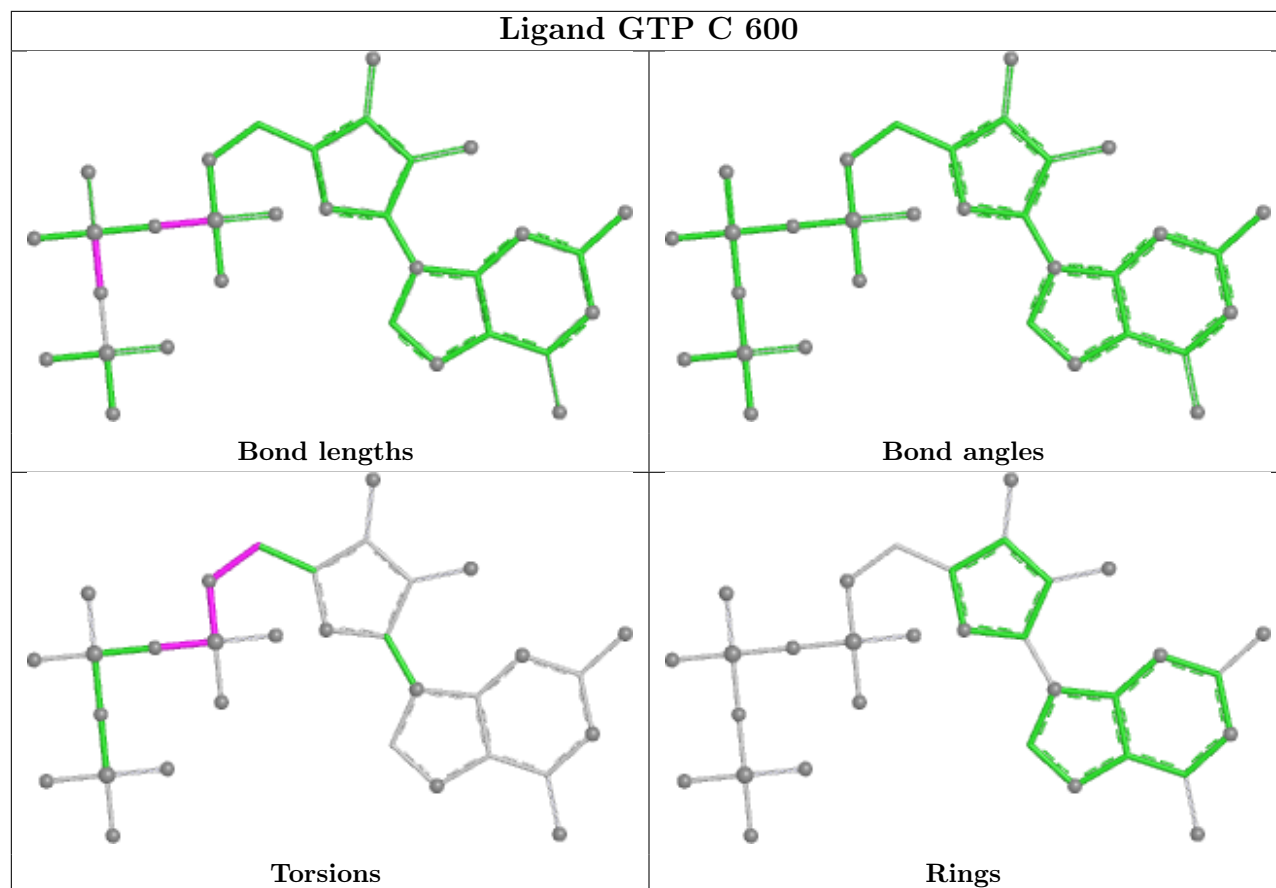
5 monomers are involved in 9 short contacts:

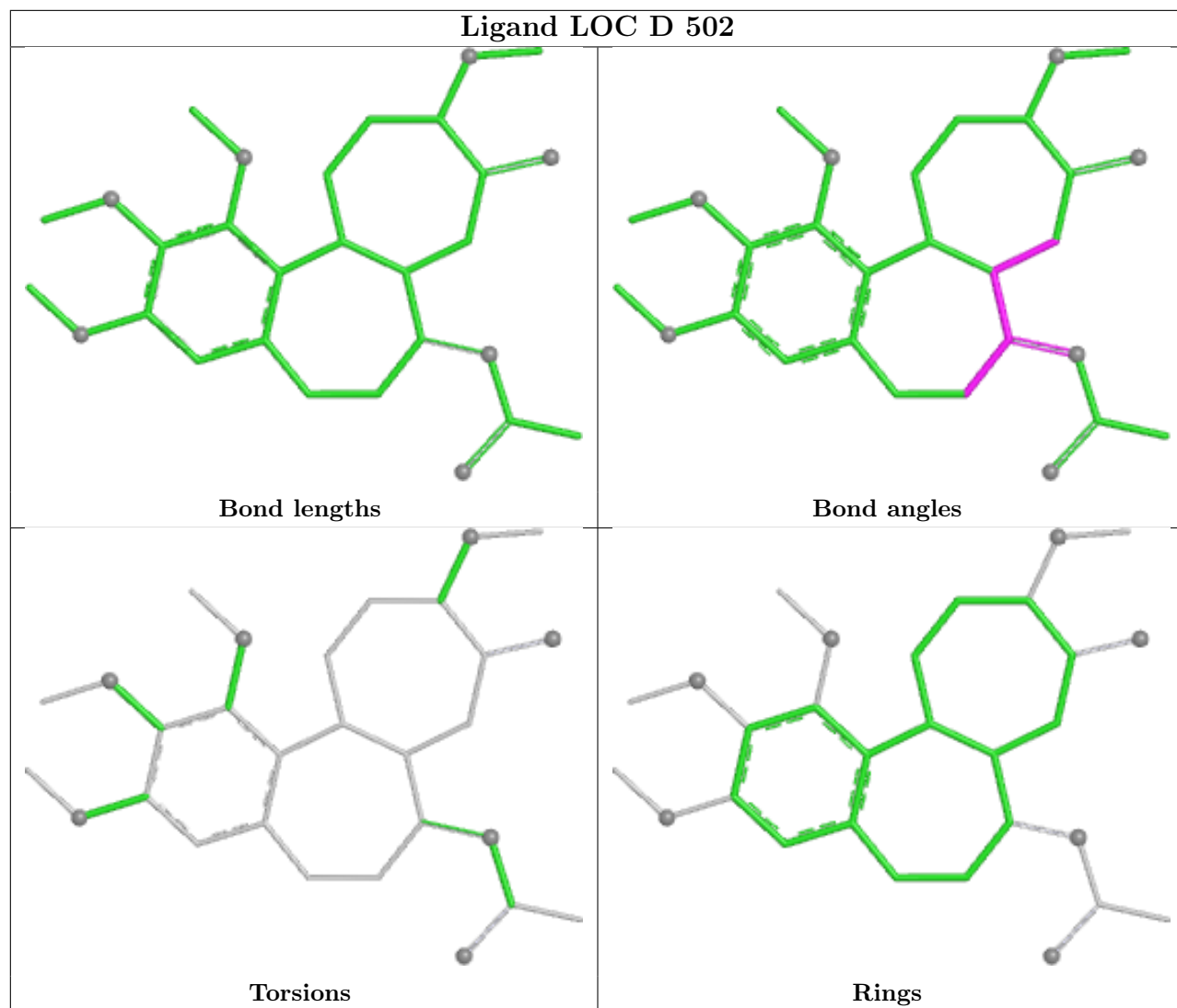
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	503	3WV	2	0
4	A	600	GTP	1	0
6	D	501	GDP	1	0
6	B	501	GDP	1	0
8	D	503	3WV	4	0

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.

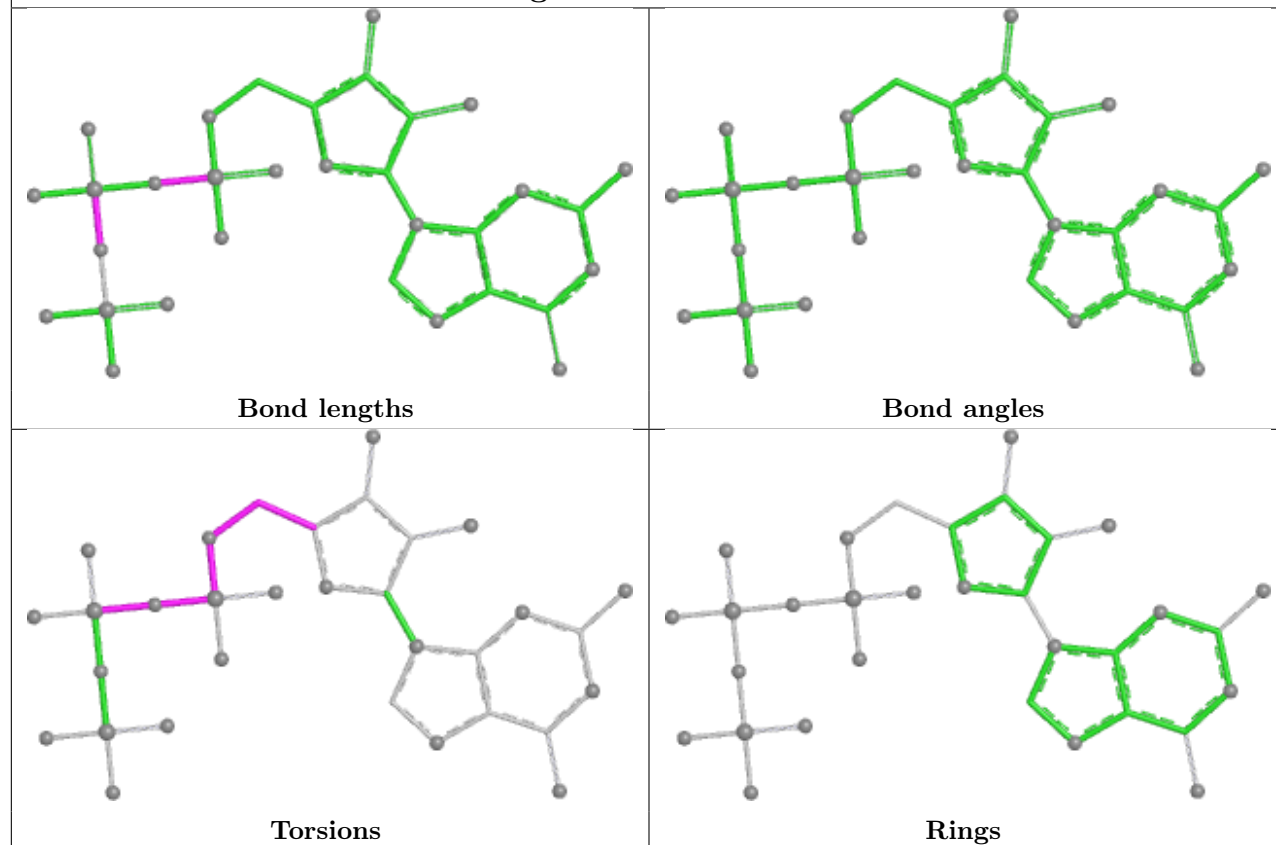




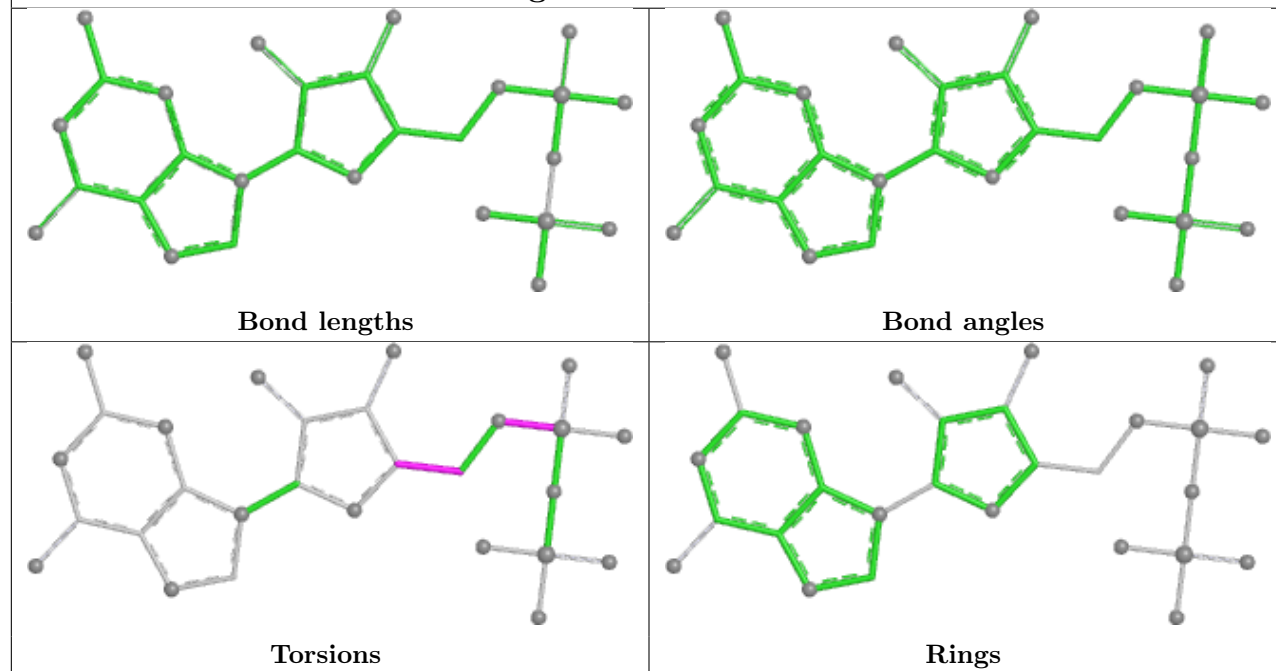


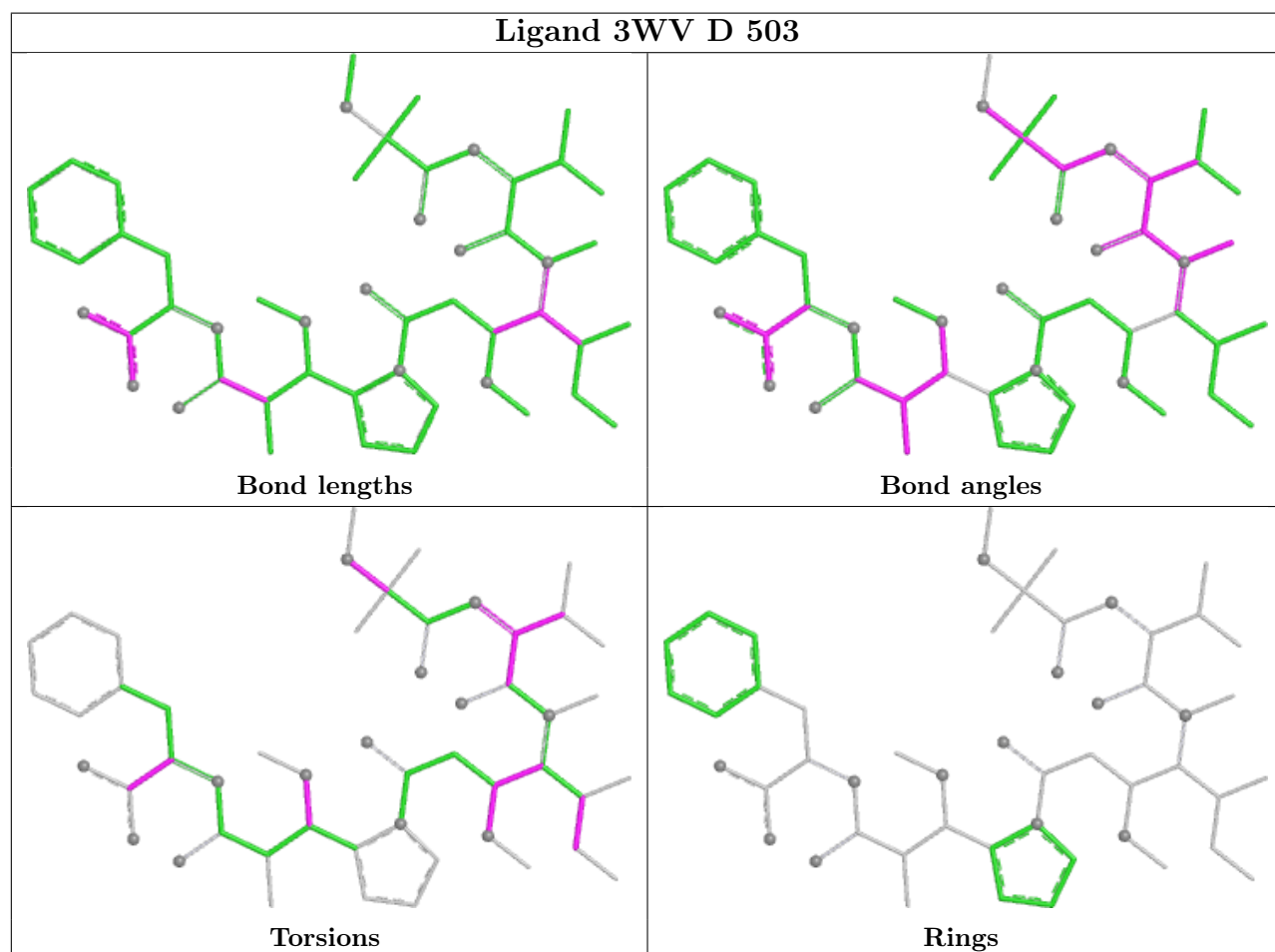
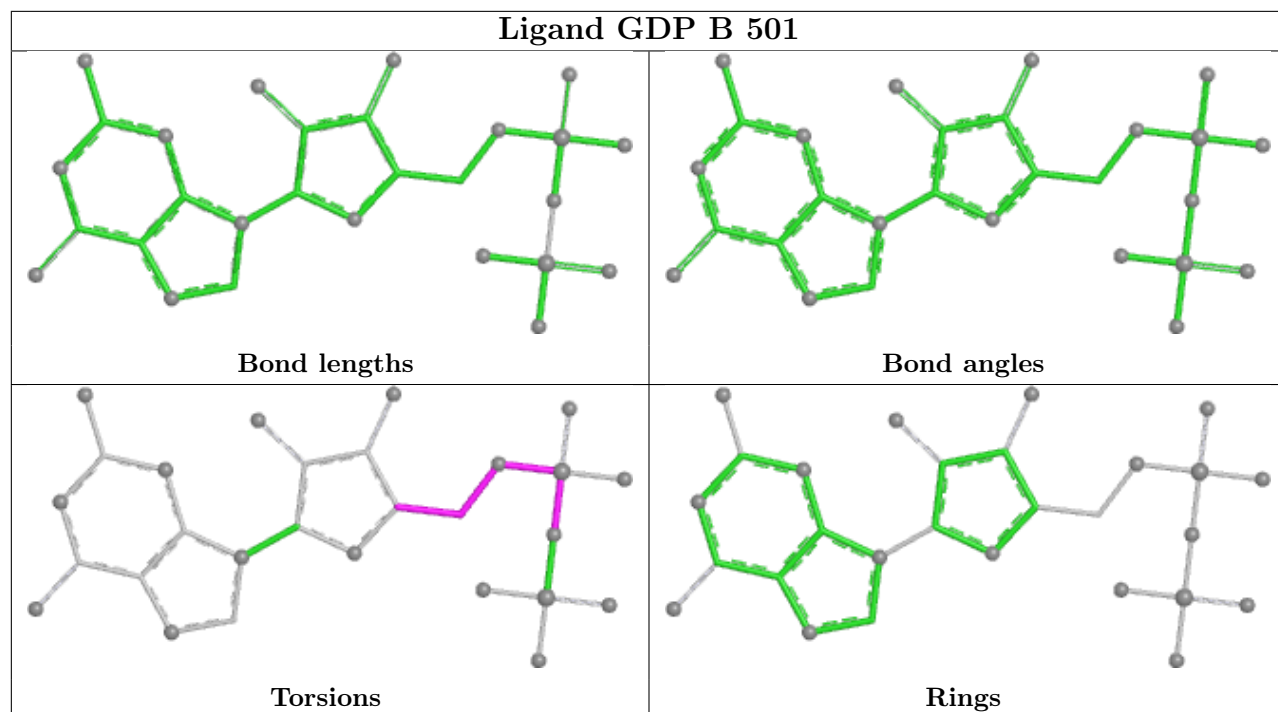


Ligand GTP A 600



Ligand GDP D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	429/451 (95%)	-0.57	1 (0%) 91 85	99, 146, 192, 212	0
1	C	430/451 (95%)	-0.61	3 (0%) 84 69	62, 113, 156, 178	2 (0%)
2	B	428/445 (96%)	-0.57	4 (0%) 81 64	91, 124, 171, 188	2 (0%)
2	D	430/445 (96%)	-0.65	0 100 100	67, 105, 143, 176	3 (0%)
3	E	123/142 (86%)	-0.72	0 100 100	115, 147, 193, 217	0
All	All	1840/1934 (95%)	-0.61	8 (0%) 88 79	62, 124, 179, 217	7 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	66	ILE	3.1
1	C	418	PHE	2.9
1	A	149	PHE	2.8
2	B	5	VAL	2.4
2	B	135	PHE	2.4
1	C	37	PRO	2.3
1	C	68	VAL	2.2
2	B	7	ILE	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

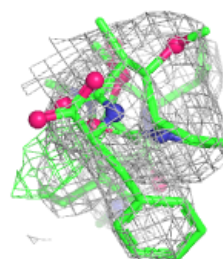
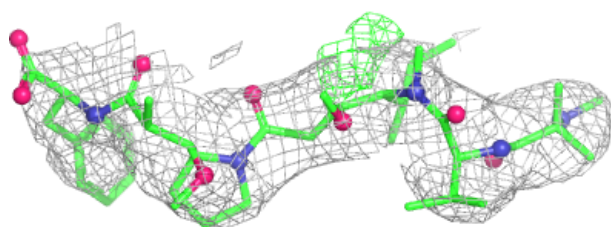
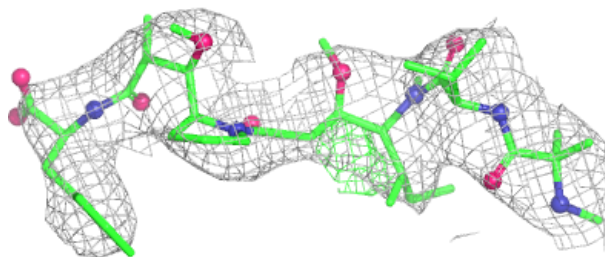
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	C	601	1/1	0.86	0.23	60,60,60,60	0
8	3WV	B	503	51/51	0.89	0.11	105,119,132,137	0
8	3WV	D	503	51/51	0.90	0.08	88,114,122,128	0
7	LOC	D	502	29/29	0.92	0.11	88,99,102,103	0
4	GTP	C	600	32/32	0.94	0.08	99,104,108,110	0
4	GTP	A	600	32/32	0.95	0.07	120,133,146,146	0
6	GDP	B	501	28/28	0.95	0.06	106,117,120,123	0
6	GDP	D	501	28/28	0.95	0.06	88,94,101,105	0
7	LOC	B	502	29/29	0.96	0.07	114,119,124,128	0
5	MG	A	601	1/1	0.96	0.10	81,81,81,81	0

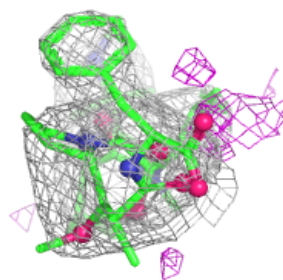
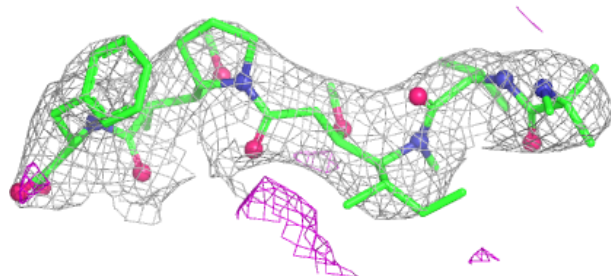
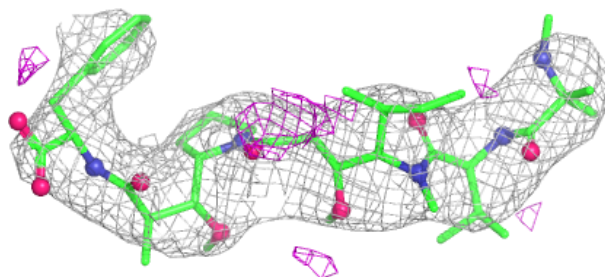
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3WV B 503:

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

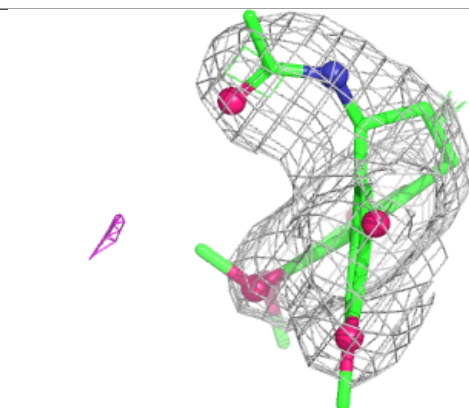
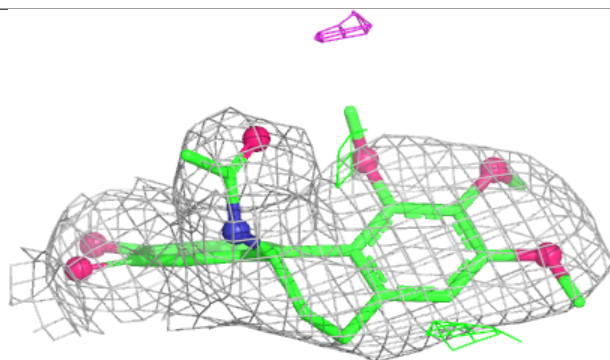
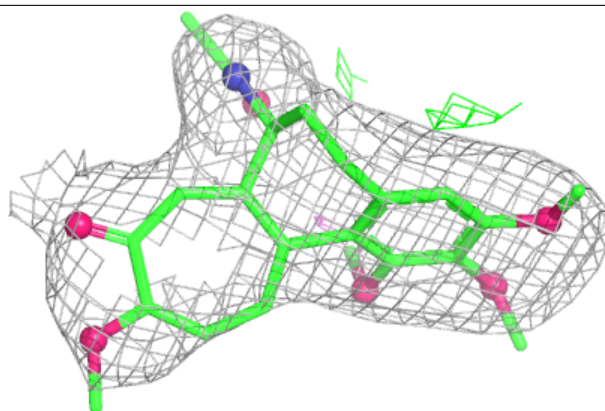
**Electron density around 3WV D 503:**

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

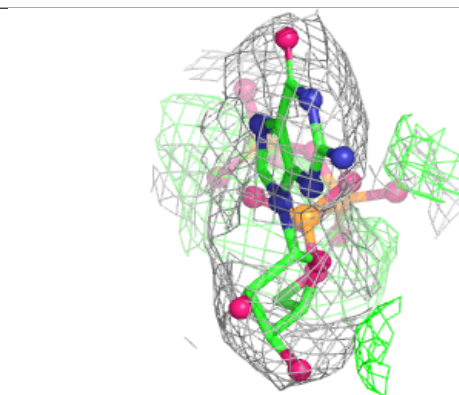
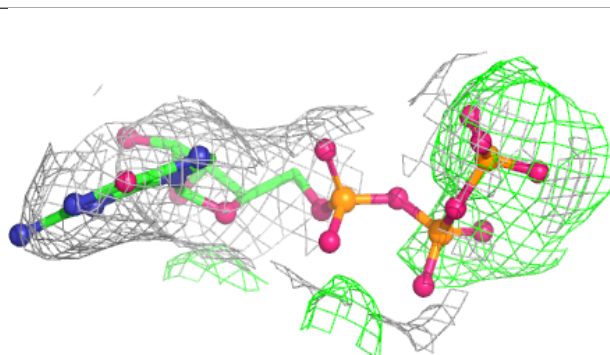
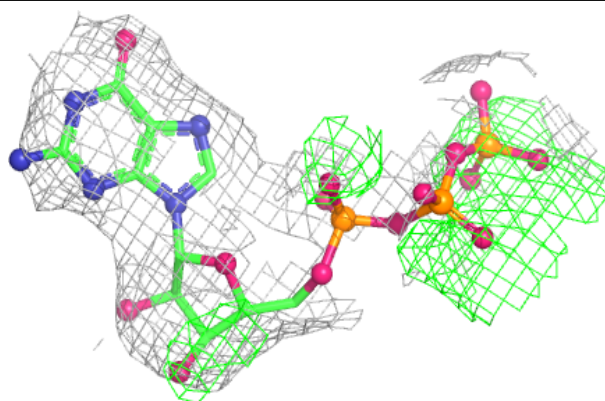


Electron density around LOC D 502:

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

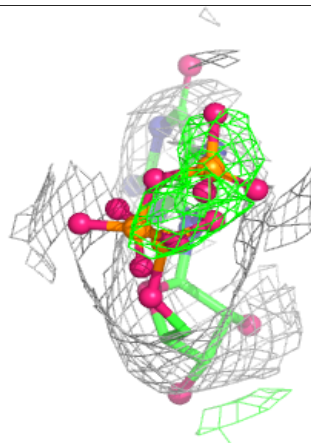
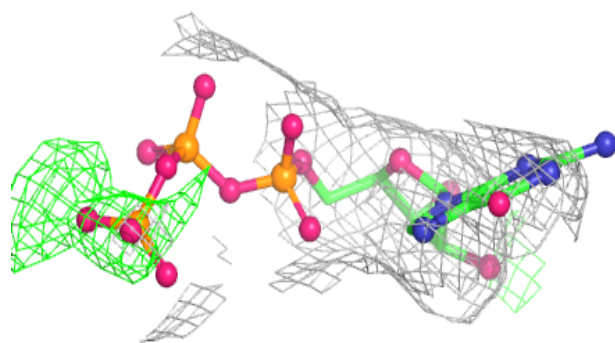
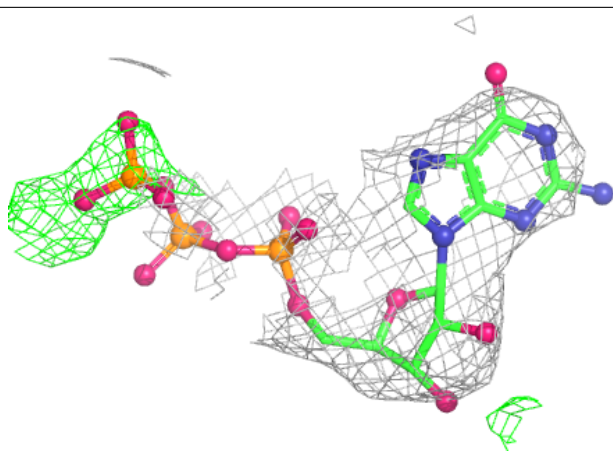
**Electron density around GTP C 600:**

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



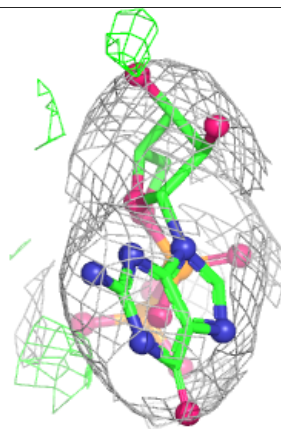
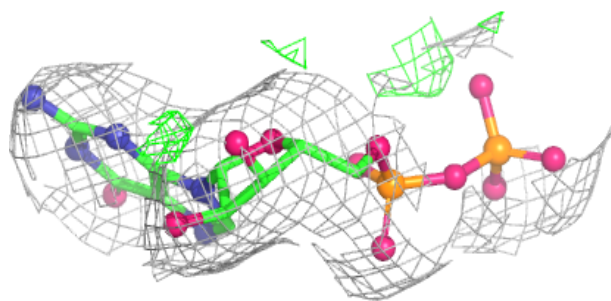
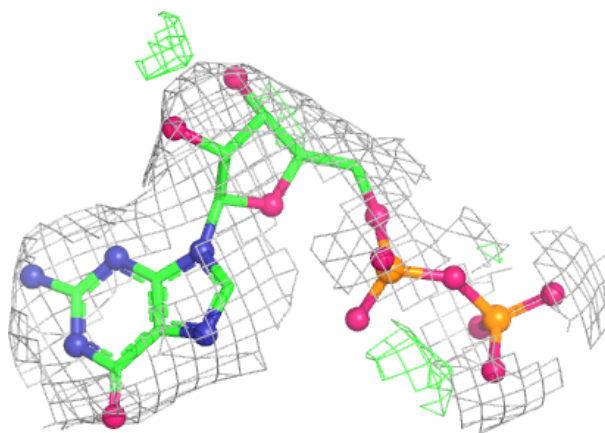
Electron density around GTP A 600:

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



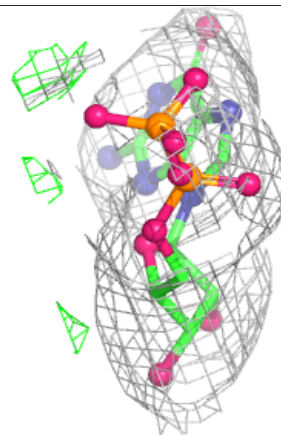
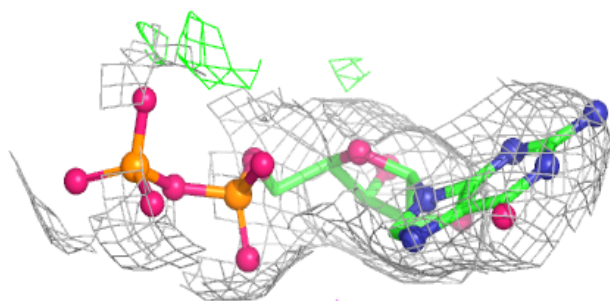
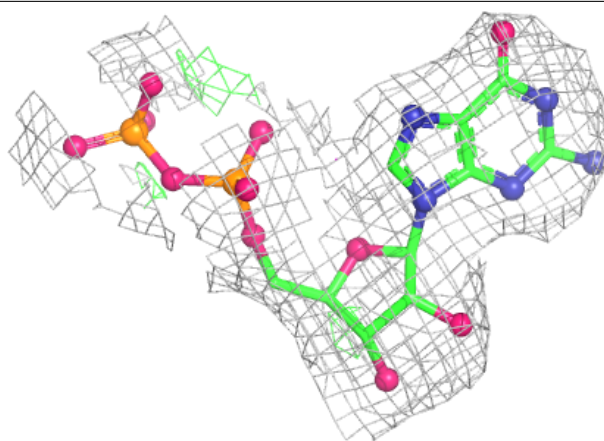
Electron density around GDP B 501:

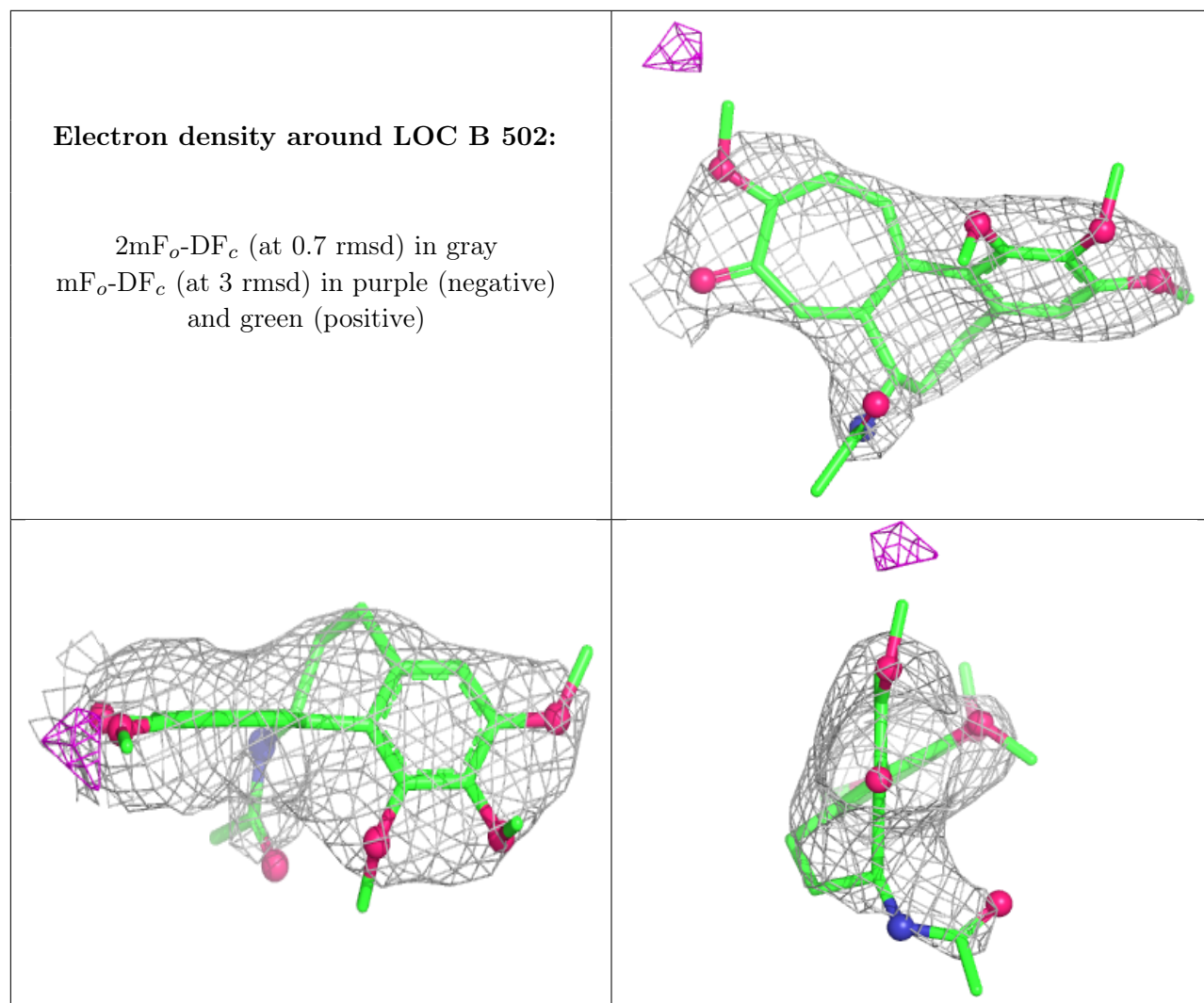
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP D 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.