



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:34 PM UTC

PDB ID : 5KX5 / pdb_00005kx5
Title : Crystal structure of tubulin-stathmin-TTL-Compound 11 complex
Authors : Parris, K.
Deposited on : 2016-07-20
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

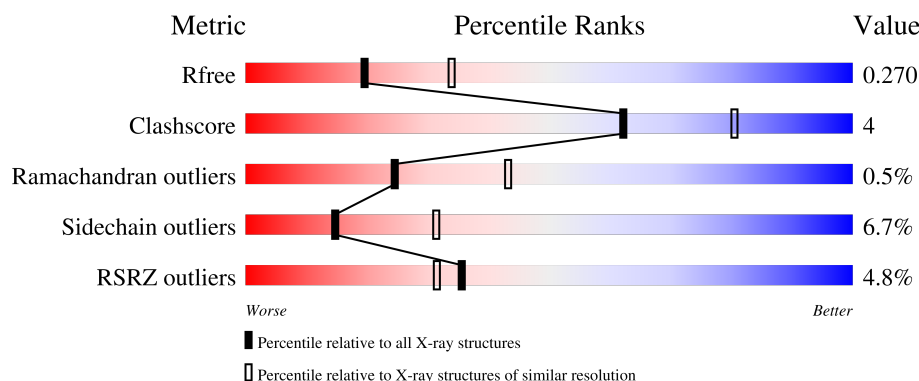
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	451	3% 80% 16% ..
1	C	451	3% 82% 15% ..
2	B	445	% 78% 16% ..
2	D	445	5% 77% 16% ..
3	E	143	6% 65% 18% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	11% 71% 16% • 12%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17802 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	441	Total	C	N	O	S	0	0	0
			3445	2179	585	659	22			
1	C	440	Total	C	N	O	S	0	2	0
			3455	2186	589	658	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	3	0
			3377	2122	578	651	26			
2	D	426	Total	C	N	O	S	0	0	0
			3343	2097	571	650	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			1012	625	185	198	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	conflict	UNP P63043
E	20	TRP	PHE	conflict	UNP P63043

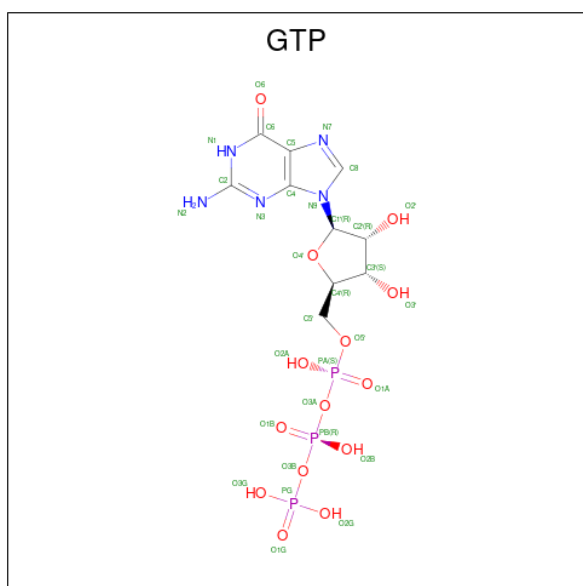
- Molecule 4 is a protein called TTL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	338	Total	C	N	O	S	0	2	0
			2788	1794	474	506	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

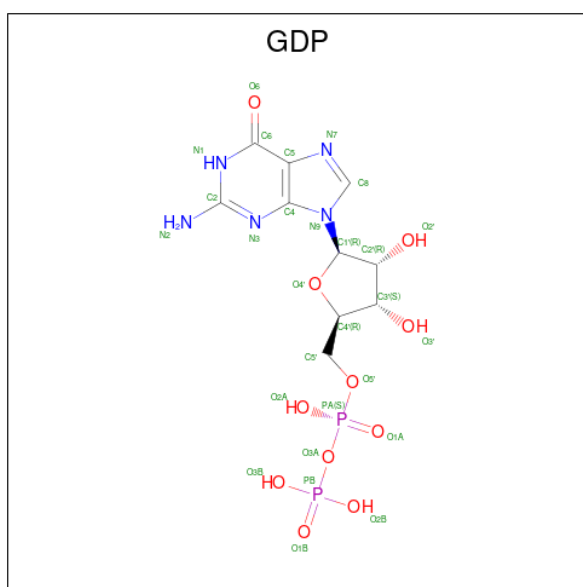
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

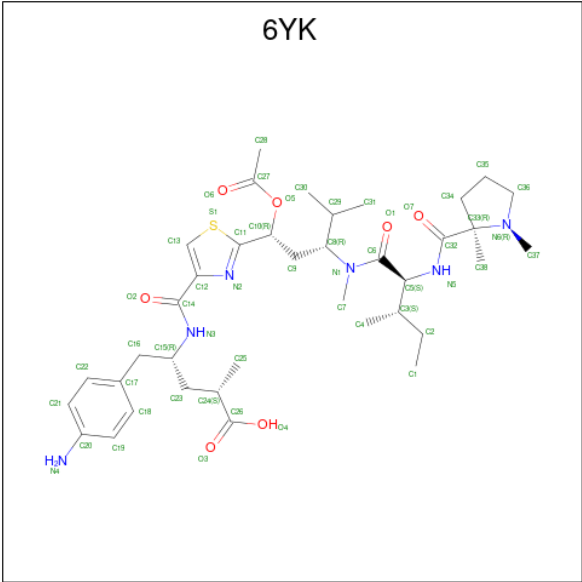
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



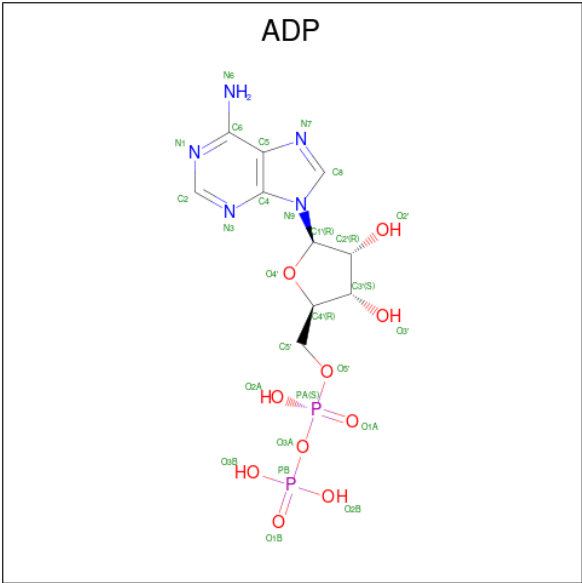
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is (2 {S},4 {R})-4-[[2-[(1 {R},3 {R})-1-acetyloxy-3-[[[(2 {S},3 {S})-2-[[[(2 {R})-1,2-dimethylpyrrolidin-2-yl]carbonylamino]-3-methyl-pentanoyl]-methyl-amino]-4-methyl-pentyl]-1,3-thiazol-4-yl]carbonylamino]-5-(4-aminophenyl)-2-methyl-pentanoic acid (CCD ID: 6YK) (formula: C₃₈H₅₈N₆O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			52	38	6	7	1		
9	D	1	Total	C	N	O	S	0	0
			52	38	6	7	1		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

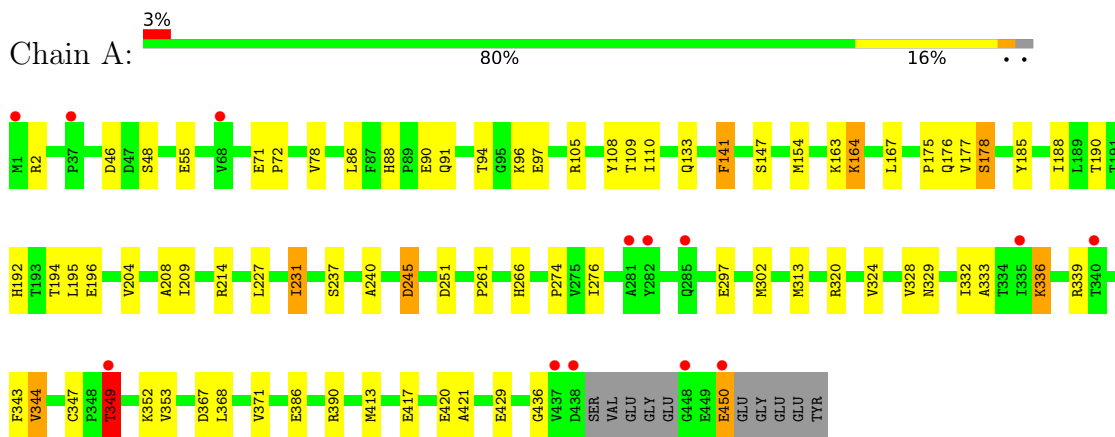
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	22	Total 22	O 22	0	0
11	B	33	Total 33	O 33	0	0
11	C	41	Total 41	O 41	0	0
11	D	7	Total 7	O 7	0	0
11	E	4	Total 4	O 4	0	0
11	F	14	Total 14	O 14	0	0

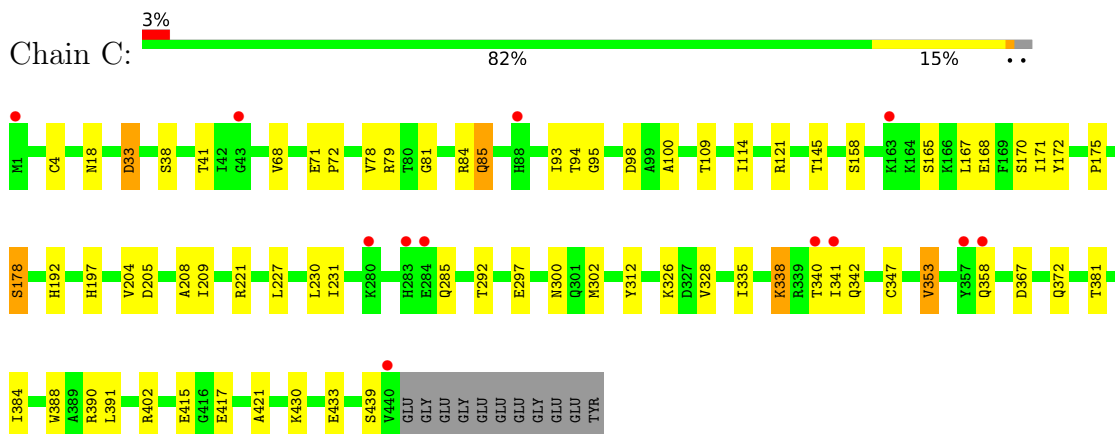
3 Residue-property plots [i](#)

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.

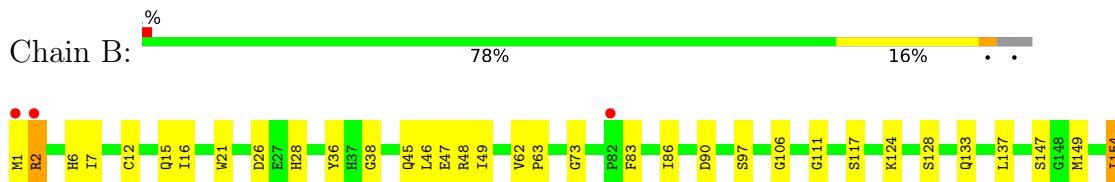
- Molecule 1: Tubulin alpha chain

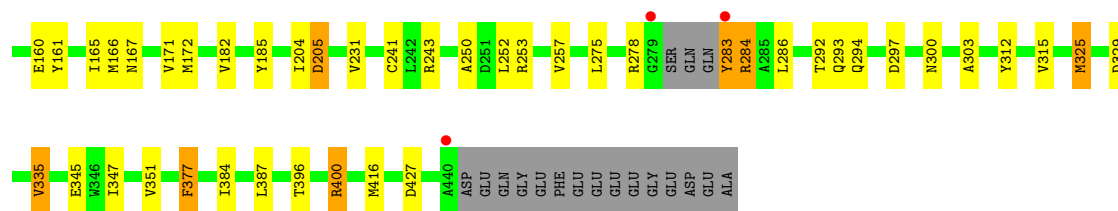


- Molecule 1: Tubulin alpha chain

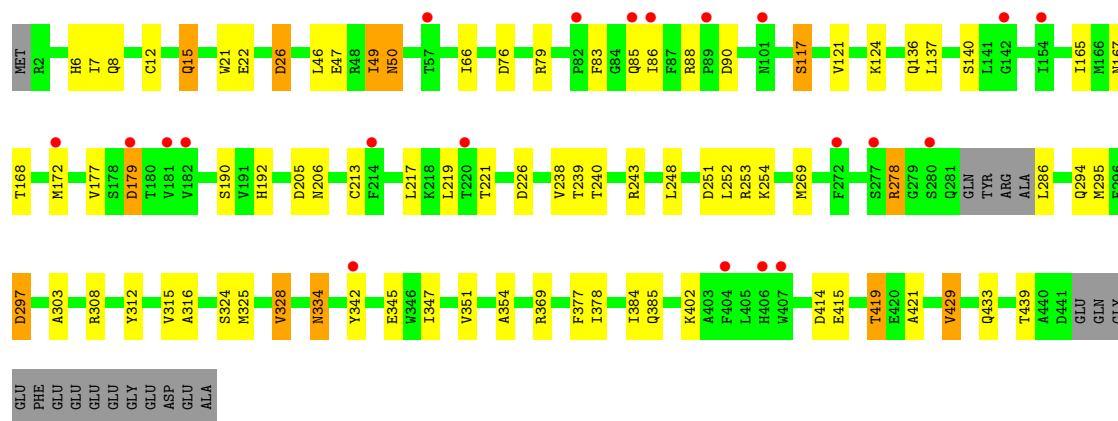
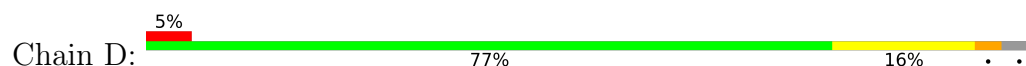


- Molecule 2: Tubulin beta chain

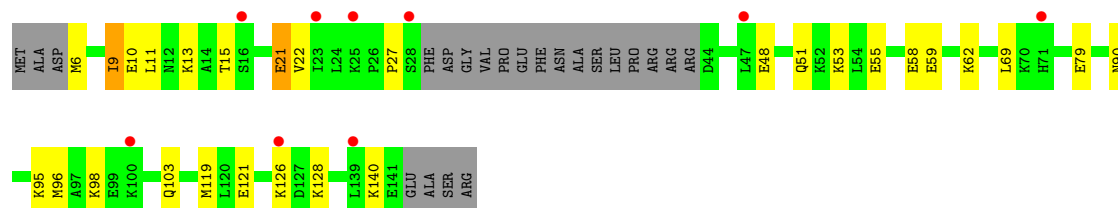




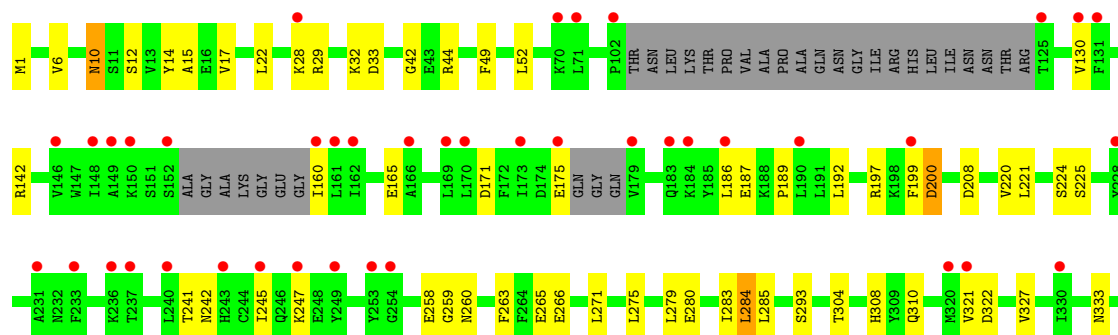
• Molecule 2: Tubulin beta chain

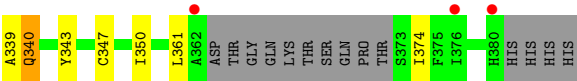


• Molecule 3: Stathmin-4



• Molecule 4: TTL protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.79Å 153.90Å 185.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.47 – 2.50 38.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (38.47-2.50) 97.2 (38.47-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.51Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.197 , 0.251 0.214 , 0.270	Depositor DCC
R_{free} test set	5070 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17802	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: GTP, 6YK, ADP, CA, GDP, 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	0.90	0/3522	1.46	21/4779 (0.4%)
1	C	0.89	0/3534	1.45	26/4800 (0.5%)
2	B	0.91	2/3457 (0.1%)	1.42	13/4681 (0.3%)
2	D	0.86	0/3416	1.43	27/4627 (0.6%)
3	E	0.88	0/1022	1.56	8/1358 (0.6%)
4	F	0.86	0/2857	1.34	10/3859 (0.3%)
All	All	0.89	2/17808 (0.0%)	1.43	105/24104 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	149	MET	SD-CE	-5.26	1.66	1.79
2	B	62	VAL	CA-C	5.21	1.57	1.53

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	179	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	333	ALA	CA-C-N	6.72	130.13	120.79
1	A	333	ALA	C-N-CA	6.72	130.13	120.79
1	A	141	PHE	CA-CB-CG	6.53	120.33	113.80
1	C	353	VAL	CA-C-N	6.36	126.57	122.18
1	C	353	VAL	C-N-CA	6.36	126.57	122.18
3	E	79	GLU	CA-C-N	6.31	129.02	120.44
3	E	79	GLU	C-N-CA	6.31	129.02	120.44
1	A	78	VAL	N-CA-C	-6.29	103.48	112.35
2	B	347	ILE	N-CA-CB	6.29	120.01	111.21
2	D	26	ASP	CA-CB-CG	6.29	118.89	112.60
1	C	98	ASP	CA-CB-CG	6.25	118.85	112.60
1	C	78	VAL	CA-C-N	6.13	128.50	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	VAL	C-N-CA	6.13	128.50	120.28
2	D	334	ASN	CA-CB-CG	6.11	118.71	112.60
4	F	42	GLY	N-CA-C	6.06	120.30	112.54
2	D	22	GLU	CA-C-N	6.01	128.13	120.56
2	D	22	GLU	C-N-CA	6.01	128.13	120.56
1	C	18	ASN	CA-C-N	5.97	128.20	120.44
1	C	18	ASN	C-N-CA	5.97	128.20	120.44
4	F	304	THR	CA-C-N	5.96	129.07	120.79
4	F	304	THR	C-N-CA	5.96	129.07	120.79
2	D	414	ASP	CA-CB-CG	5.90	118.50	112.60
4	F	322	ASP	CA-CB-CG	5.90	118.50	112.60
2	D	419	THR	CA-C-N	5.87	128.07	120.44
2	D	419	THR	C-N-CA	5.87	128.07	120.44
1	A	240	ALA	CA-C-N	5.86	128.72	120.28
1	A	240	ALA	C-N-CA	5.86	128.72	120.28
2	D	226	ASP	CA-C-N	5.85	128.12	120.28
2	D	226	ASP	C-N-CA	5.85	128.12	120.28
2	D	402	LYS	CA-C-N	5.85	129.01	120.71
2	D	402	LYS	C-N-CA	5.85	129.01	120.71
2	D	415	GLU	CA-C-N	5.82	128.00	120.44
2	D	415	GLU	C-N-CA	5.82	128.00	120.44
4	F	208	ASP	CA-CB-CG	5.79	118.39	112.60
4	F	200	ASP	CA-CB-CG	5.66	118.26	112.60
2	B	427	ASP	CA-CB-CG	5.65	118.25	112.60
1	C	388	TRP	CA-C-N	5.64	127.78	120.44
1	C	388	TRP	C-N-CA	5.64	127.78	120.44
1	A	420	GLU	N-CA-C	-5.62	104.79	111.03
1	C	145	THR	CA-C-N	5.57	126.26	120.03
1	C	145	THR	C-N-CA	5.57	126.26	120.03
2	D	297	ASP	CA-CB-CG	5.55	118.15	112.60
2	B	297	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	436	GLY	N-CA-C	5.53	120.78	113.37
2	B	283	TYR	CA-C-N	5.49	131.06	122.17
2	B	283	TYR	C-N-CA	5.49	131.06	122.17
4	F	12	SER	CA-C-N	5.46	127.55	120.56
4	F	12	SER	C-N-CA	5.46	127.55	120.56
1	A	429	GLU	CA-C-N	5.43	127.55	120.28
1	A	429	GLU	C-N-CA	5.43	127.55	120.28
1	C	81	GLY	CA-C-N	5.42	127.80	120.38
1	C	81	GLY	C-N-CA	5.42	127.80	120.38
1	C	433	GLU	CA-C-N	5.39	127.45	120.44
1	C	433	GLU	C-N-CA	5.39	127.45	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ILE	CA-C-N	5.38	126.05	120.03
1	A	231	ILE	C-N-CA	5.38	126.05	120.03
2	D	347	ILE	N-CA-CB	5.37	118.72	111.21
1	C	390	ARG	CA-C-N	5.32	127.41	120.28
1	C	390	ARG	C-N-CA	5.32	127.41	120.28
4	F	15	ALA	N-CA-C	-5.28	105.60	111.36
1	A	208	ALA	CA-C-N	5.26	127.66	120.46
1	A	208	ALA	C-N-CA	5.26	127.66	120.46
3	E	9	ILE	CA-C-N	5.25	131.56	121.54
3	E	9	ILE	C-N-CA	5.25	131.56	121.54
1	C	208	ALA	CA-C-N	5.24	127.64	120.46
1	C	208	ALA	C-N-CA	5.24	127.64	120.46
1	C	205	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	154	ILE	CA-C-N	5.22	127.28	120.28
2	B	154	ILE	C-N-CA	5.22	127.28	120.28
1	C	417	GLU	CA-C-N	5.21	127.53	120.44
1	C	417	GLU	C-N-CA	5.21	127.53	120.44
2	D	433	GLN	CA-C-N	5.20	127.56	120.54
2	D	433	GLN	C-N-CA	5.20	127.56	120.54
2	D	251	ASP	CA-C-N	5.18	127.48	120.38
2	D	251	ASP	C-N-CA	5.18	127.48	120.38
2	B	329	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	338	LYS	CA-C-N	5.16	131.40	121.54
1	C	338	LYS	C-N-CA	5.16	131.40	121.54
2	B	147	SER	CA-C-N	5.15	125.55	119.94
2	B	147	SER	C-N-CA	5.15	125.55	119.94
2	D	88	ARG	N-CA-C	-5.14	103.30	109.72
1	C	33	ASP	CA-CB-CG	5.13	117.73	112.60
2	B	205	ASP	CA-CB-CG	5.12	117.72	112.60
2	D	117	SER	CA-C-N	5.12	127.12	120.56
2	D	117	SER	C-N-CA	5.12	127.12	120.56
4	F	171	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	185	TYR	CA-C-N	5.10	127.12	120.28
1	A	185	TYR	C-N-CA	5.10	127.12	120.28
2	B	97	SER	N-CA-C	5.10	116.53	110.97
2	B	377	PHE	CA-CB-CG	5.08	118.88	113.80
1	C	95	GLY	N-CA-C	-5.07	105.35	112.60
3	E	51	GLN	CA-C-N	5.07	127.03	120.44
3	E	51	GLN	C-N-CA	5.07	127.03	120.44
1	A	96	LYS	CA-C-N	5.04	129.96	123.00
1	A	96	LYS	C-N-CA	5.04	129.96	123.00
1	A	237	SER	CA-C-N	5.04	127.58	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	SER	C-N-CA	5.04	127.58	120.42
1	A	349	THR	CB-CA-C	5.04	118.33	110.67
2	D	240	THR	CA-C-N	5.01	127.50	120.28
2	D	240	THR	C-N-CA	5.01	127.50	120.28
2	D	328	VAL	CA-C-N	5.01	126.99	120.28
2	D	328	VAL	C-N-CA	5.01	126.99	120.28
3	E	69	LEU	CA-C-N	5.01	127.25	120.44
3	E	69	LEU	C-N-CA	5.01	127.25	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	3445	0	3349	31	0
1	C	3455	0	3364	25	0
2	B	3377	0	3265	35	0
2	D	3343	0	3216	33	0
3	E	1012	0	1025	6	0
4	F	2788	0	2768	21	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	0	0
9	B	52	0	0	1	0
9	D	52	0	0	1	0
10	F	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	22	0	0	0	0
11	B	33	0	0	0	0
11	C	41	0	0	0	0
11	D	7	0	0	0	0
11	E	4	0	0	0	0
11	F	14	0	0	0	0
All	All	17802	0	17047	143	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 4.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:HIS:CE1	2:B:243:ARG:HH11	2.12	0.67
1:A:97:GLU:HG3	2:B:1:MET:HG2	1.76	0.67
2:B:15:GLN:HG2	9:B:504:6YK:C19	2.25	0.66
1:A:195:LEU:HD12	1:A:266:HIS:HE1	1.60	0.66
2:B:28:HIS:HE1	2:B:243:ARG:HH11	1.44	0.66
1:A:245:ASP:OD2	3:E:15:THR:HG22	1.94	0.66
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.77	0.65
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.78	0.64
4:F:14:TYR:HA	4:F:17:VAL:HB	1.81	0.62
1:C:285:GLN:HE22	1:C:372:GLN:H	1.49	0.61
1:A:175:PRO:HA	1:A:178:SER:HB2	1.83	0.60
1:A:163:LYS:H	1:A:163:LYS:HD3	1.66	0.59
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.86	0.57
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.86	0.57
1:C:209:ILE:HD11	1:C:302:MET:SD	2.44	0.57
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.85	0.57
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.87	0.56
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.87	0.56
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.87	0.56
2:B:28:HIS:HE1	2:B:243:ARG:HD2	1.70	0.56
1:C:221:ARG:HD2	2:D:325:MET:HE3	1.88	0.56
2:D:324:SER:O	2:D:328:VAL:HG23	2.06	0.55
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.40	0.55
2:D:295:MET:HE3	2:D:377:PHE:HB2	1.89	0.55
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.89	0.54
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.88	0.54
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.90	0.53
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.89	0.53
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.89	0.53
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.90	0.53
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.91	0.53
1:A:192:HIS:CG	1:A:421:ALA:HA	2.44	0.52
2:B:2:ARG:H	2:B:133:GLN:HG3	1.74	0.52
2:B:83:PHE:O	2:B:86:ILE:HG22	2.09	0.52
1:A:209:ILE:HD11	1:A:302:MET:SD	2.49	0.52
2:B:182:VAL:O	2:B:185:TYR:HB2	2.10	0.52
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.44	0.52
2:B:241:CYS:O	2:B:250:ALA:HA	2.10	0.51
4:F:347:CYS:HA	4:F:350:ILE:HD12	1.92	0.51
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.92	0.51
2:D:385:GLN:HB2	2:D:429:VAL:HG22	1.93	0.51
1:A:72:PRO:HA	1:A:94:THR:HG21	1.93	0.51
2:D:83:PHE:O	2:D:86:ILE:HG22	2.10	0.51
1:A:154:MET:HG3	1:A:194:THR:HG23	1.93	0.51
1:C:72:PRO:HA	1:C:94:THR:HG21	1.93	0.51
4:F:224:SER:HB2	4:F:241:THR:HG22	1.91	0.50
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.30	0.50
2:D:15:GLN:HG2	9:D:504:6YK:C19	2.43	0.49
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.95	0.49
2:B:283:TYR:HB2	2:B:284:ARG:HG3	1.94	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.49
2:B:396:THR:O	2:B:400[B]:ARG:HB2	2.13	0.49
1:C:100:ALA:HA	2:D:254:LYS:HE2	1.95	0.49
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.95	0.48
2:D:312:TYR:HE1	2:D:377:PHE:HZ	1.59	0.47
1:A:352:LYS:HG2	3:E:21:GLU:HG3	1.96	0.47
1:C:33:ASP:HA	1:C:85:GLN:HB2	1.97	0.47
2:D:46:LEU:HD23	2:D:49:ILE:HD13	1.97	0.47
3:E:58:GLU:HG2	3:E:62:LYS:HD2	1.96	0.47
1:C:171:ILE:HD13	1:C:204:VAL:HB	1.96	0.47
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.96	0.47
2:D:50:ASN:ND2	2:D:50:ASN:H	2.12	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.46
1:A:88:HIS:HB2	1:A:91:GLN:HG3	1.97	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.45	0.46
1:A:163:LYS:HG2	1:A:164:LYS:HD2	1.97	0.46
1:A:450:GLU:HG3	4:F:333:ASN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ARG:O	2:B:257:VAL:HG23	2.16	0.46
2:B:38:GLY:HA3	2:B:45:GLN:HE22	1.81	0.45
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.81	0.45
2:D:7:ILE:O	2:D:137:LEU:HD12	2.16	0.45
2:B:325:MET:HE3	2:B:325:MET:HB2	1.90	0.45
2:D:12:CYS:CB	2:D:140:SER:HB3	2.47	0.45
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.98	0.45
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.52	0.45
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.97	0.45
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.52	0.45
2:B:160:GLU:HG2	2:B:161:TYR:CE2	2.50	0.45
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.45
2:B:48:ARG:HB2	2:B:243:ARG:O	2.16	0.45
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.34	0.45
1:C:79:ARG:O	1:C:84:ARG:HB2	2.16	0.45
2:D:76:ASP:HA	2:D:79:ARG:NH1	2.32	0.45
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.44
4:F:271:LEU:HD23	4:F:275:LEU:HD13	1.99	0.44
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.44
1:C:158:SER:OG	1:C:197:HIS:HD2	2.01	0.44
1:C:402:ARG:HE	1:C:415:GLU:CD	2.26	0.44
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.88	0.44
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.98	0.44
2:D:7:ILE:O	2:D:137:LEU:HA	2.18	0.44
4:F:321:VAL:HG22	4:F:327:VAL:HG22	1.99	0.44
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.99	0.44
4:F:187:GLU:O	4:F:189:PRO:HD3	2.18	0.43
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.53	0.43
2:D:316:ALA:HB3	2:D:378:ILE:HB	2.00	0.43
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.01	0.43
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE2	2.53	0.43
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.83	0.43
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.99	0.43
2:D:239:THR:O	2:D:243:ARG:HG3	2.18	0.43
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.99	0.43
1:C:285:GLN:HG3	1:C:372:GLN:HE21	1.82	0.43
2:D:238:VAL:HG12	2:D:378:ILE:HG12	2.01	0.43
4:F:197:ARG:HB2	4:F:224:SER:O	2.19	0.43
1:A:329:ASN:HB3	3:E:6:MET:HE1	2.01	0.43
1:A:97:GLU:HG2	1:A:105:ARG:HH21	1.84	0.43
2:D:172:MET:HB2	2:D:205:ASP:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:225:SER:HB3	4:F:260:ASN:HD21	1.83	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.42
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.00	0.42
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.00	0.42
1:C:312:TYR:CD2	1:C:341:ILE:HG23	2.54	0.42
2:B:400[B]:ARG:HH11	2:B:400[B]:ARG:HB3	1.85	0.42
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	2.02	0.42
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.02	0.42
2:B:46:LEU:HA	2:B:49:ILE:HB	2.01	0.42
2:D:165:ILE:HD11	2:D:253:ARG:HG3	2.02	0.41
4:F:6:VAL:HB	4:F:29:ARG:CZ	2.50	0.41
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.02	0.41
1:C:285:GLN:NE2	1:C:372:GLN:H	2.18	0.41
4:F:242:ASN:HB2	4:F:245:ILE:HD12	2.02	0.41
1:C:297:GLU:HB3	1:C:300:ASN:HD22	1.86	0.41
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.01	0.41
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.55	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
4:F:220[A]:VAL:HG11	4:F:339:ALA:HB2	2.02	0.41
4:F:258:GLU:HA	4:F:259:GLY:HA2	1.88	0.41
2:B:172:MET:HG3	2:B:387:LEU:HD21	2.03	0.41
1:C:175:PRO:HA	1:C:178:SER:HB2	2.03	0.41
1:A:332:ILE:HD13	3:E:22:VAL:HG11	2.02	0.41
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.56	0.41
2:B:286:LEU:HD21	2:B:294:GLN:NE2	2.36	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.02	0.40
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.02	0.40
1:A:297:GLU:HG2	1:A:339:ARG:HH22	1.86	0.40
1:C:192:HIS:CG	1:C:421:ALA:HA	2.57	0.40
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.03	0.40
1:A:386:GLU:O	1:A:390:ARG:HG3	2.21	0.40
1:C:209:ILE:CD1	1:C:302:MET:SD	3.10	0.40
2:B:315:VAL:HB	2:B:351:VAL:HG22	2.03	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	437/451 (97%)	415 (95%)	20 (5%)	2 (0%)	24	43
1	C	440/451 (98%)	428 (97%)	11 (2%)	1 (0%)	43	63
2	B	426/445 (96%)	413 (97%)	9 (2%)	4 (1%)	14	27
2	D	422/445 (95%)	399 (94%)	22 (5%)	1 (0%)	43	63
3	E	118/143 (82%)	113 (96%)	3 (2%)	2 (2%)	7	13
4	F	330/384 (86%)	310 (94%)	19 (6%)	1 (0%)	36	55
All	All	2173/2319 (94%)	2078 (96%)	84 (4%)	11 (0%)	24	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2	ARG
2	B	73	GLY
3	E	10	GLU
1	C	109	THR
3	E	27	PRO
2	B	128	SER
2	B	278	ARG
1	A	109	THR
1	A	245	ASP
4	F	361	LEU
2	D	278	ARG

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	370/378 (98%)	344 (93%)	26 (7%)	14	29
1	C	372/378 (98%)	349 (94%)	23 (6%)	16	34
2	B	371/383 (97%)	356 (96%)	15 (4%)	28	54
2	D	368/383 (96%)	343 (93%)	25 (7%)	14	31
3	E	109/126 (86%)	92 (84%)	17 (16%)	2	5
4	F	308/342 (90%)	286 (93%)	22 (7%)	13	29
All	All	1898/1990 (95%)	1770 (93%)	128 (7%)	15	31

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	48	SER
1	A	55	GLU
1	A	71	GLU
1	A	86	LEU
1	A	90	GLU
1	A	110	ILE
1	A	141	PHE
1	A	164	LYS
1	A	167	LEU
1	A	176	GLN
1	A	177	VAL
1	A	178	SER
1	A	188	ILE
1	A	196	GLU
1	A	214	ARG
1	A	251	ASP
1	A	276	ILE
1	A	320	ARG
1	A	324	VAL
1	A	336	LYS
1	A	344	VAL
1	A	349	THR
1	A	367	ASP
1	A	368	LEU
1	A	450	GLU
2	B	26	ASP
2	B	47	GLU
2	B	90	ASP
2	B	117	SER

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Mol	Chain	Res	Type
2	B	124	LYS
2	B	167	ASN
2	B	284	ARG
2	B	293	GLN
2	B	325	MET
2	B	335	VAL
2	B	345	GLU
2	B	384	ILE
2	B	400[A]	ARG
2	B	400[B]	ARG
2	B	416	MET
1	C	4	CYS
1	C	38	SER
1	C	41	THR
1	C	68	VAL
1	C	71	GLU
1	C	85	GLN
1	C	165	SER
1	C	167	LEU
1	C	168	GLU
1	C	170	SER
1	C	178	SER
1	C	326	LYS
1	C	338	LYS
1	C	340	THR
1	C	342	GLN
1	C	347	CYS
1	C	358[A]	GLN
1	C	358[B]	GLN
1	C	367	ASP
1	C	381	THR
1	C	384	ILE
1	C	430	LYS
1	C	439	SER
2	D	8	GLN
2	D	15	GLN
2	D	26	ASP
2	D	47	GLU
2	D	49	ILE
2	D	50	ASN
2	D	85	GLN
2	D	90	ASP

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Mol	Chain	Res	Type
2	D	117	SER
2	D	124	LYS
2	D	179	ASP
2	D	190	SER
2	D	219	LEU
2	D	221	THR
2	D	278	ARG
2	D	286	LEU
2	D	294	GLN
2	D	297	ASP
2	D	334	ASN
2	D	345	GLU
2	D	369	ARG
2	D	384	ILE
2	D	419	THR
2	D	429	VAL
2	D	439	THR
3	E	11	LEU
3	E	13	LYS
3	E	21	GLU
3	E	48	GLU
3	E	53	LYS
3	E	55	GLU
3	E	59	GLU
3	E	90	ASN
3	E	95	LYS
3	E	96	MET
3	E	98	LYS
3	E	103	GLN
3	E	119	MET
3	E	121	GLU
3	E	126	LYS
3	E	128	LYS
3	E	140	LYS
4	F	10	ASN
4	F	22	LEU
4	F	32	LYS
4	F	33	ASP
4	F	130	VAL
4	F	142	ARG
4	F	160	ILE
4	F	165	GLU

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Mol	Chain	Res	Type
4	F	175	GLU
4	F	186	LEU
4	F	192	LEU
4	F	200	ASP
4	F	247	LYS
4	F	265	GLU
4	F	266	GLU
4	F	284	LEU
4	F	285	LEU
4	F	293	SER
4	F	308	HIS
4	F	310	GLN
4	F	340	GLN
4	F	374	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	216	ASN
1	A	301	GLN
1	A	380	ASN
1	A	393	HIS
2	B	11	GLN
2	B	28	HIS
2	B	45	GLN
2	B	96	GLN
2	B	101	ASN
2	B	192	HIS
2	B	193	GLN
2	B	294	GLN
2	B	300	ASN
2	B	349	ASN
1	C	31	GLN
1	C	50	ASN
1	C	101	ASN
1	C	139	HIS
1	C	197	HIS
1	C	256	GLN
1	C	283	HIS
1	C	300	ASN
1	C	356	ASN

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Mol	Chain	Res	Type
1	C	372	GLN
2	D	45	GLN
2	D	50	ASN
2	D	167	ASN
2	D	192	HIS
2	D	349	ASN
2	D	385	GLN
2	D	433	GLN
3	E	12	ASN
3	E	64	GLN
3	E	115	HIS
3	E	136	ASN
4	F	10	ASN
4	F	45	ASN
4	F	260	ASN
4	F	269	GLN
4	F	310	GLN
4	F	333	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 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	$\# Z > 2$
9	6YK	B	504	-	52,54,54	0.96	1 (1%)	65,77,77	0.91	1 (1%)
10	ADP	F	401	-	28,29,29	0.54	0	43,45,45	0.60	1 (2%)
8	GDP	D	501	6	29,30,30	0.37	0	45,47,47	0.66	1 (2%)
9	6YK	D	504	-	52,54,54	1.01	1 (1%)	65,77,77	1.08	3 (4%)
8	GDP	B	501	-	29,30,30	0.45	0	45,47,47	0.71	1 (2%)
5	GTP	A	501	6	33,34,34	0.50	0	50,54,54	0.64	0
5	GTP	C	501	6	33,34,34	0.43	0	50,54,54	0.70	2 (4%)

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
9	6YK	B	504	-	-	6/64/77/77	0/3/3/3
10	ADP	F	401	-	-	2/16/32/32	0/3/3/3
8	GDP	D	501	6	-	6/16/32/32	0/3/3/3
9	6YK	D	504	-	-	17/64/77/77	0/3/3/3
8	GDP	B	501	-	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
5	GTP	C	501	6	-	5/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	504	6YK	C33-C32	6.64	1.61	1.54
9	B	504	6YK	C33-C32	6.05	1.61	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	6YK	C38-C33-C32	-5.32	103.55	110.45
9	D	504	6YK	C38-C33-C32	-5.11	103.82	110.45
9	D	504	6YK	C35-C34-C33	-4.41	100.50	104.20
5	C	501	GTP	O5'-PA-O1A	2.66	119.46	108.94
8	B	501	GDP	O2B-PB-O3A	2.66	113.54	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	504	6YK	C31-C29-C8	2.41	117.55	111.52
10	F	401	ADP	O2B-PB-O3A	2.33	112.44	104.64
8	D	501	GDP	O2B-PB-O3A	2.29	112.33	104.64
5	C	501	GTP	O3G-PG-O1G	2.22	119.49	110.83

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	504	6YK	C13-C12-C14-O2
9	B	504	6YK	C13-C12-C14-N3
9	D	504	6YK	O7-C32-C33-N6
9	D	504	6YK	N5-C32-C33-N6
9	D	504	6YK	C30-C29-C8-N1
9	D	504	6YK	C31-C29-C8-N1
9	D	504	6YK	C30-C29-C8-C9
9	D	504	6YK	O5-C10-C11-N2
9	D	504	6YK	C13-C12-C14-O2
9	D	504	6YK	C13-C12-C14-N3
9	D	504	6YK	C1-C2-C3-C4
9	D	504	6YK	C1-C2-C3-C5
9	B	504	6YK	N2-C12-C14-O2
9	D	504	6YK	N2-C12-C14-O2
9	B	504	6YK	N2-C12-C14-N3
9	D	504	6YK	N2-C12-C14-N3
9	D	504	6YK	C31-C29-C8-C9
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PB-O3A-PA-O2A
10	F	401	ADP	PB-O3A-PA-O1A
9	B	504	6YK	N5-C32-C33-C38
8	B	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
9	D	504	6YK	O7-C32-C33-C34
9	D	504	6YK	N5-C32-C33-C34
8	D	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
9	D	504	6YK	C29-C8-N1-C7
5	A	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O1A
9	D	504	6YK	C23-C24-C26-O3
9	B	504	6YK	O7-C32-C33-C38
5	C	501	GTP	PG-O3B-PB-O2B
8	D	501	GDP	PB-O3A-PA-O1A
10	F	401	ADP	PB-O3A-PA-O2A

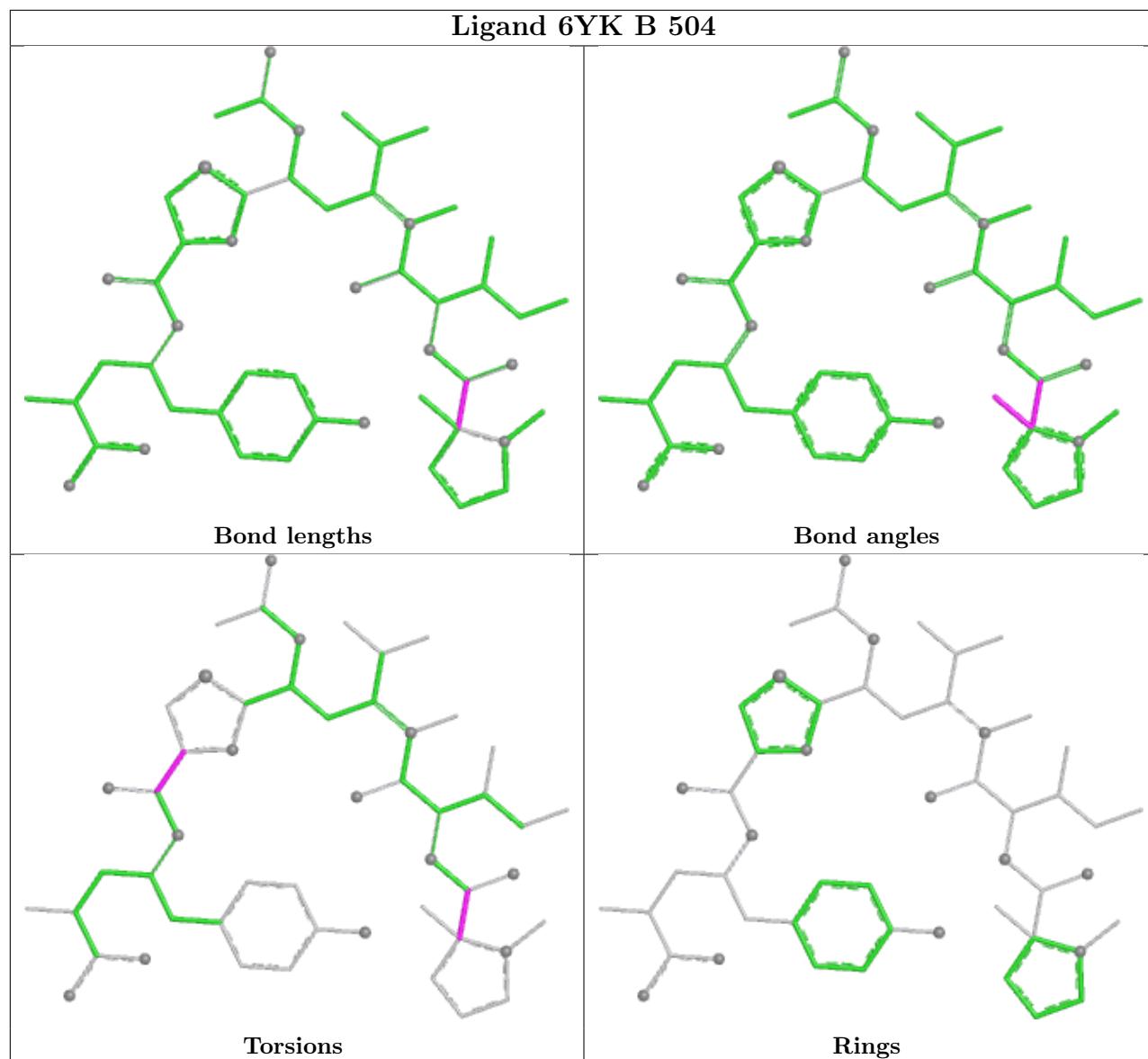
There are no ring outliers.

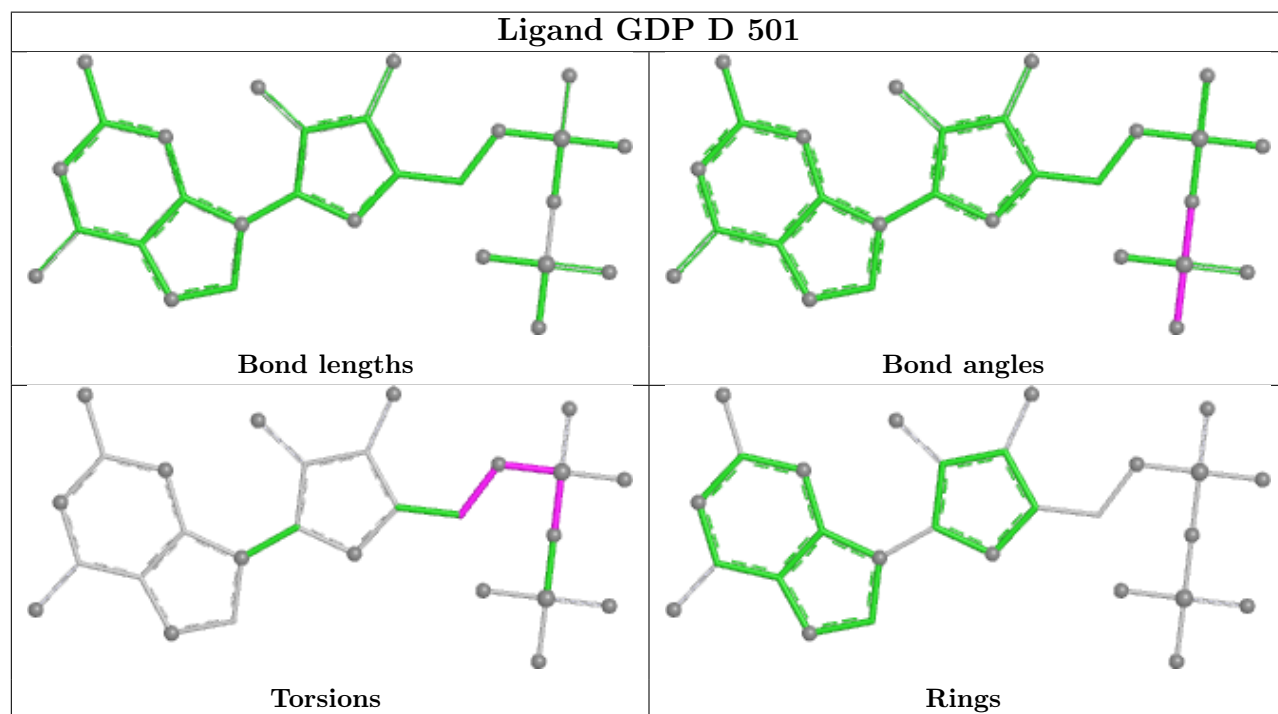
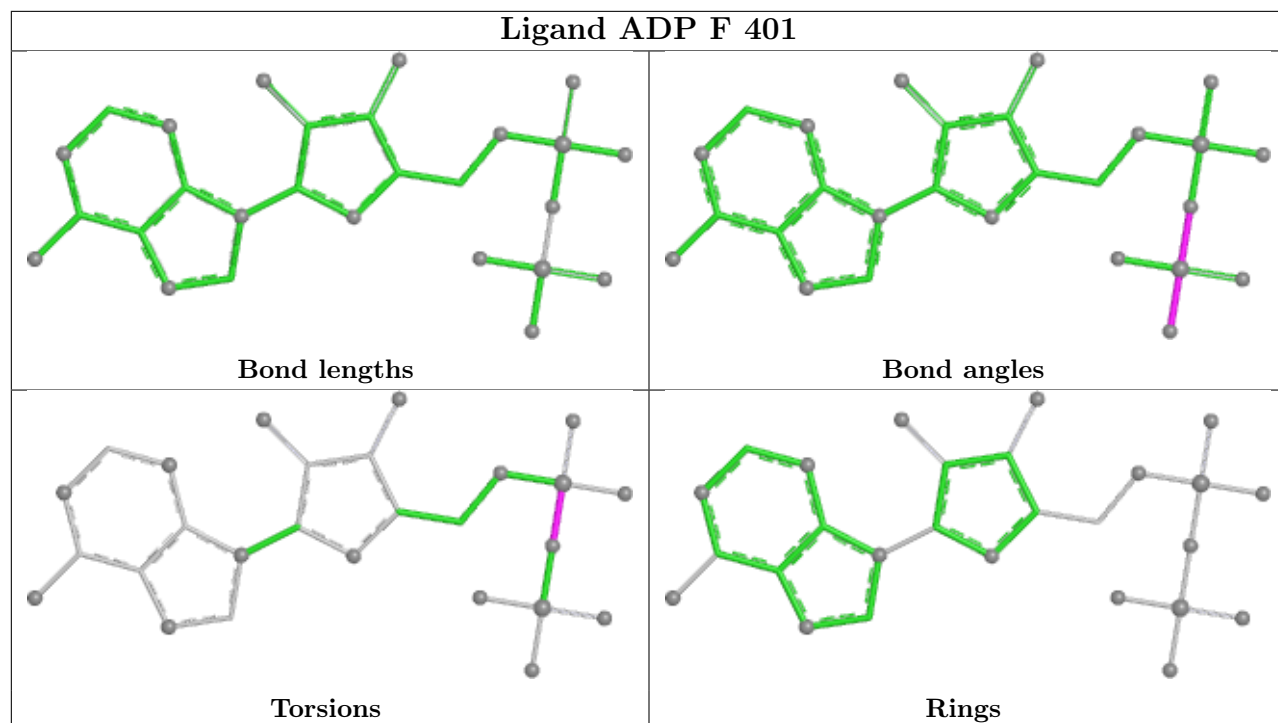
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	6YK	1	0
9	D	504	6YK	1	0
8	B	501	GDP	1	0

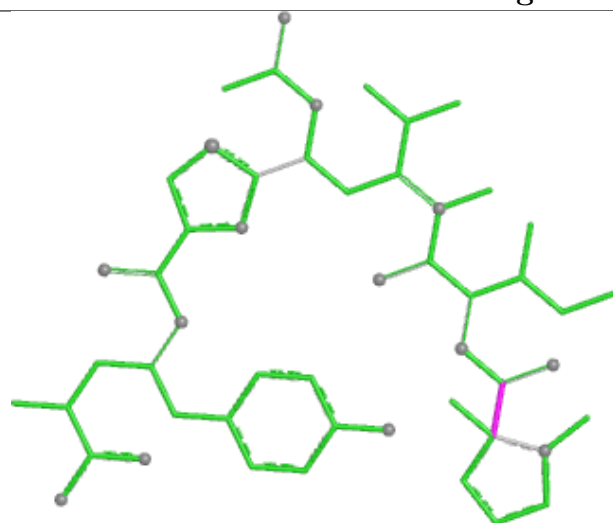
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 6YK B 504

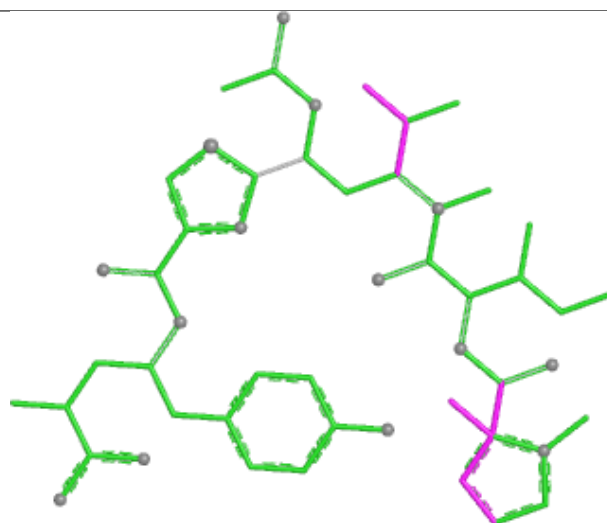




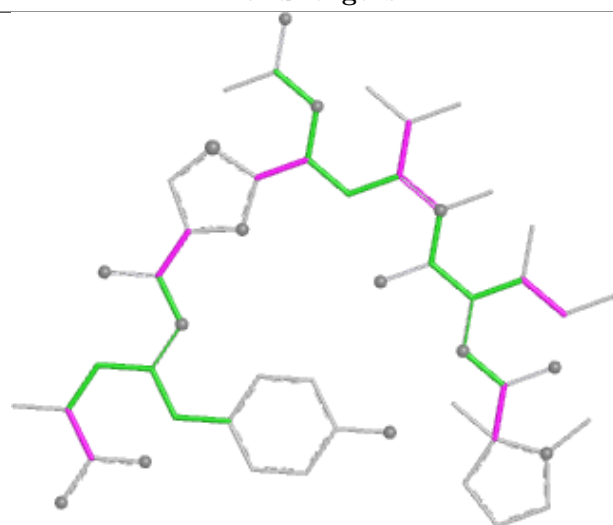
Ligand 6YK D 504



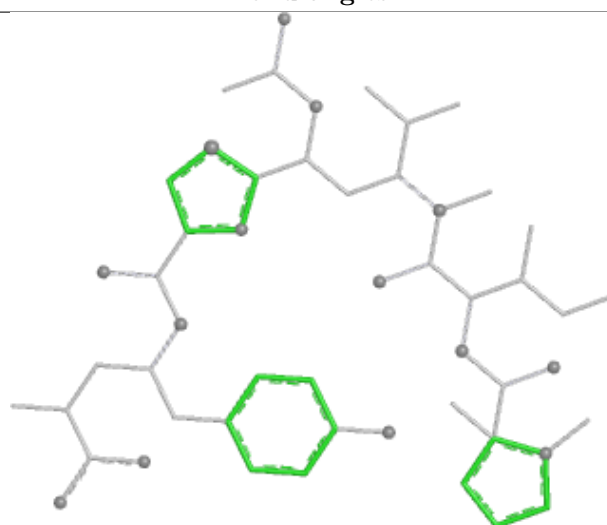
Bond lengths



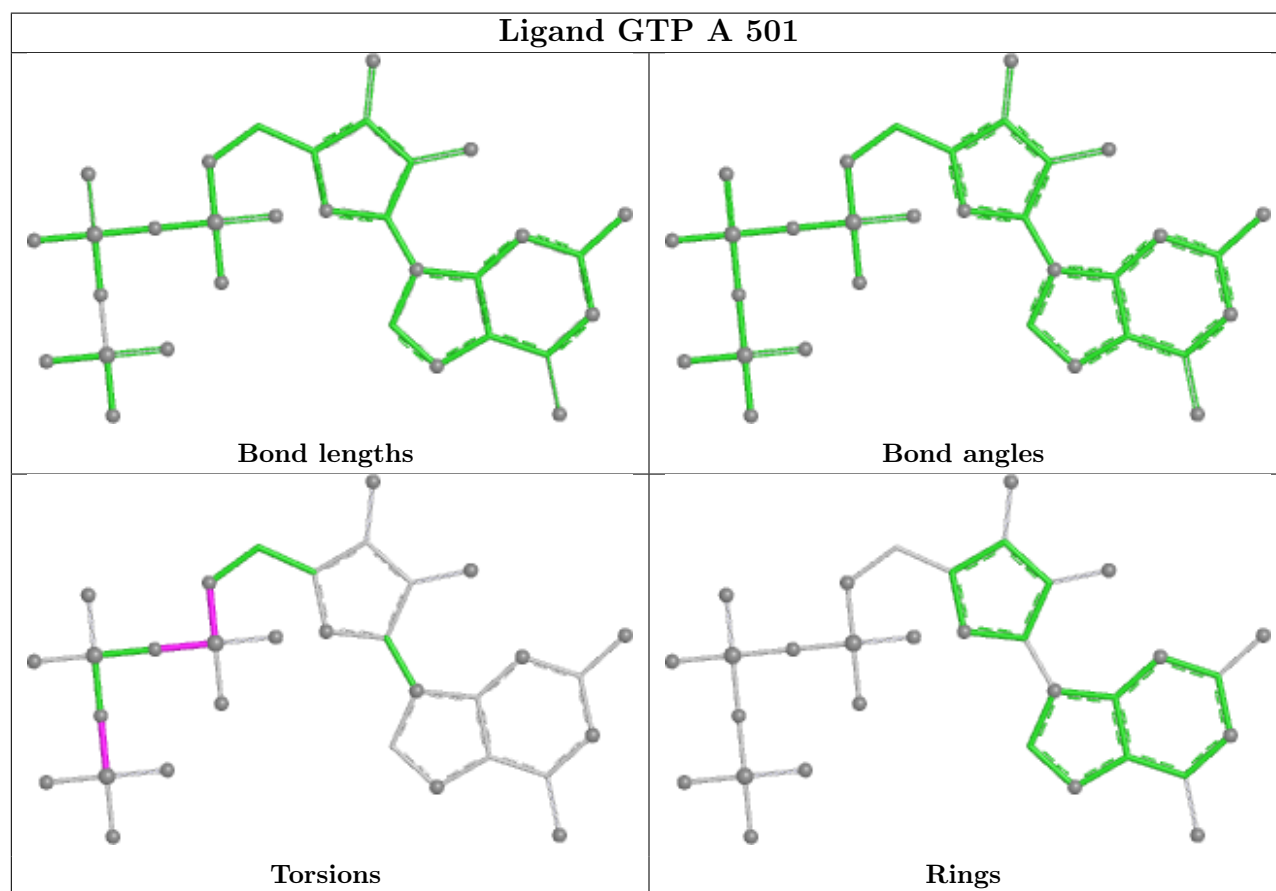
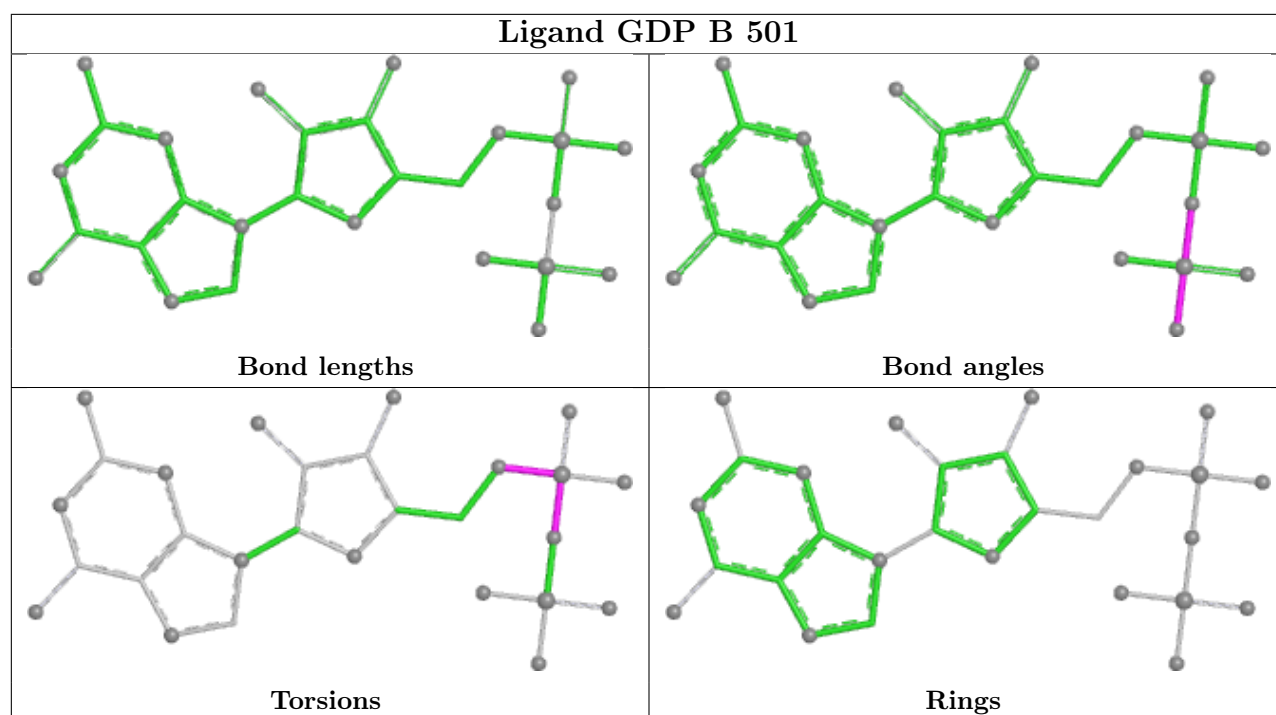
Bond angles

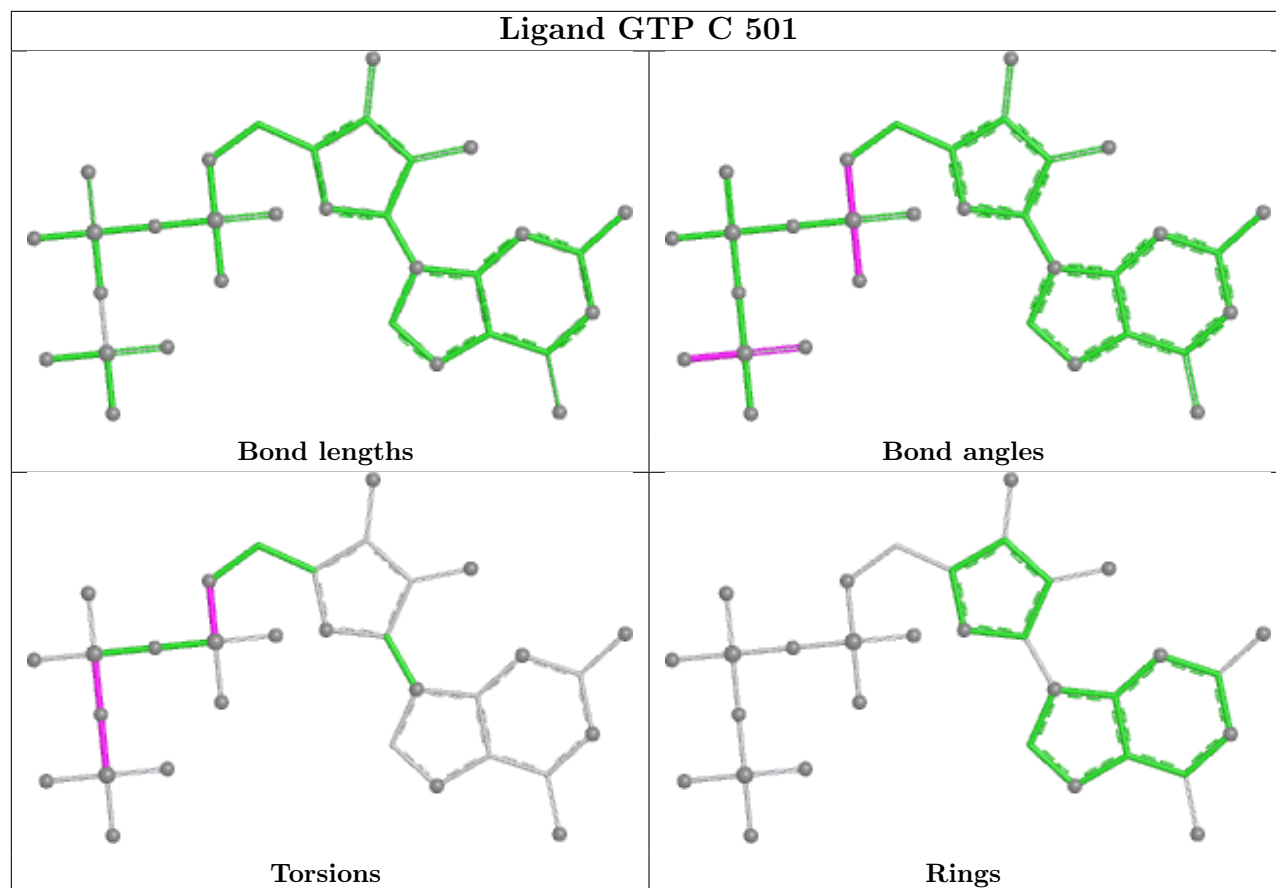


Torsions



Rings





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	441/451 (97%)	0.29	13 (2%)	53	49	38, 61, 92, 146	0
1	C	440/451 (97%)	-0.04	12 (2%)	56	51	28, 51, 76, 106	2 (0%)
2	B	427/445 (95%)	-0.01	6 (1%)	73	70	24, 52, 85, 101	5 (1%)
2	D	426/445 (95%)	0.65	21 (4%)	35	31	48, 72, 97, 126	5 (1%)
3	E	121/143 (84%)	0.68	9 (7%)	20	18	31, 71, 99, 112	1 (0%)
4	F	338/384 (88%)	0.93	44 (13%)	7	6	46, 84, 142, 164	2 (0%)
All	All	2193/2319 (94%)	0.36	105 (4%)	35	31	24, 63, 106, 164	15 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	160	ILE	7.1
1	C	163	LYS	4.4
4	F	166	ALA	4.3
2	B	1	MET	4.2
4	F	240	LEU	4.2
2	B	283	TYR	3.7
1	C	440	VAL	3.7
4	F	362	ALA	3.7
4	F	125	THR	3.6
2	D	407	TRP	3.4
4	F	152	SER	3.4
3	E	28	SER	3.3
1	C	284	GLU	3.2
4	F	236	LYS	3.2
4	F	253	TYR	3.1
4	F	179	VAL	3.1
1	A	335	ILE	3.0
4	F	130	VAL	3.0
4	F	237	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	71[A]	HIS	3.0
2	D	82	PRO	3.0
1	A	282	TYR	2.9
4	F	228	TYR	2.9
2	D	277	SER	2.8
4	F	169	LEU	2.8
1	C	341	ILE	2.8
2	B	82	PRO	2.8
1	C	358[A]	GLN	2.8
1	C	283	HIS	2.8
4	F	245	ILE	2.7
1	C	88[A]	HIS	2.7
2	D	404	PHE	2.7
4	F	233	PHE	2.7
1	A	285	GLN	2.7
4	F	247	LYS	2.6
1	A	68	VAL	2.6
2	D	57	THR	2.6
4	F	231	ALA	2.6
4	F	330	ILE	2.6
1	A	450	GLU	2.6
3	E	16	SER	2.6
3	E	126	LYS	2.6
1	C	1	MET	2.6
4	F	249	TYR	2.6
4	F	199	PHE	2.5
1	C	43	GLY	2.5
3	E	139	LEU	2.5
2	D	101	ASN	2.5
2	D	220	THR	2.5
2	D	86	ILE	2.5
4	F	173	ILE	2.5
1	A	1	MET	2.5
1	A	349	THR	2.5
1	C	340	THR	2.5
4	F	148	ILE	2.4
1	A	448	GLY	2.4
1	A	438	ASP	2.4
4	F	186	LEU	2.4
4	F	380	HIS	2.4
3	E	23	ILE	2.4
2	D	214	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	150	LYS	2.4
1	C	357	TYR	2.4
2	D	272	PHE	2.4
2	D	406	HIS	2.3
4	F	70	LYS	2.3
2	D	181	VAL	2.3
4	F	175	GLU	2.3
4	F	243	HIS	2.3
2	D	172	MET	2.3
1	C	280	LYS	2.3
2	D	142	GLY	2.3
2	D	280	SER	2.3
4	F	376	ILE	2.3
3	E	100	LYS	2.3
4	F	131	PHE	2.3
2	D	89	PRO	2.3
4	F	183	GLN	2.2
2	D	154	ILE	2.2
1	A	437	VAL	2.2
4	F	162	ILE	2.2
2	D	182	VAL	2.2
2	B	440	ALA	2.2
4	F	184	LYS	2.2
2	D	85	GLN	2.2
2	B	279	GLY	2.2
2	B	2	ARG	2.2
3	E	25	LYS	2.2
1	A	340	THR	2.1
4	F	161	LEU	2.1
1	A	37	PRO	2.1
4	F	320	MET	2.1
3	E	47	LEU	2.1
4	F	71	LEU	2.1
4	F	190	LEU	2.1
2	D	342	TYR	2.1
4	F	102	PRO	2.1
4	F	321	VAL	2.1
4	F	149	ALA	2.1
4	F	28	LYS	2.1
1	A	281	ALA	2.1
4	F	254	GLY	2.1
2	D	179	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	146	VAL	2.0
4	F	170	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

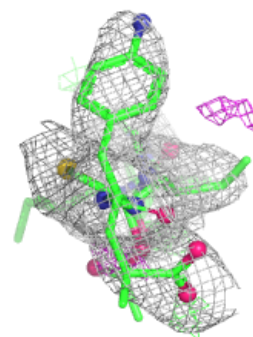
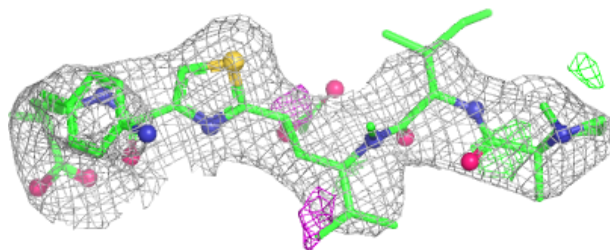
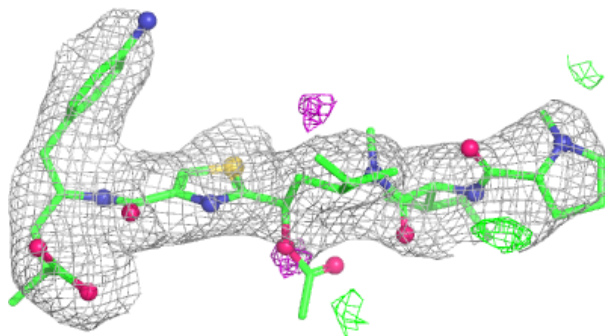
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	B	503	1/1	0.81	0.12	101,101,101,101	0
9	6YK	D	504	52/52	0.82	0.16	86,102,117,119	0
6	MG	B	502	1/1	0.84	0.30	57,57,57,57	0
6	MG	D	503	1/1	0.86	0.11	61,61,61,61	0
6	MG	B	505	1/1	0.87	0.19	78,78,78,78	0
6	MG	A	502	1/1	0.87	0.26	50,50,50,50	0
10	ADP	F	401	27/27	0.87	0.12	91,103,121,122	0
6	MG	D	502	1/1	0.88	0.12	65,65,65,65	0
7	CA	E	201	1/1	0.90	0.15	113,113,113,113	0
8	GDP	D	501	28/28	0.93	0.09	58,62,67,74	0
6	MG	C	502	1/1	0.95	0.24	47,47,47,47	0
9	6YK	B	504	52/52	0.95	0.09	35,49,65,76	0
5	GTP	A	501	32/32	0.96	0.08	40,47,51,53	0
5	GTP	C	501	32/32	0.96	0.07	37,44,49,54	0
7	CA	A	503	1/1	0.97	0.07	94,94,94,94	0
7	CA	C	503	1/1	0.98	0.05	71,71,71,71	0
8	GDP	B	501	28/28	0.98	0.06	31,40,43,47	0

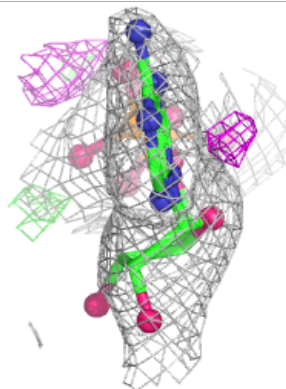
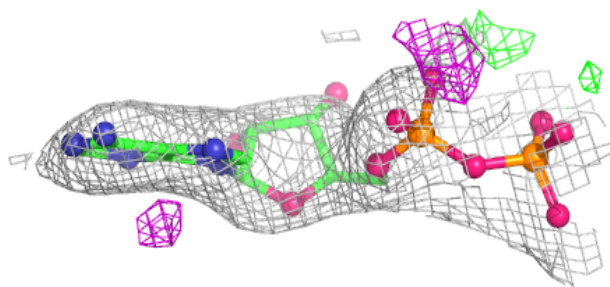
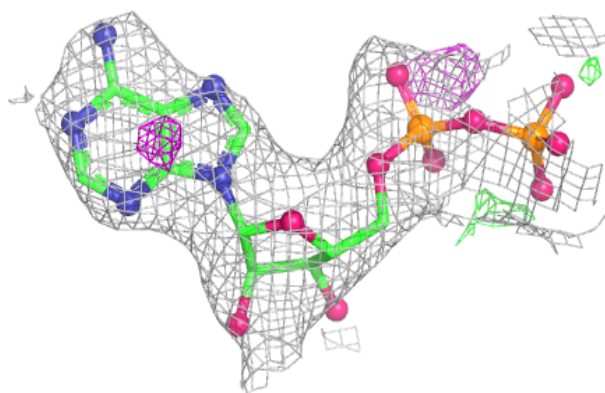
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6YK D 504:

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

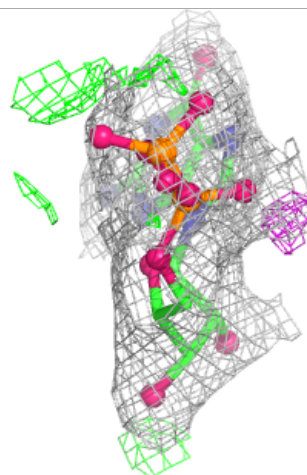
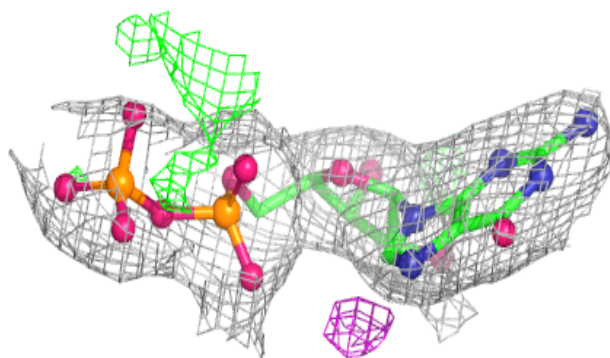
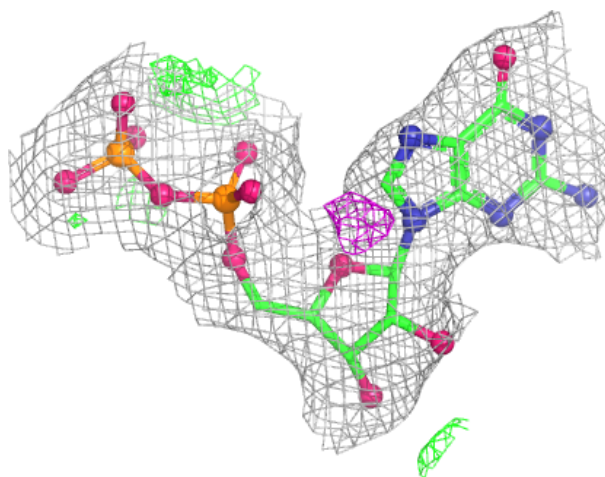
**Electron density around ADP F 401:**

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



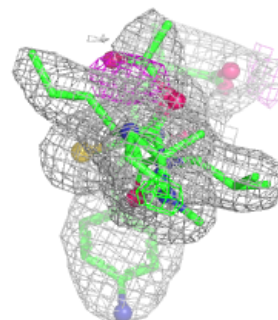
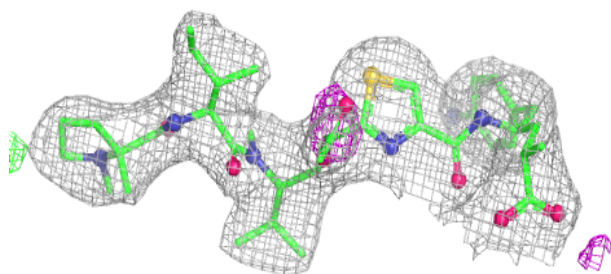
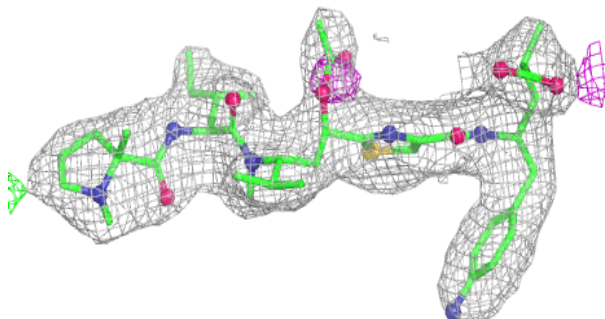
Electron density around GDP D 501:

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and green (positive)

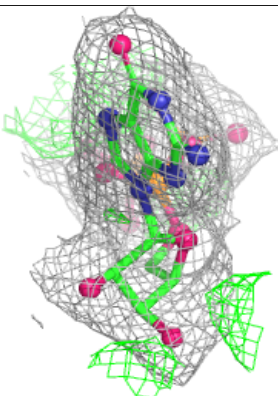
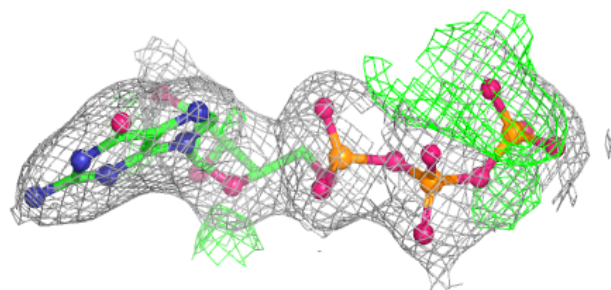
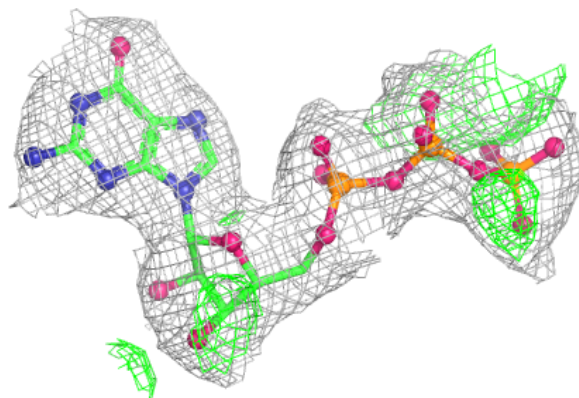


Electron density around 6YK B 504:

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

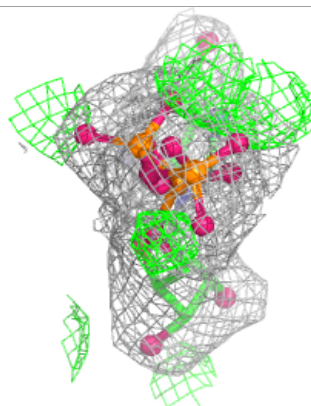
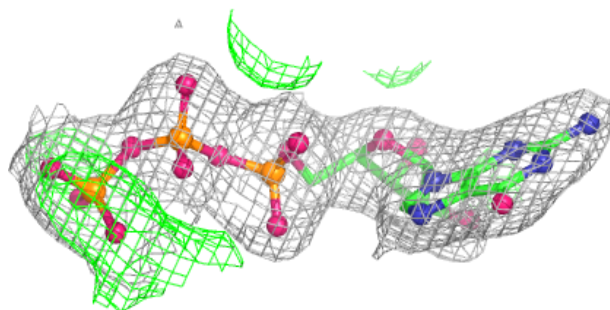
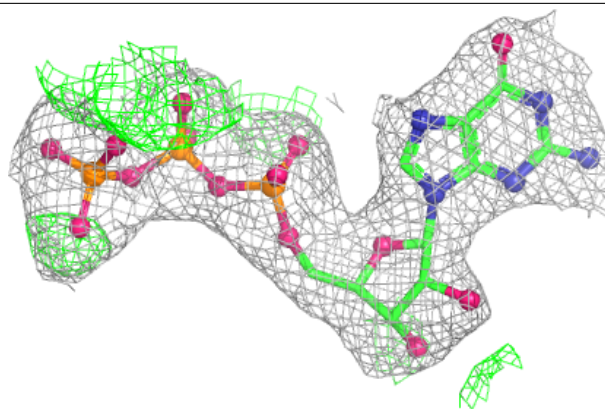
**Electron density around GTP A 501:**

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

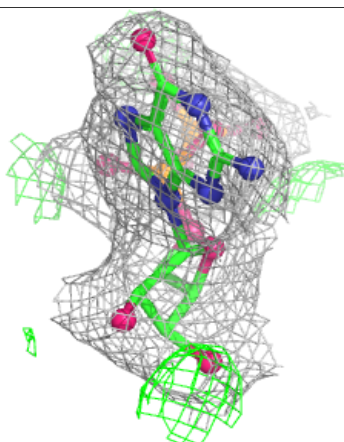
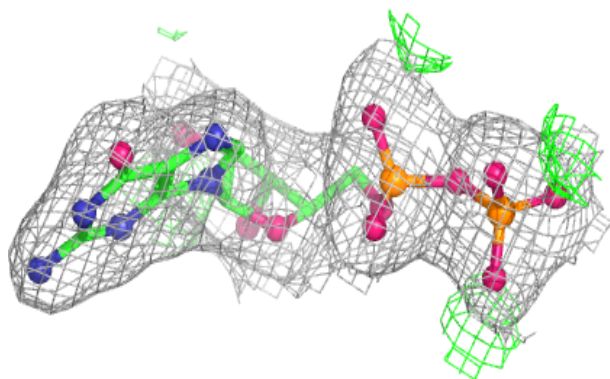
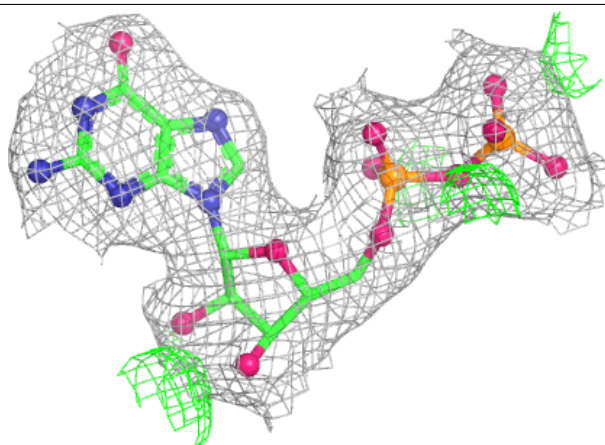


Electron density around GTP C 501:

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

**Electron density around GDP B 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.