



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 08:15 PM EDT

PDB ID : 4X1Y
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

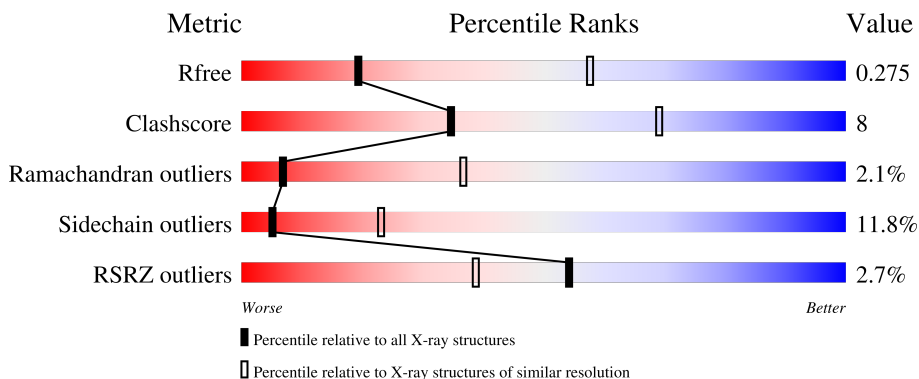
1 Overall quality at a glance

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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	
1	C	451	
2	B	445	
2	D	445	
3	E	142	

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
			Total	C	N	O	S			
1	A	429	3363	2132	572	638	21	0	0	0
1	C	430	3351	2124	569	635	23	0	2	0

- Molecule 2 is a protein called Tubulin beta chain.

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

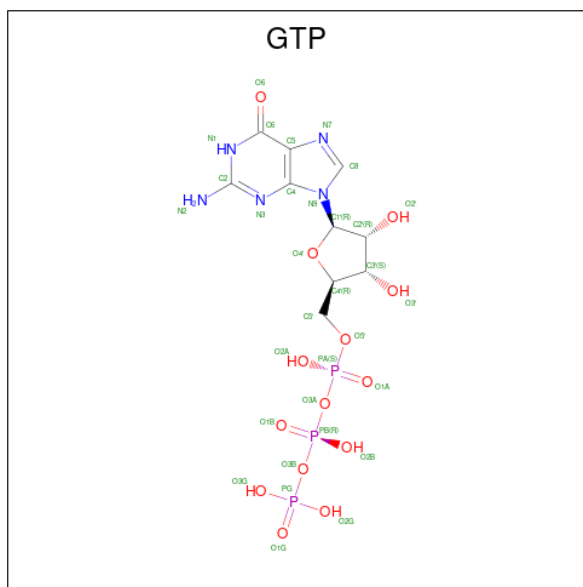
- Molecule 3 is a protein called Stathmin-4.

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

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 (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

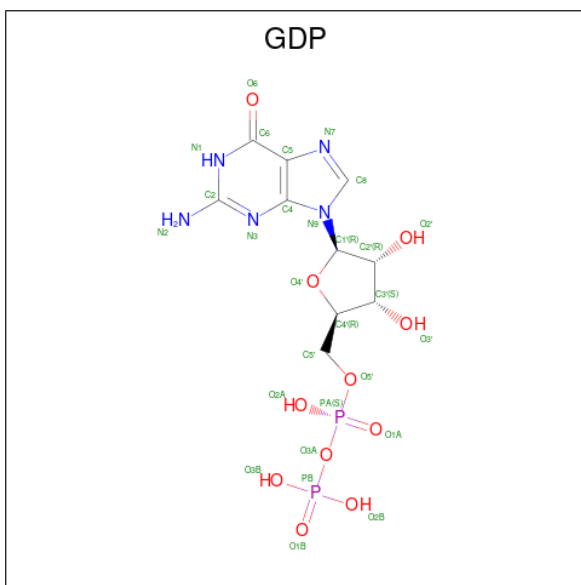


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

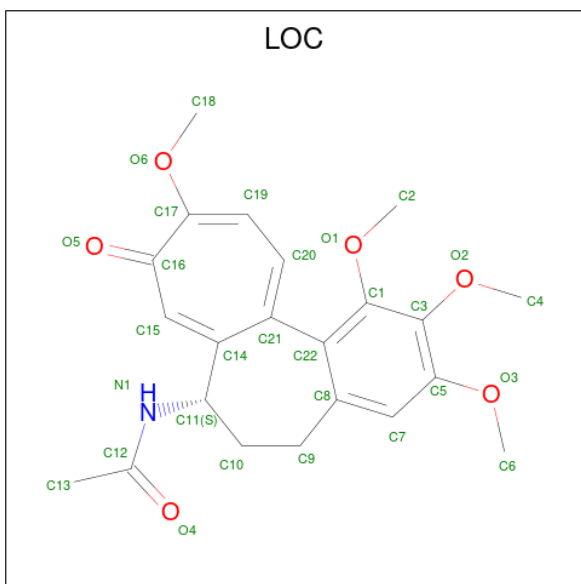
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 7 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (three-letter code: LOC) (formula: C₂₂H₂₅NO₆).



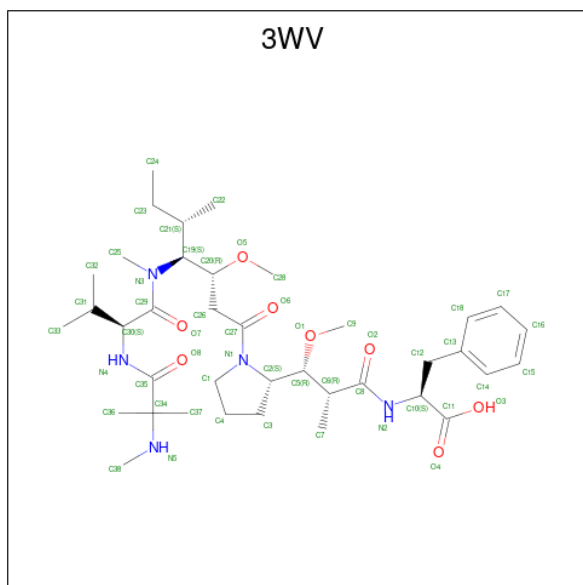
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	29	22	1	6	0	0

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

- 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 (three-letter code: 3WV) (formula: C₃₈H₆₃N₅O₈).

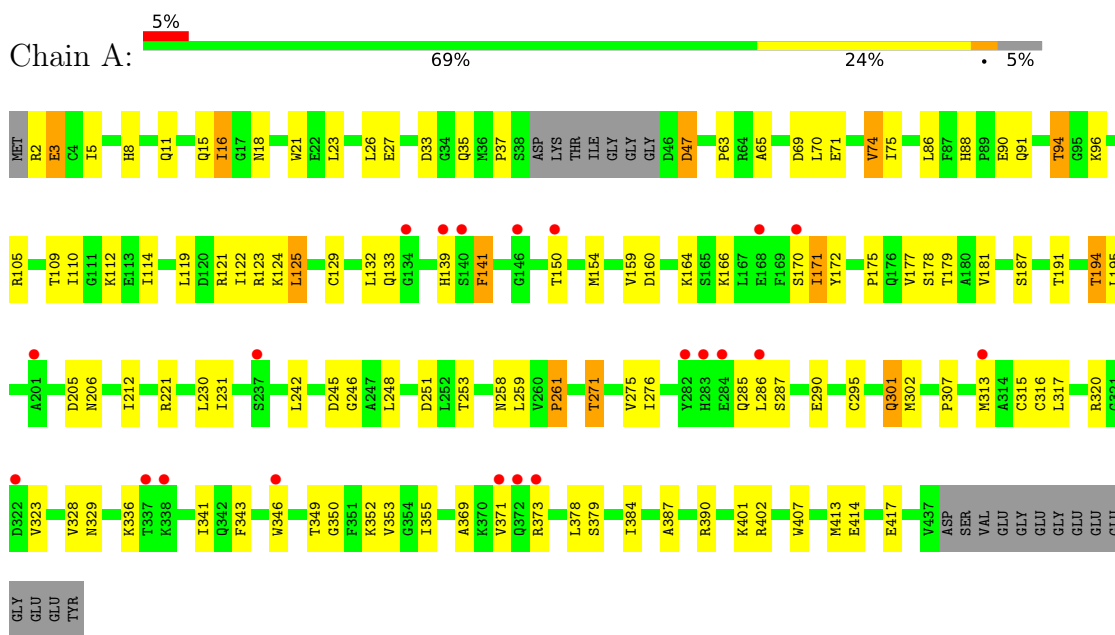


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	51	38	5	8	0	0
8	D	1	51	38	5	8	0	0

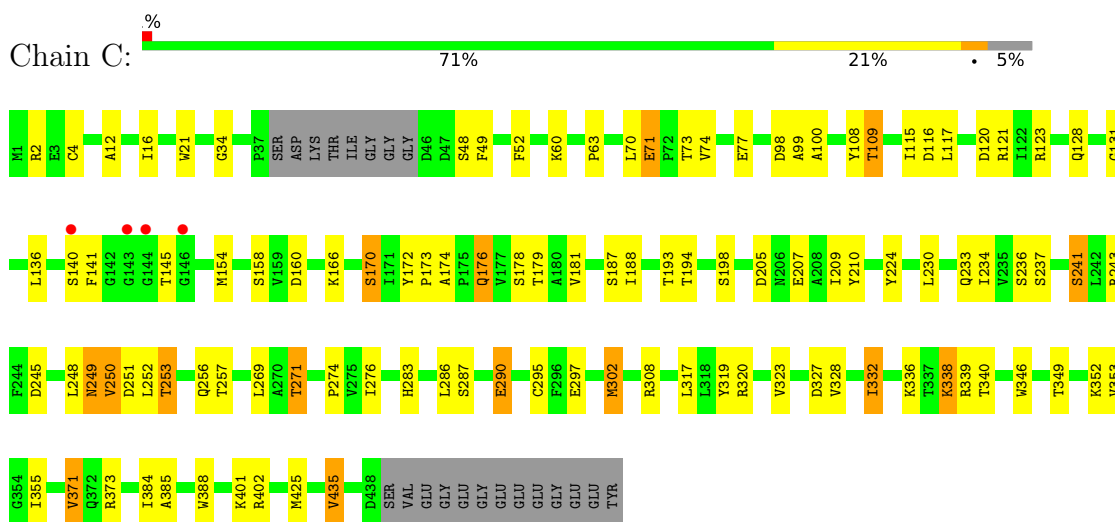
3 Residue-property plots [i](#)

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

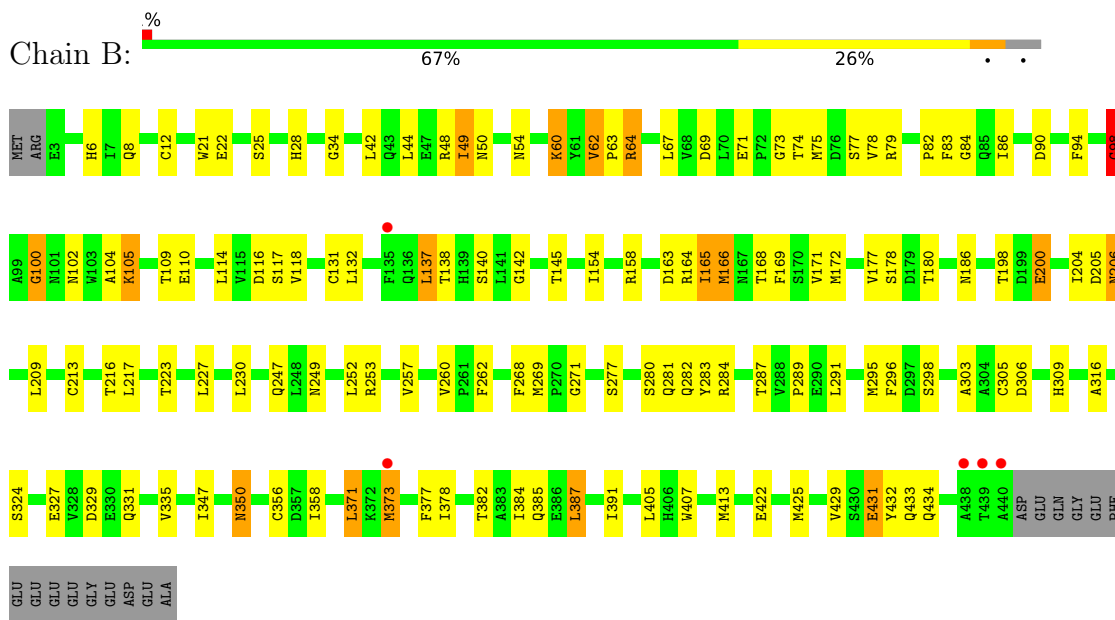
- Molecule 1: Tubulin alpha chain



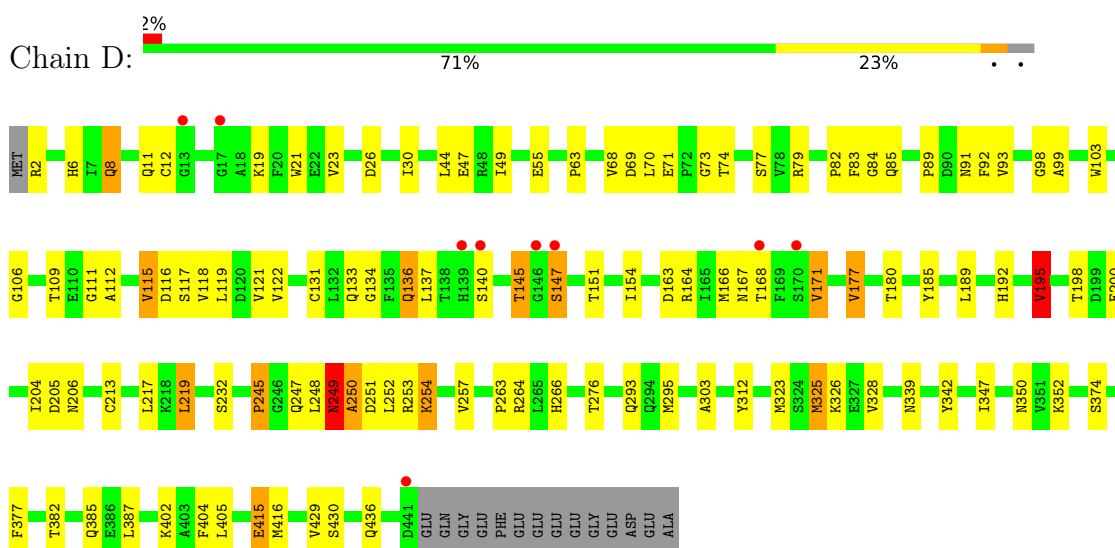
- Molecule 1: Tubulin alpha chain



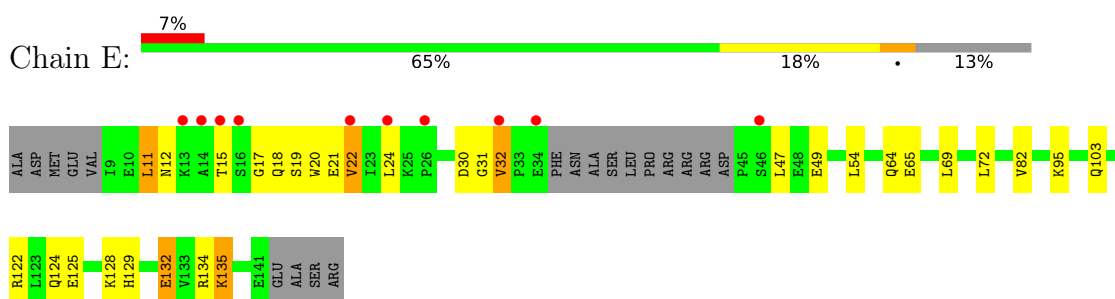
- Molecule 2: Tubulin beta chain



• 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 28.82 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.59-3.19) 91.4 (28.82-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.90Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.188 , 0.273 0.207 , 0.275	Depositor DCC
R_{free} test set	2285 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	95.4	Xtrriage
Anisotropy	0.535	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3WV, GDP, GTP, LOC, 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	0.51	0/3440	0.74	0/4671
1	C	0.53	0/3432	0.78	0/4662
2	B	0.54	0/3417	0.81	1/4634 (0.0%)
2	D	0.53	0/3446	0.77	2/4670 (0.0%)
3	E	0.50	0/1019	0.72	0/1355
All	All	0.53	0/14754	0.77	3/19992 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	248	LEU	C-N-CA	6.11	136.96	121.70
2	B	98	GLY	N-CA-C	5.85	127.72	113.10
2	D	249	ASN	C-N-CA	5.62	135.76	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3363	0	3274	57	0
1	C	3351	0	3258	50	0
2	B	3342	0	3198	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3369	0	3237	62	0
3	E	1008	0	1022	13	0
4	A	32	0	12	1	0
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	240	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 8.

All (240) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:O	2:D:23:VAL:HG23	1.95	0.66
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:CE	1:C:302:MET:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:HD21	6:D:501:GDP:HN22	1.53	0.57
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
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: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
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
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:200:GLU:HB3	2:B:268:PHE:HE1	1.76	0.51
2:D:415:GLU:H	2:D:415:GLU:CD	2.14	0.51
2:B:217:LEU:HD11	2:B:230:LEU:HD21	1.92	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:MET:O	2:B:429:VAL:HG23	2.14	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
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
1:A:258:ASN:HA	1:A:352:LYS:HZ3	1.82	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:425:MET:HB3	1:C:425:MET:HE3	1.91	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
1:C:176:GLN:H	1:C:176:GLN:CD	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:98:GLY:C	2:B:100:GLY:H	2.24	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
2:B:205:ASP:O	2:B:209:LEU:HG	2.22	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%)	9	43
1	C	428/451 (95%)	377 (88%)	41 (10%)	10 (2%)	6	34
2	B	426/445 (96%)	384 (90%)	31 (7%)	11 (3%)	5	31
2	D	429/445 (96%)	396 (92%)	25 (6%)	8 (2%)	8	39
3	E	119/142 (84%)	112 (94%)	4 (3%)	3 (2%)	5	32
All	All	1827/1934 (94%)	1647 (90%)	141 (8%)	39 (2%)	7	37

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
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%)	317 (88%)	45 (12%)	4	21
1	C	359/378 (95%)	312 (87%)	47 (13%)	4	19
2	B	364/383 (95%)	322 (88%)	42 (12%)	5	24
2	D	369/383 (96%)	337 (91%)	32 (9%)	10	37
3	E	107/125 (86%)	89 (83%)	18 (17%)	2	10
All	All	1561/1647 (95%)	1377 (88%)	184 (12%)	5	23

All (184) 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	33	ASP
1	A	35	GLN
1	A	47	ASP
1	A	71	GLU
1	A	74	VAL
1	A	86	LEU
1	A	94	THR
1	A	105	ARG
1	A	109	THR
1	A	124	LYS
1	A	125	LEU
1	A	141	PHE
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	194	THR

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Mol	Chain	Res	Type
1	A	221	ARG
1	A	230	LEU
1	A	242	LEU
1	A	245	ASP
1	A	253	THR
1	A	271	THR
1	A	285	GLN
1	A	295	CYS
1	A	301	GLN
1	A	302	MET
1	A	315	CYS
1	A	320	ARG
1	A	323	VAL
1	A	336	LYS
1	A	343	PHE
1	A	371	VAL
1	A	379	SER
1	A	384	ILE
1	A	401	LYS
1	A	402	ARG
1	A	414	GLU
1	A	417	GLU
2	B	25	SER
2	B	42	LEU
2	B	49	ILE
2	B	62	VAL
2	B	64	ARG
2	B	67	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	132	LEU
2	B	137	LEU
2	B	158	ARG
2	B	163	ASP
2	B	165	ILE
2	B	166	MET
2	B	171	VAL

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Mol	Chain	Res	Type
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	247	GLN
2	B	277	SER
2	B	291	LEU
2	B	296	PHE
2	B	298	SER
2	B	329	ASP
2	B	350	ASN
2	B	356	CYS
2	B	358	ILE
2	B	371	LEU
2	B	373	MET
2	B	387	LEU
2	B	405	LEU
2	B	422	GLU
2	B	431	GLU
1	C	2	ARG
1	C	16	ILE
1	C	48	SER
1	C	49	PHE
1	C	71	GLU
1	C	74	VAL
1	C	77	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	176	GLN
1	C	178	SER
1	C	179	THR
1	C	181	VAL

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Mol	Chain	Res	Type
1	C	187	SER
1	C	188	ILE
1	C	193	THR
1	C	198	SER
1	C	224	TYR
1	C	233	GLN
1	C	236	SER
1	C	245	ASP
1	C	248	LEU
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	297	GLU
1	C	302	MET
1	C	327	ASP
1	C	332	ILE
1	C	338	LYS
1	C	339	ARG
1	C	349	THR
1	C	352	LYS
1	C	371	VAL
1	C	401	LYS
1	C	402	ARG
1	C	435	VAL
2	D	8	GLN
2	D	26	ASP
2	D	55	GLU
2	D	77	SER
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
2	D	219	LEU

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Mol	Chain	Res	Type
2	D	245	PRO
2	D	247	GLN
2	D	249	ASN
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	387	LEU
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	64	GLN
3	E	65	GLU
3	E	69	LEU
3	E	72	LEU
3	E	82	VAL
3	E	95	LYS
3	E	103	GLN
3	E	122	ARG
3	E	124	GLN
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 (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	28	HIS

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Mol	Chain	Res	Type
1	A	91	GLN
1	A	139	HIS
1	A	206	ASN
1	A	258	ASN
1	A	301	GLN
1	A	329	ASN
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN
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	426	ASN
2	B	434	GLN
2	B	436	GLN
1	C	8	HIS
1	C	176	GLN
2	D	6	HIS
2	D	14	ASN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	206	ASN
2	D	249	ASN
2	D	266	HIS
2	D	293	GLN
2	D	331	GLN
2	D	339	ASN
2	D	385	GLN
2	D	433	GLN
3	E	111	ASN
3	E	129	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 monosaccharides 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
6	GDP	B	501	-	24,30,30	0.72	0	30,47,47	0.86	1 (3%)
4	GTP	C	600	5	26,34,34	0.72	1 (3%)	32,54,54	0.68	0
4	GTP	A	600	5	26,34,34	0.75	1 (3%)	32,54,54	0.77	0
7	LOC	B	502	-	31,31,31	0.65	1 (3%)	44,44,44	0.88	1 (2%)
6	GDP	D	501	-	24,30,30	0.85	0	30,47,47	0.68	0
8	3WV	B	503	-	51,52,52	1.14	6 (11%)	56,73,73	1.57	9 (16%)
7	LOC	D	502	-	31,31,31	0.52	0	44,44,44	0.76	2 (4%)
8	3WV	D	503	-	51,52,52	1.17	6 (11%)	56,73,73	1.78	13 (23%)

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
6	GDP	B	501	-	-	7/12/32/32	0/3/3/3
4	GTP	C	600	5	-	5/18/38/38	0/3/3/3
4	GTP	A	600	5	-	6/18/38/38	0/3/3/3
7	LOC	B	502	-	-	0/12/25/25	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	D	501	-	-	5/12/32/32	0/3/3/3
8	3WV	B	503	-	-	18/72/85/85	0/2/2/2
7	LOC	D	502	-	-	0/12/25/25	0/3/3/3
8	3WV	D	503	-	-	13/72/85/85	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	3WV	C19-N3	5.24	1.58	1.47
8	B	503	3WV	C19-N3	4.67	1.57	1.47
8	B	503	3WV	C20-C19	3.40	1.60	1.52
8	B	503	3WV	O4-C11	3.13	1.31	1.22
8	D	503	3WV	O4-C11	3.04	1.31	1.22
7	B	502	LOC	C11-C14	3.04	1.58	1.53
8	D	503	3WV	C6-C8	3.01	1.57	1.52
8	B	503	3WV	C21-C19	2.62	1.60	1.54
8	B	503	3WV	C6-C8	2.61	1.56	1.52
8	D	503	3WV	O3-C11	-2.59	1.22	1.30
8	D	503	3WV	C20-C19	2.57	1.58	1.52
8	B	503	3WV	O3-C11	-2.31	1.23	1.30
4	C	600	GTP	C8-N7	-2.17	1.31	1.35
8	D	503	3WV	C21-C19	2.13	1.59	1.54
4	A	600	GTP	C8-N7	-2.08	1.31	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	3WV	C25-N3-C19	-5.45	108.73	119.46
7	B	502	LOC	C14-C11-N1	5.25	118.48	114.34
8	B	503	3WV	C25-N3-C19	-4.84	109.94	119.46
8	B	503	3WV	C19-N3-C29	4.79	134.05	120.34
8	B	503	3WV	C22-C21-C19	4.55	123.78	111.20
8	D	503	3WV	C31-C30-C29	4.30	119.43	110.73
8	D	503	3WV	C30-C29-N3	4.18	127.36	118.74
8	D	503	3WV	O1-C5-C6	4.07	115.48	105.83
8	D	503	3WV	O7-C29-C30	-3.60	112.97	119.99
8	D	503	3WV	C25-N3-C29	3.46	133.51	122.26
8	D	503	3WV	C31-C30-N4	3.27	119.51	111.43
8	B	503	3WV	C6-C8-N2	-3.03	111.86	116.44
8	B	503	3WV	O1-C5-C6	2.98	112.90	105.83
8	D	503	3WV	C35-C34-N5	-2.93	105.78	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	3WV	O3-C11-C10	2.89	122.99	113.40
8	B	503	3WV	O4-C11-C10	-2.88	112.78	122.26
8	D	503	3WV	O3-C11-C10	2.73	122.48	113.40
8	B	503	3WV	C35-C34-N5	-2.66	106.22	110.54
8	D	503	3WV	O4-C11-C10	-2.56	113.86	122.26
6	B	501	GDP	PA-O3A-PB	2.53	141.52	132.83
8	D	503	3WV	C7-C6-C8	-2.13	104.51	108.78
7	D	502	LOC	C10-C11-C14	2.10	113.26	110.58
7	D	502	LOC	C11-C14-C15	-2.10	115.14	117.12
8	D	503	3WV	C30-N4-C35	2.06	125.93	121.30
8	B	503	3WV	C25-N3-C29	-2.05	115.58	122.26
8	D	503	3WV	C29-C30-N4	2.01	112.75	108.03

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
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	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

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Mol	Chain	Res	Type	Atoms
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
4	A	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	PB-O3A-PA-O1A
8	B	503	3WV	C19-C21-C23-C24
4	A	600	GTP	C5'-O5'-PA-O1A
8	B	503	3WV	N3-C19-C21-C23
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	C3'-C4'-C5'-O5'
4	A	600	GTP	C4'-C5'-O5'-PA
8	B	503	3WV	C21-C19-N3-C29
8	D	503	3WV	C21-C19-N3-C29
6	B	501	GDP	O4'-C4'-C5'-O5'
6	D	501	GDP	O4'-C4'-C5'-O5'
6	D	501	GDP	C3'-C4'-C5'-O5'
8	B	503	3WV	O7-C29-N3-C19
8	D	503	3WV	C19-C20-C26-C27
4	C	600	GTP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C4'-C5'-O5'-PA
4	A	600	GTP	PA-O3A-PB-O2B
6	B	501	GDP	PB-O3A-PA-O1A
4	A	600	GTP	C3'-C4'-C5'-O5'
4	C	600	GTP	C4'-C5'-O5'-PA

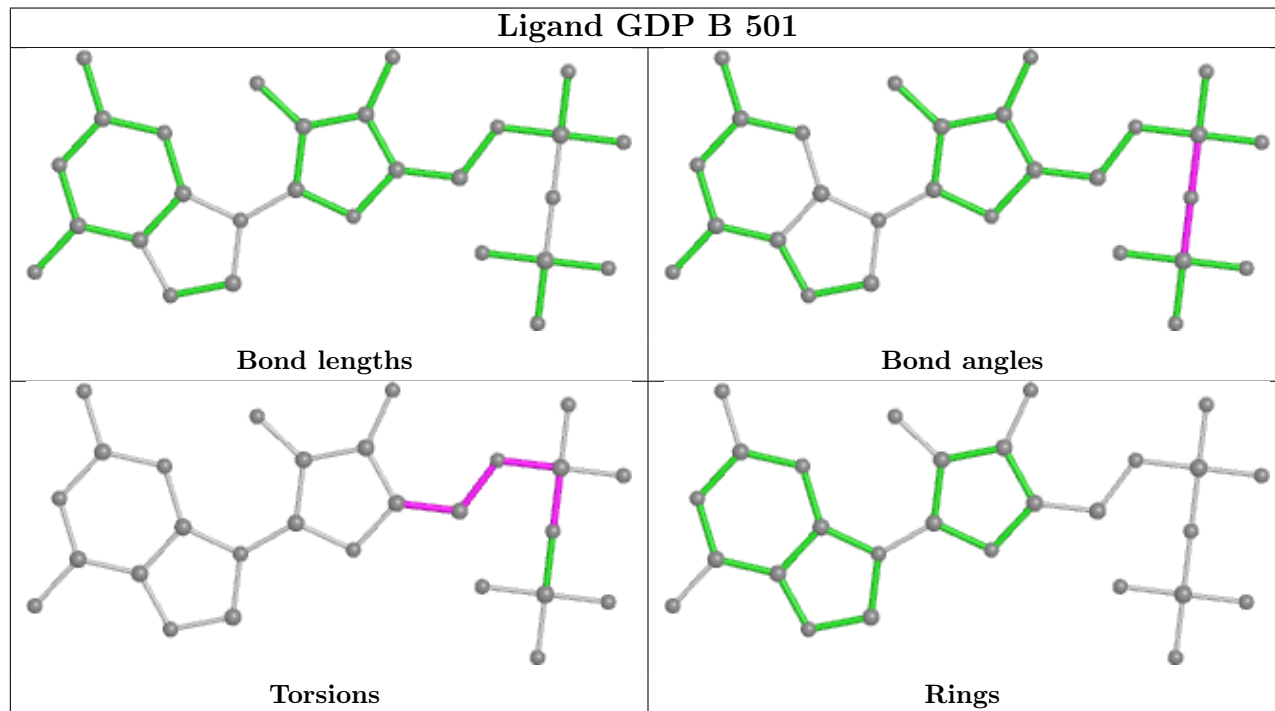
There are no ring outliers.

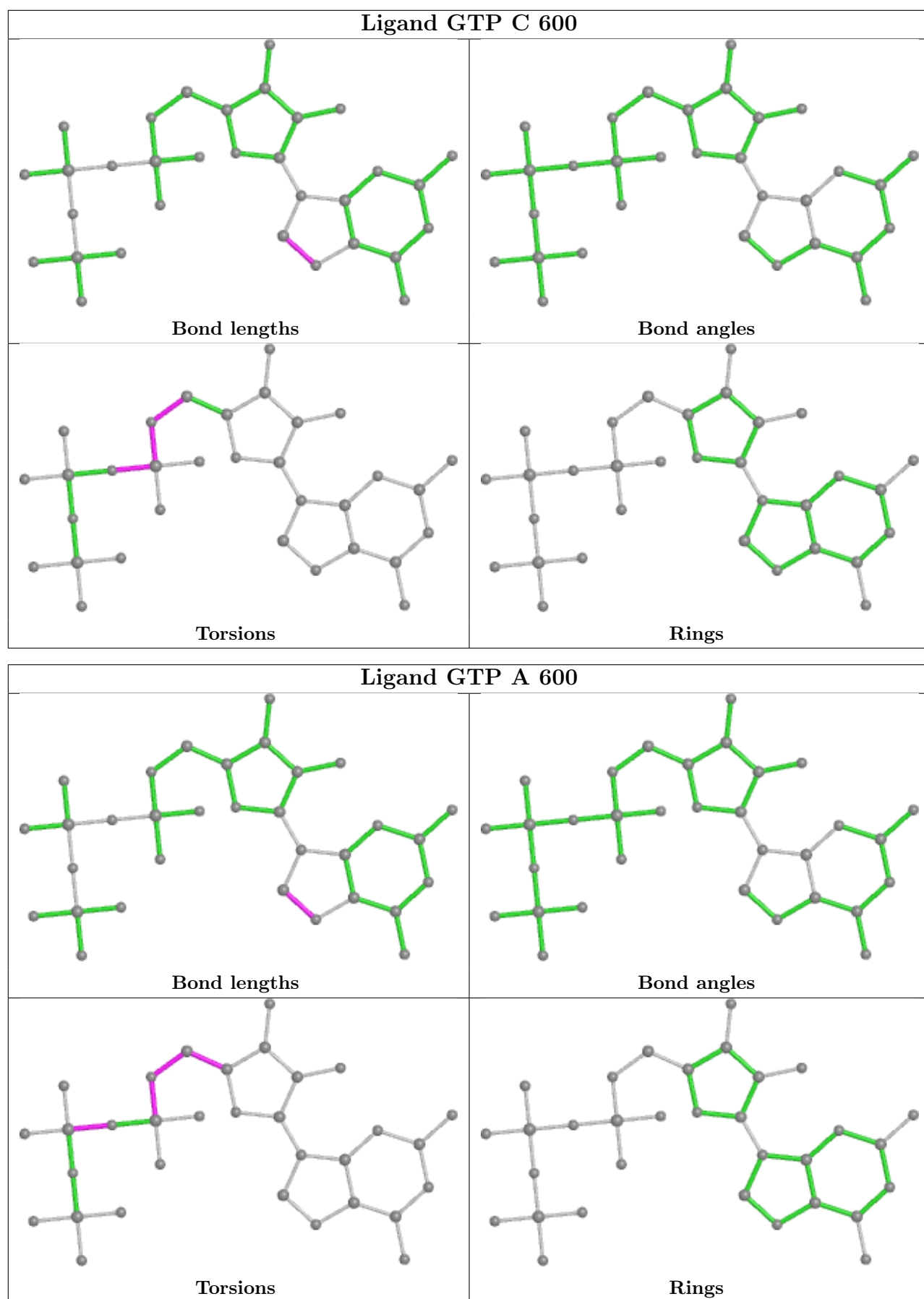
5 monomers are involved in 9 short contacts:

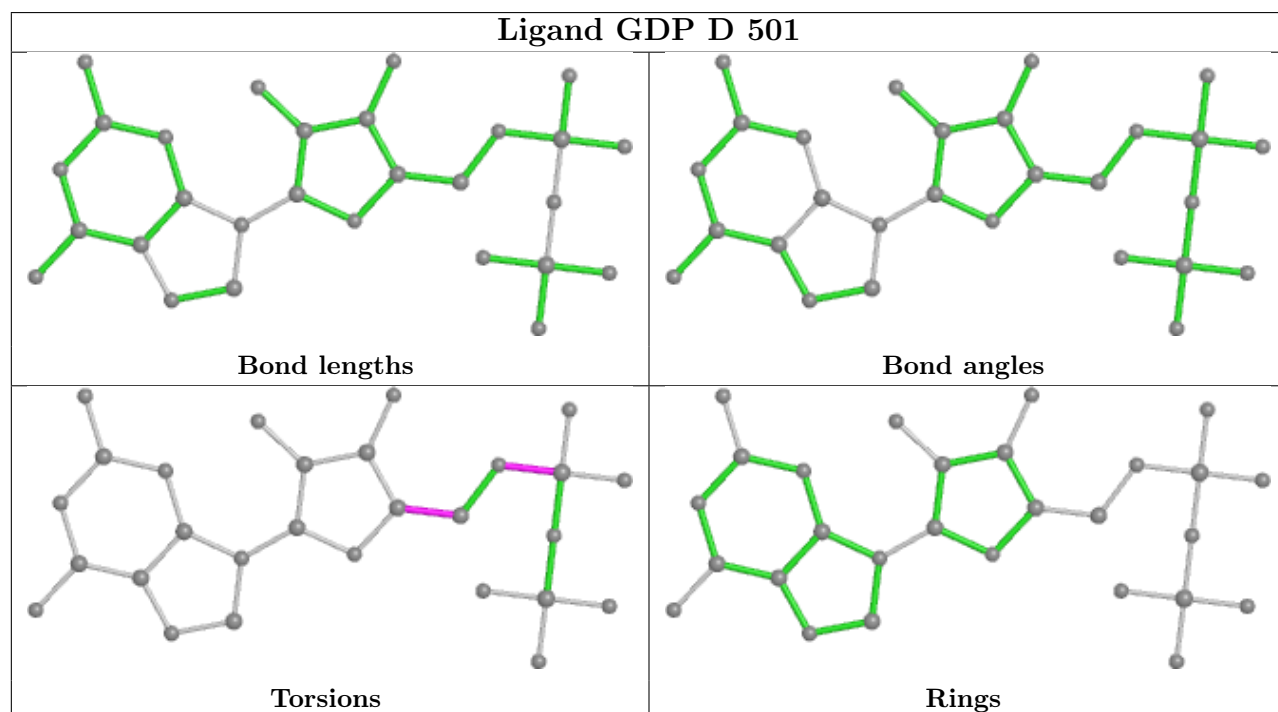
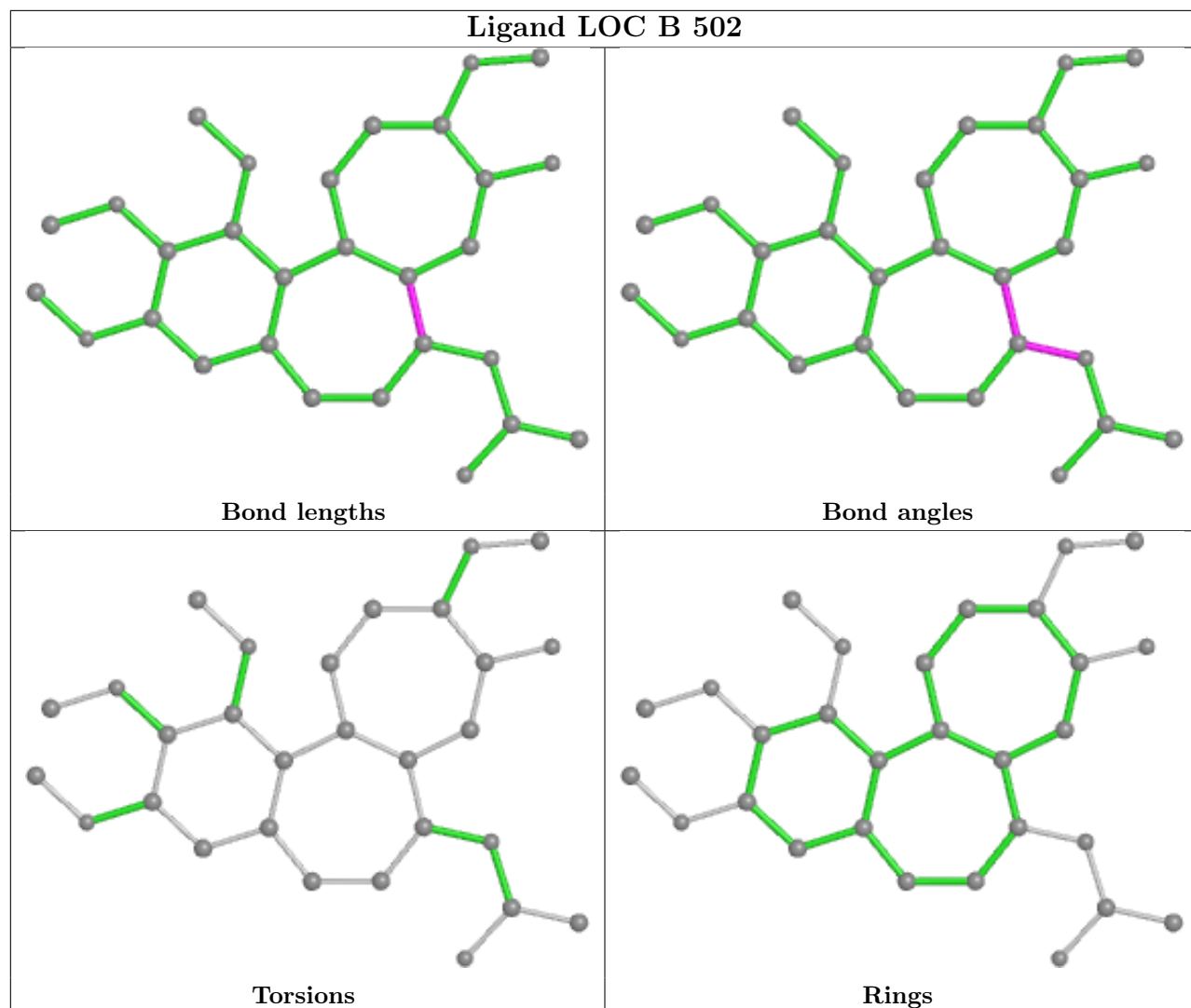
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GDP	1	0
4	A	600	GTP	1	0
6	D	501	GDP	1	0
8	B	503	3WV	2	0
8	D	503	3WV	4	0

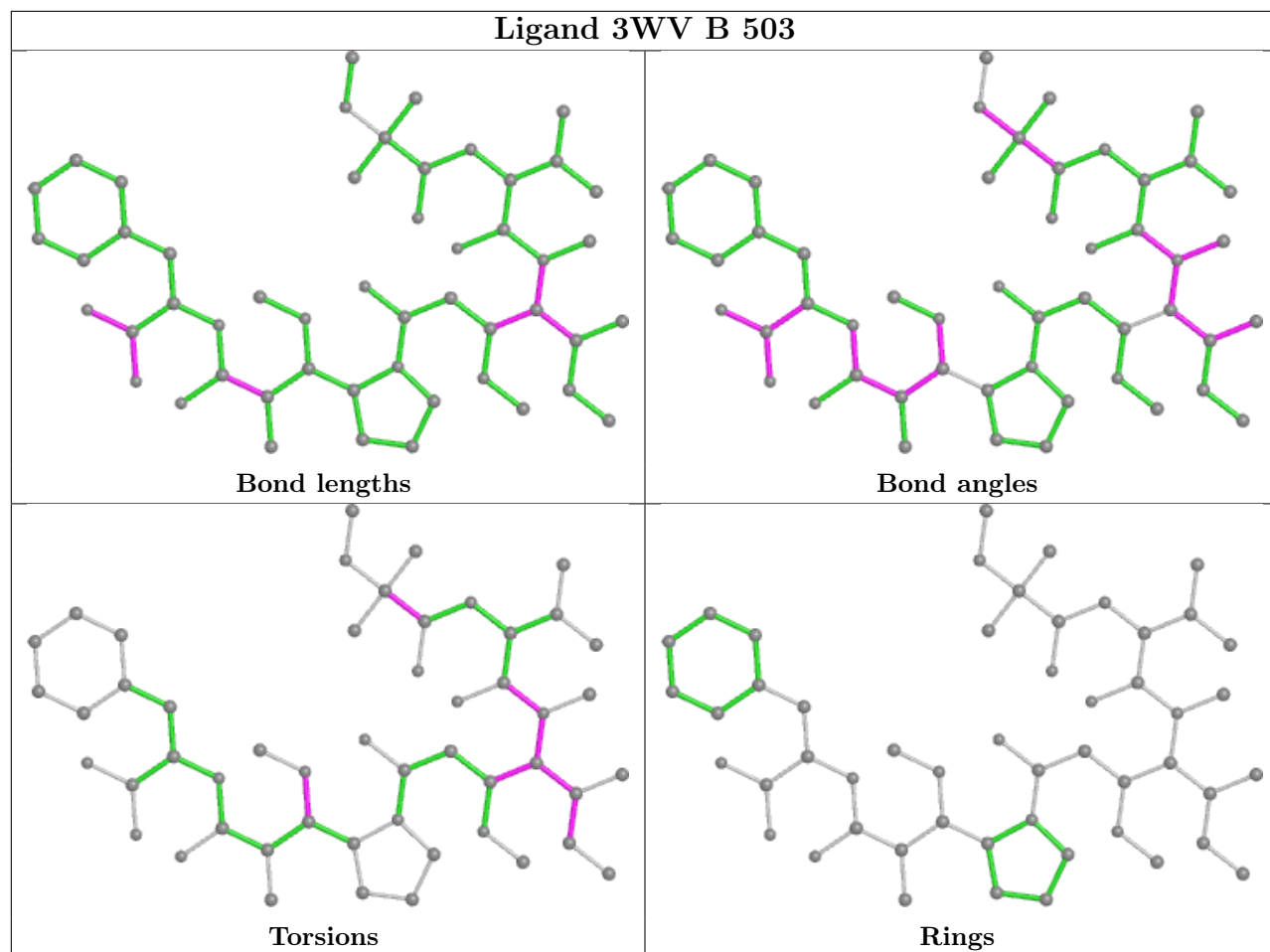
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

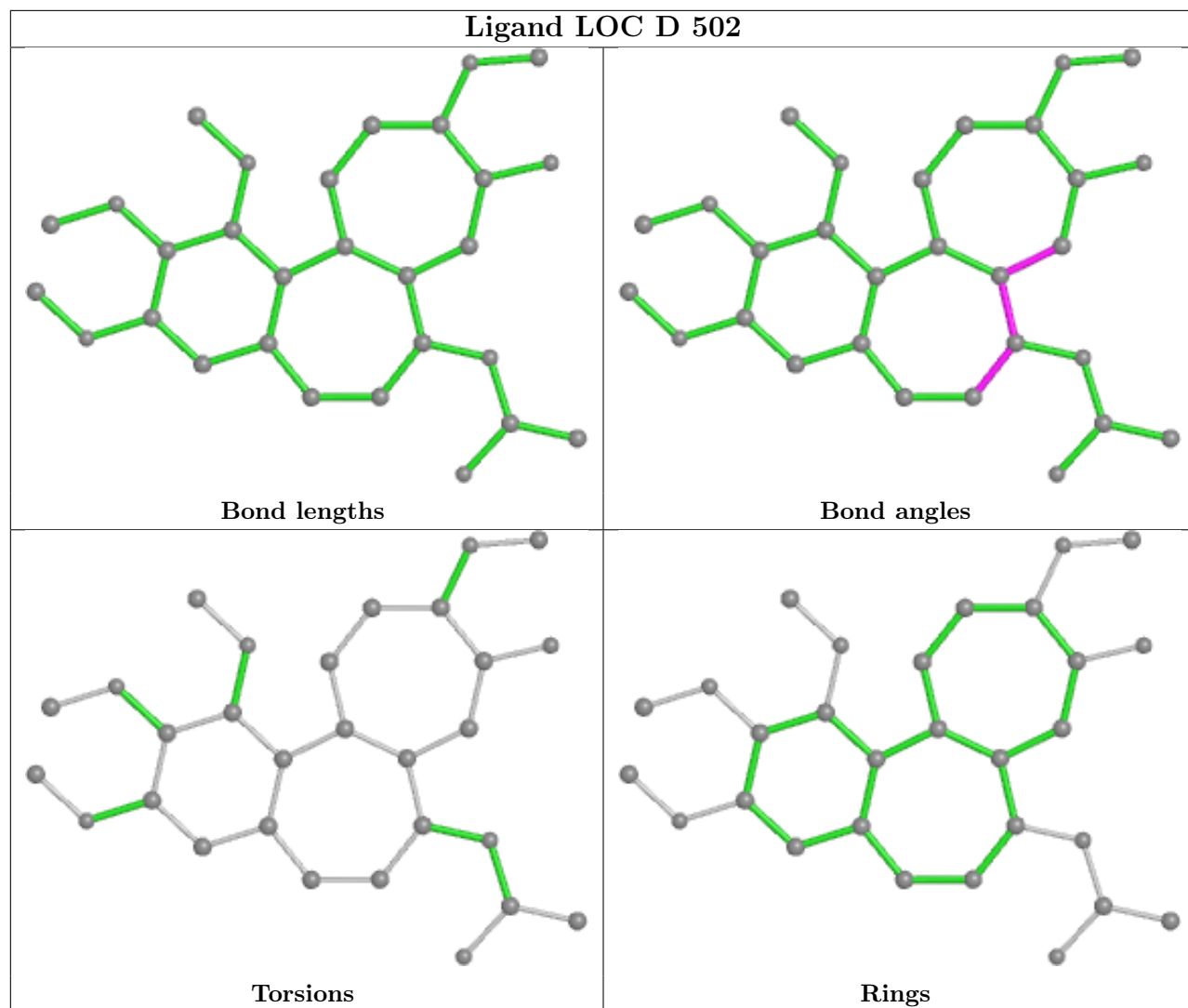
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

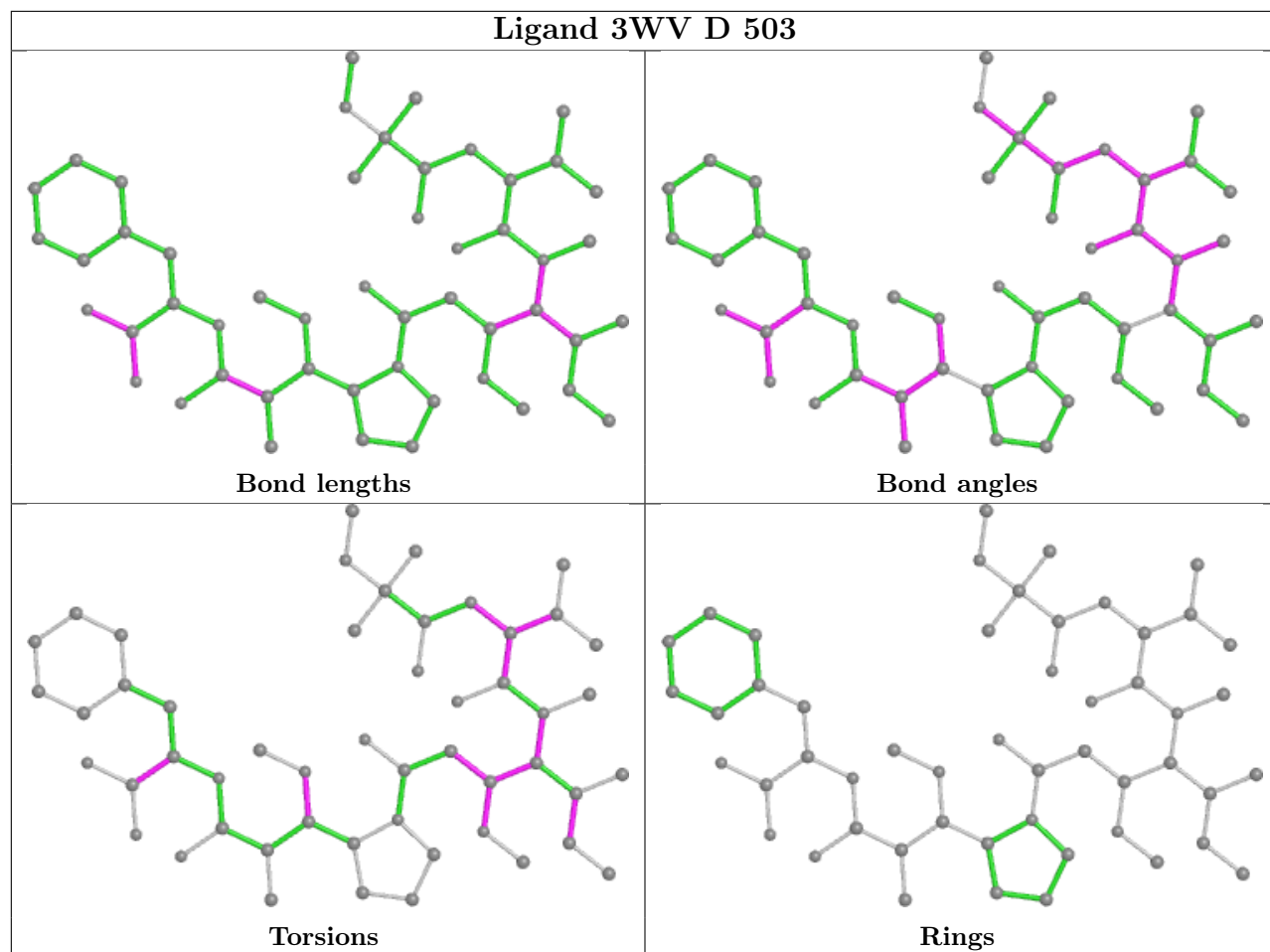












5.7 Other polymers [\(i\)](#)

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

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	429/451 (95%)	0.01	21 (4%) 29 17	99, 146, 192, 212	0
1	C	430/451 (95%)	-0.28	4 (0%) 84 75	86, 113, 156, 178	0
2	B	428/445 (96%)	-0.24	5 (1%) 79 67	91, 124, 171, 188	2 (0%)
2	D	430/445 (96%)	-0.27	9 (2%) 63 49	80, 105, 143, 176	2 (0%)
3	E	123/142 (86%)	0.16	10 (8%) 12 6	115, 147, 193, 217	0
All	All	1840/1934 (95%)	-0.17	49 (2%) 54 39	80, 124, 179, 217	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	LYS	4.3
2	B	439	THR	4.2
1	A	373	ARG	4.2
1	A	346	TRP	4.1
1	A	313	MET	4.0
2	D	140	SER	4.0
2	B	373	MET	3.7
2	B	438	ALA	3.6
1	A	322	ASP	3.6
1	A	283	HIS	3.5
1	A	146	GLY	3.3
3	E	16	SER	3.3
1	A	134	GLY	3.3
3	E	14	ALA	3.2
1	A	170	SER	3.2
1	A	371	VAL	3.1
1	A	337	THR	3.0
1	A	150	THR	3.0
3	E	22	VAL	2.9
1	A	286	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	147	SER	2.9
2	D	170	SER	2.9
3	E	26	PRO	2.9
2	D	441	ASP	2.8
1	A	139	HIS	2.7
2	D	168	THR	2.7
3	E	34	GLU	2.7
3	E	24	LEU	2.7
1	A	372	GLN	2.7
1	A	201	ALA	2.5
2	D	146	GLY	2.4
1	A	237	SER	2.4
3	E	46	SER	2.3
1	C	144	GLY	2.2
2	D	139	HIS	2.3
1	C	140	SER	2.2
2	D	13	GLY	2.2
1	A	282	TYR	2.2
3	E	13	LYS	2.2
2	B	440	ALA	2.1
2	B	135	PHE	2.1
1	A	284	GLU	2.1
1	A	140	SER	2.1
3	E	32	VAL	2.1
3	E	15	THR	2.1
1	C	146	GLY	2.1
2	D	17	GLY	2.0
1	C	143	GLY	2.0
1	A	168	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

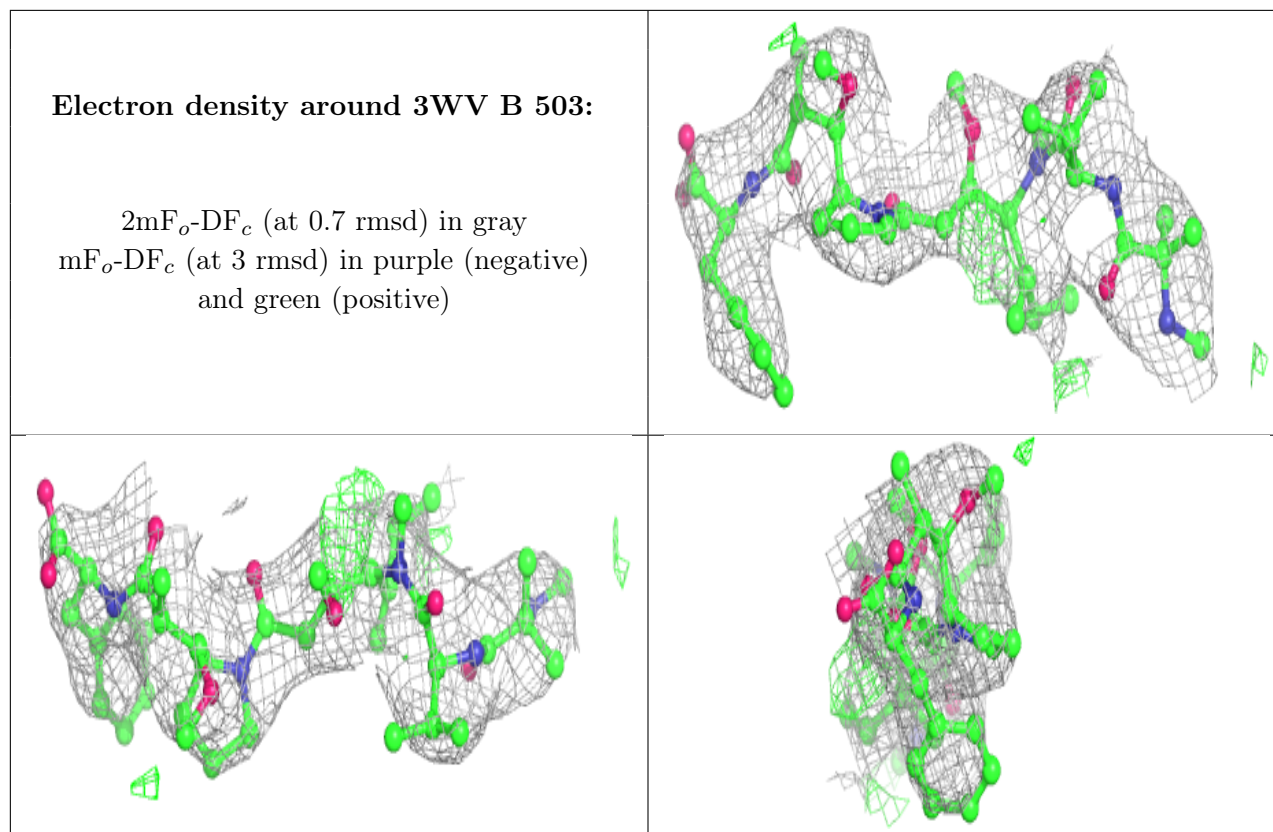
There are no monosaccharides in this entry.

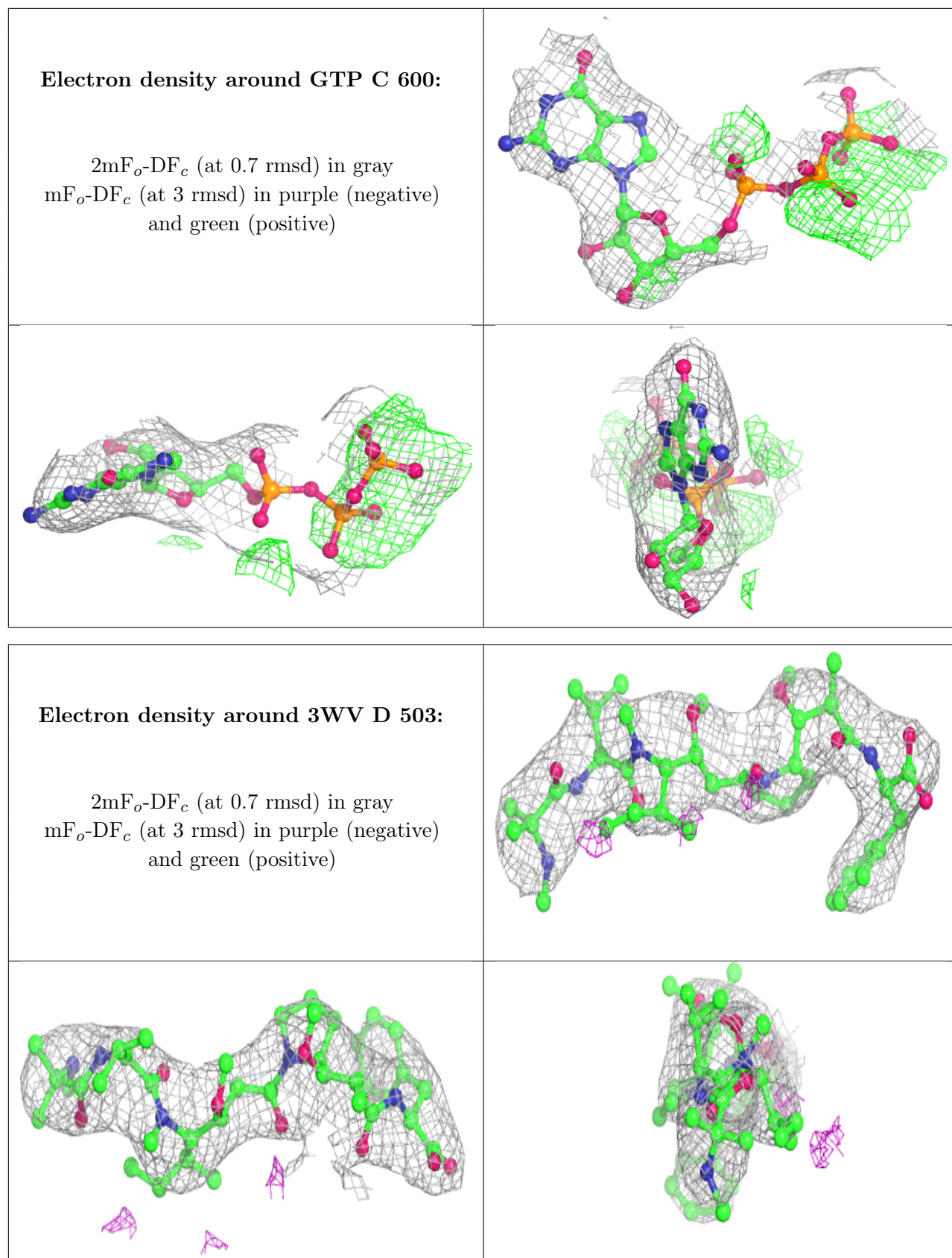
6.4 Ligands [i](#)

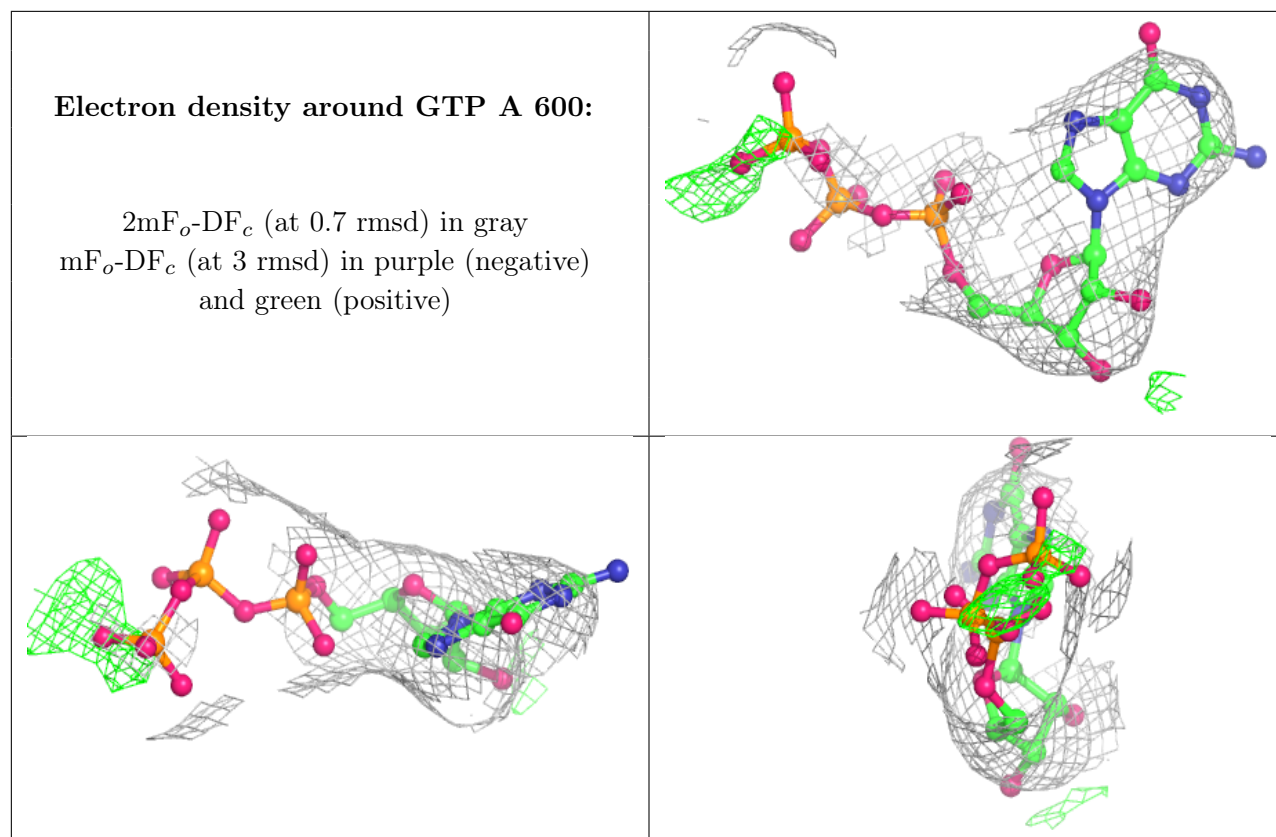
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	3WV	B	503	51/51	0.90	0.21	105,119,132,137	0
4	GTP	C	600	32/32	0.92	0.25	99,104,108,110	0
8	3WV	D	503	51/51	0.92	0.29	88,114,122,128	0
4	GTP	A	600	32/32	0.93	0.27	120,133,146,146	0
7	LOC	D	502	29/29	0.93	0.23	88,99,102,103	0
6	GDP	D	501	28/28	0.94	0.22	88,94,101,105	0
7	LOC	B	502	29/29	0.96	0.16	114,119,124,128	0
6	GDP	B	501	28/28	0.97	0.21	106,117,120,123	0
5	MG	A	601	1/1	0.98	0.31	81,81,81,81	0
5	MG	C	601	1/1	0.99	0.43	60,60,60,60	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.

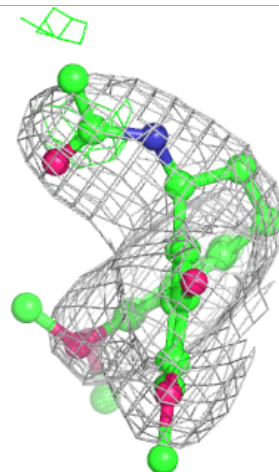
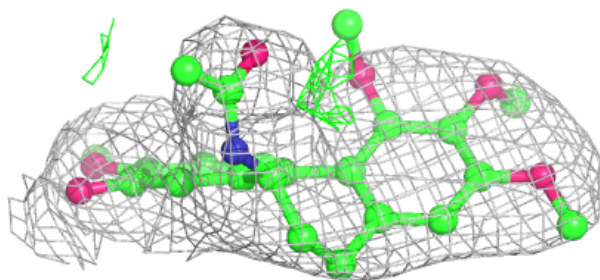
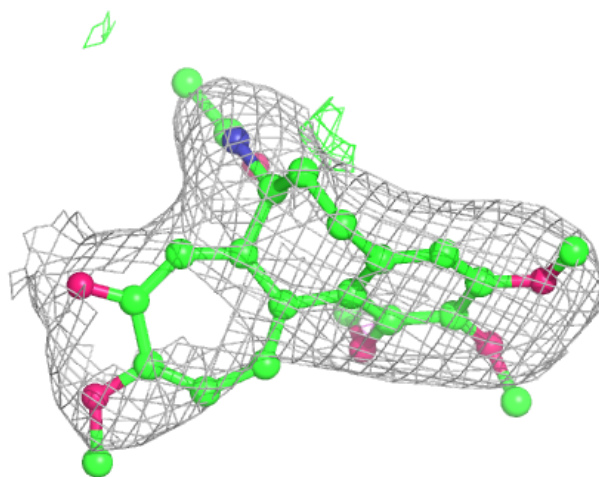






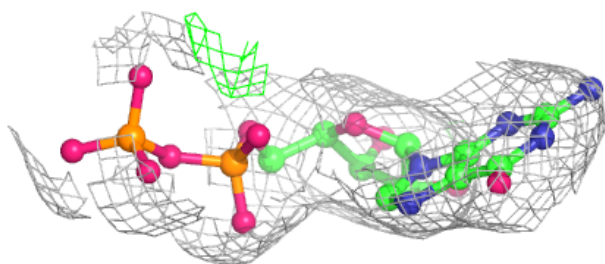
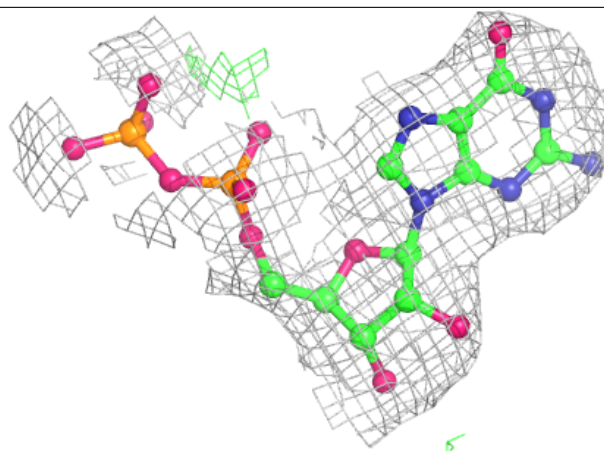
Electron density around LOC D 502:

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



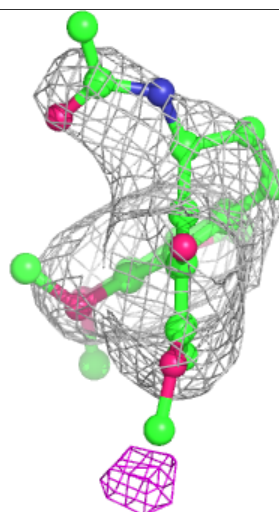
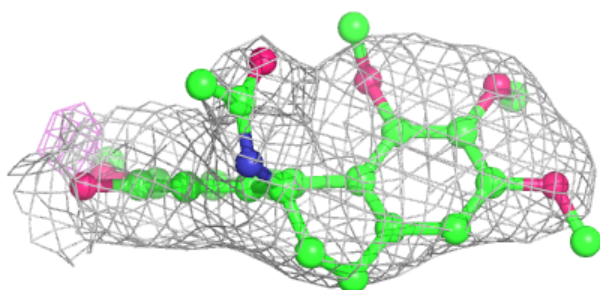
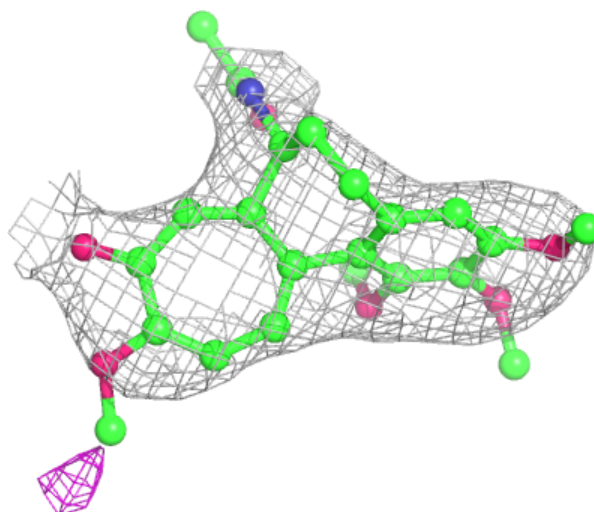
Electron density around GDP D 501:

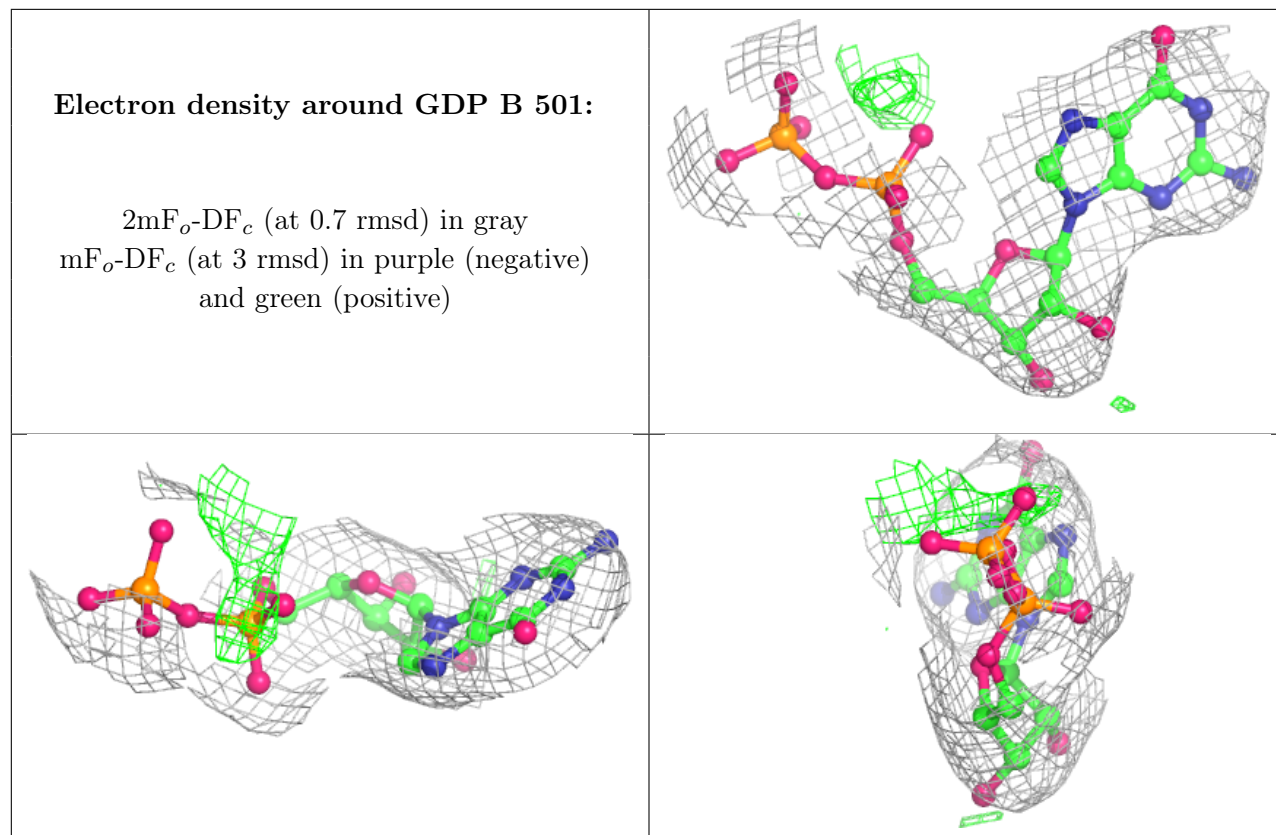
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LOC B 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.