



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:21 PM UTC

PDB ID : 4ZHQ / pdb_00004zhq
Title : Crystal structure of Tubulin-Stathmin-TTL-MMAE Complex
Authors : Wang, Y.; Zhang, R.
Deposited on : 2015-04-26
Resolution : 2.55 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

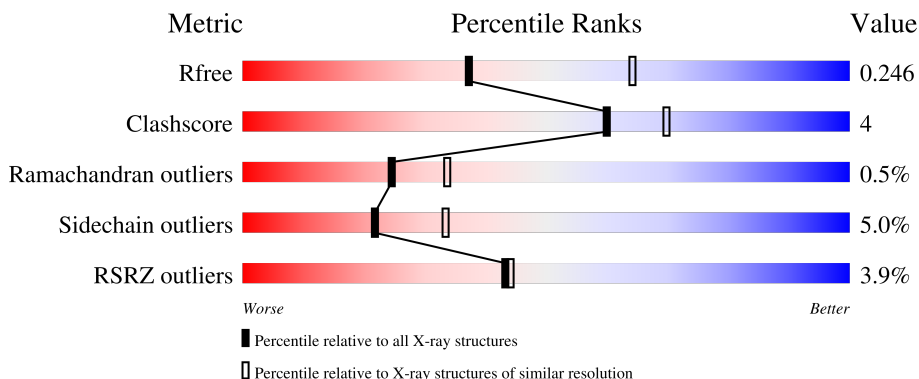
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	143	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	C	506	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17988 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	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	0	0
			3360	2111	576	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- 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
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	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	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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

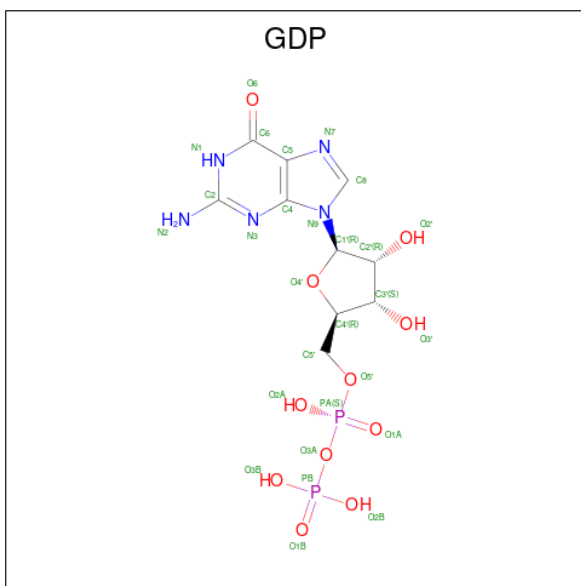
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



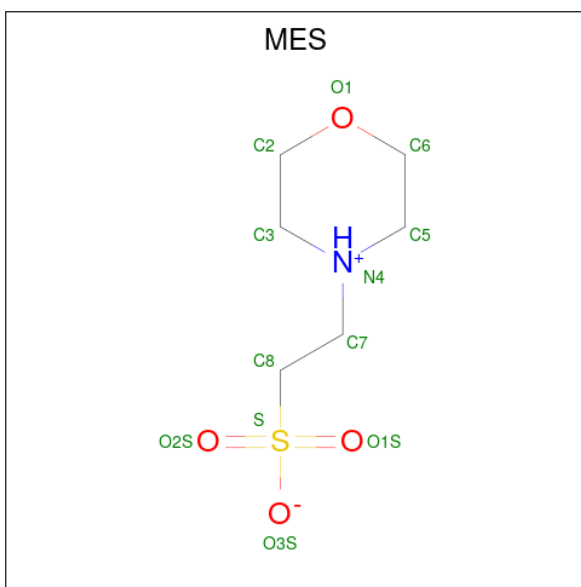
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

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



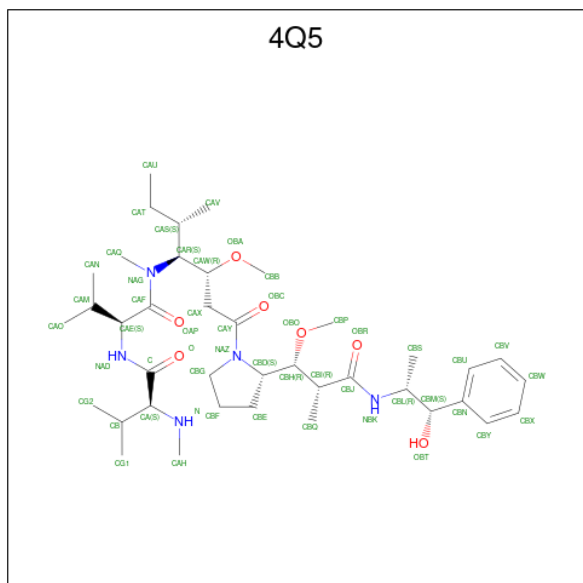
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



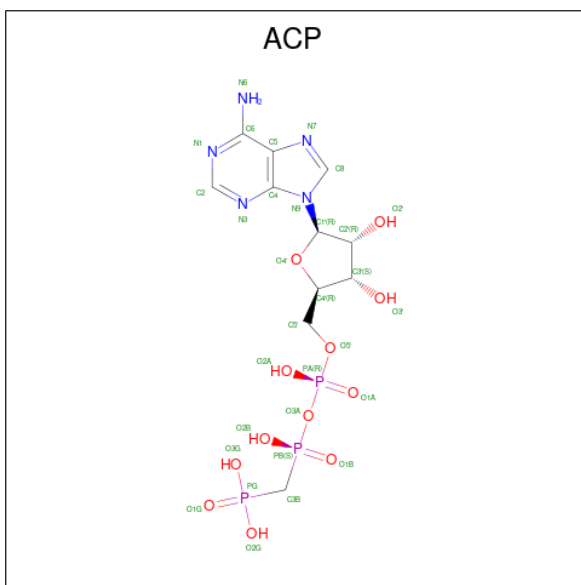
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 12	C 6	N 1	O 4	S 1	0	0
10	B	1	Total 12	C 6	N 1	O 4	S 1	0	0

- Molecule 11 is N-methyl-L-valyl-N-[(3R,4S,5S)-1-{(2S)-2-[(1R,2R)-3-{[(1S,2R)-1-hydroxy-1-phenylpropan-2-yl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (CCD ID: 4Q5) (formula: $C_{39}H_{67}N_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			51	39	5	7		

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



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

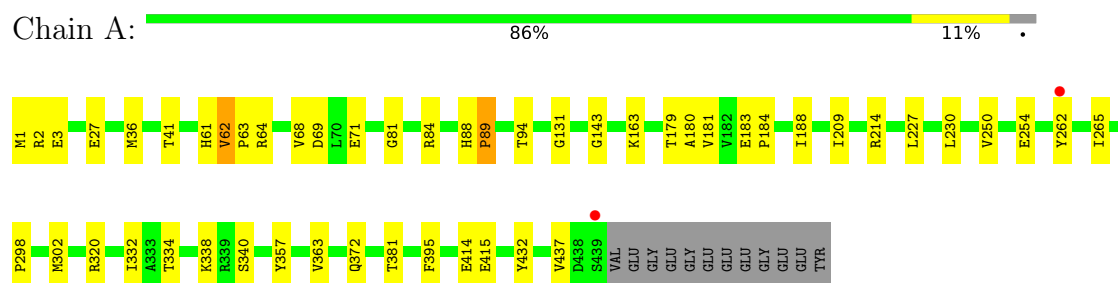
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	63	Total O 63 63	0	0
13	B	66	Total O 66 66	0	0
13	C	110	Total O 110 110	0	0
13	D	19	Total O 19 19	0	0
13	E	2	Total O 2 2	0	0
13	F	37	Total O 37 37	0	0

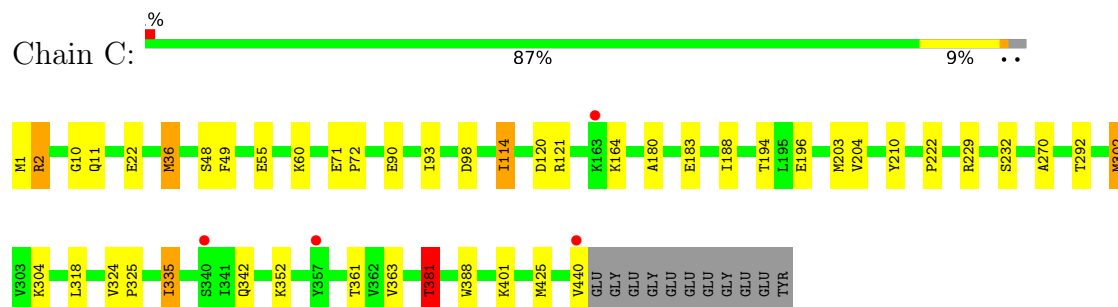
3 Residue-property plots [i](#)

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

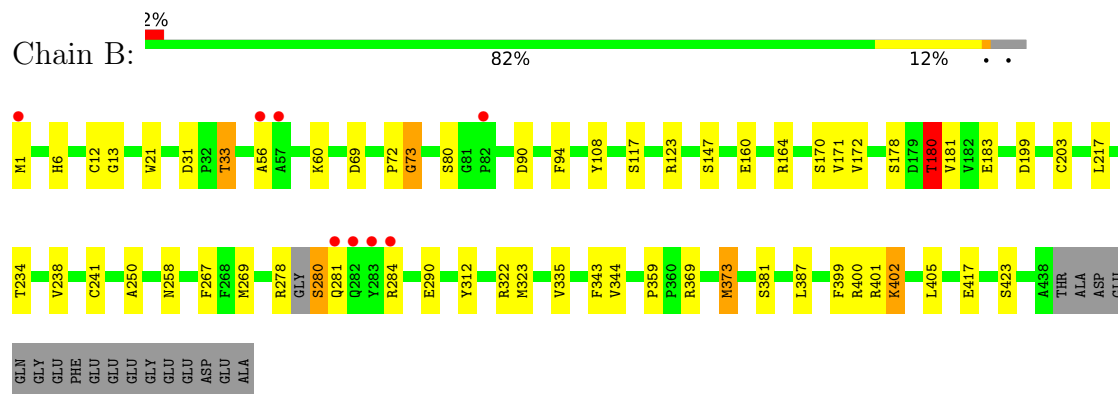
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

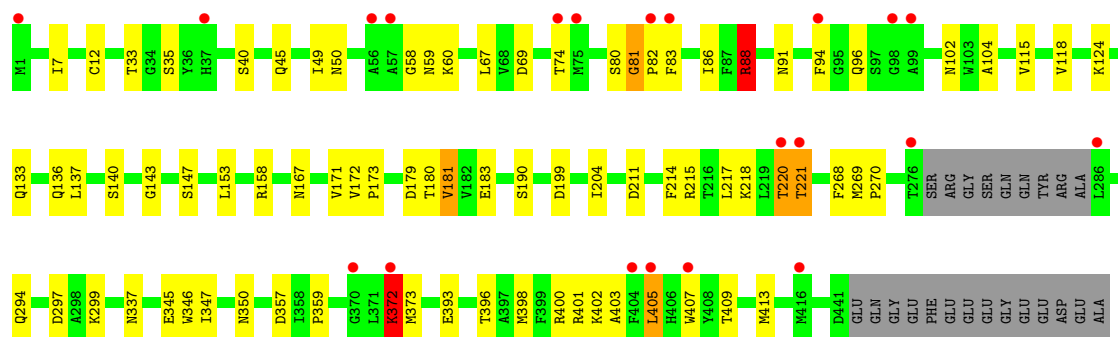


- Molecule 2: Tubulin beta chain

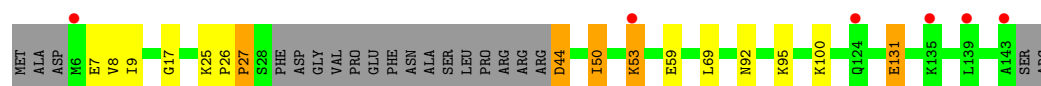
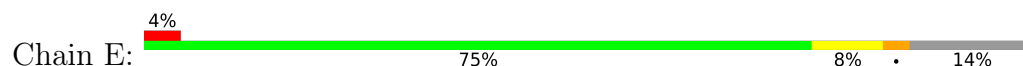


- Molecule 2: Tubulin beta chain

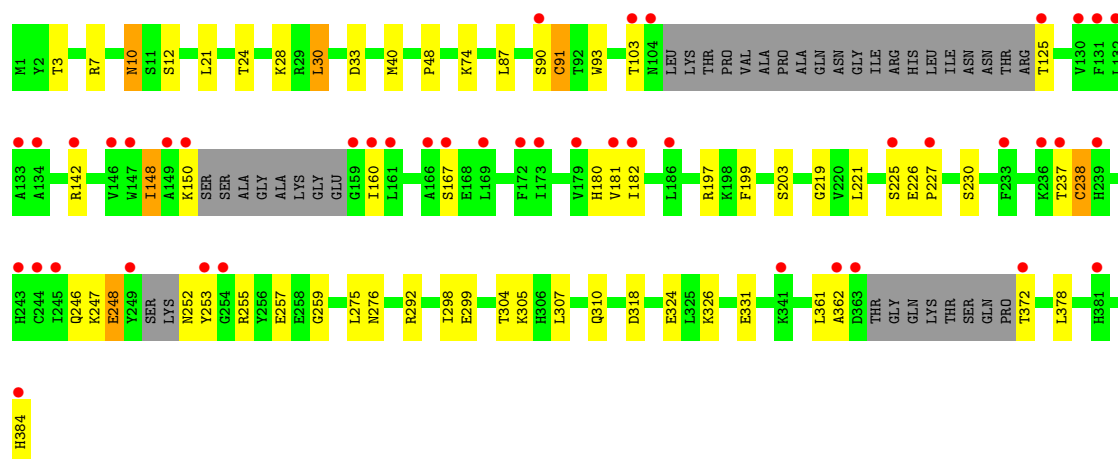
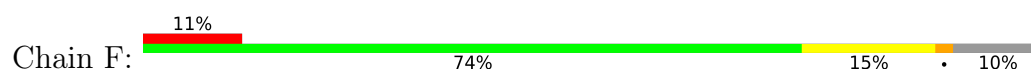




- Molecule 3: Stathmin-4



- Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.94Å 156.81Å 182.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.55 39.34 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.34-2.55) 99.6 (39.34-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.190 , 0.245 0.192 , 0.246	Depositor DCC
R_{free} test set	4896 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17988	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: ACP, GOL, GDP, MG, 4Q5, CA, MES, GTP

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	0.97	1/3508 (0.0%)	1.05	4/4762 (0.1%)
1	C	1.06	0/3524	1.08	7/4785 (0.1%)
2	B	1.05	5/3434 (0.1%)	1.07	7/4651 (0.2%)
2	D	0.93	3/3384 (0.1%)	1.07	11/4586 (0.2%)
3	E	1.01	0/1022	1.17	5/1356 (0.4%)
4	F	0.78	0/2916	0.94	3/3940 (0.1%)
All	All	0.97	9/17788 (0.1%)	1.05	37/24080 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	172	VAL	C-N	6.49	1.41	1.33
2	B	170	SER	C-O	-6.00	1.17	1.24
2	B	171	VAL	C-O	-5.94	1.16	1.23
2	D	172	VAL	C-N	5.80	1.40	1.33
2	B	183	GLU	C-O	-5.63	1.19	1.24
2	B	359	PRO	C-N	5.63	1.40	1.33
2	D	171	VAL	C-O	-5.38	1.18	1.24
1	A	62	VAL	CA-CB	5.25	1.58	1.54
2	D	173	PRO	N-CD	5.24	1.55	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	221	THR	N-CA-C	-10.57	87.29	108.12
2	D	220	THR	N-CA-C	9.28	123.86	112.54
1	C	381	THR	CB-CA-C	-7.74	94.09	109.33
2	B	359	PRO	CA-C-N	-7.62	112.48	120.03
2	B	359	PRO	C-N-CA	-7.62	112.48	120.03
2	D	359	PRO	CA-C-N	-7.21	113.27	120.98
2	D	359	PRO	C-N-CA	-7.21	113.27	120.98
2	D	372	LYS	N-CA-C	-6.77	105.15	113.41
2	D	373	MET	N-CA-C	6.52	119.07	108.76
1	A	262	TYR	CA-C-N	6.21	127.61	119.84
1	A	262	TYR	C-N-CA	6.21	127.61	119.84
2	B	172	VAL	CA-C-N	-6.19	114.24	120.31
2	B	172	VAL	C-N-CA	-6.19	114.24	120.31
3	E	44	ASP	CA-C-N	6.10	127.47	119.84
3	E	44	ASP	C-N-CA	6.10	127.47	119.84
4	F	219	GLY	N-CA-C	-6.08	104.42	112.81
2	B	335	VAL	CB-CA-C	-5.99	104.30	111.97
2	D	172	VAL	CA-C-N	-5.61	114.19	120.14
2	D	172	VAL	C-N-CA	-5.61	114.19	120.14
3	E	50	ILE	N-CA-C	5.56	115.65	110.42
1	A	363	VAL	N-CA-C	-5.55	103.51	108.95
1	C	22	GLU	N-CA-C	-5.46	105.23	111.07
3	E	131	GLU	N-CA-C	-5.35	105.09	111.03
1	C	302	MET	CB-CG-SD	-5.32	96.75	112.70
4	F	230	SER	N-CA-C	5.22	119.37	113.15
1	C	36	MET	CA-C-N	5.22	126.37	119.84
1	C	36	MET	C-N-CA	5.22	126.37	119.84
2	B	269	MET	CB-CA-C	-5.19	104.11	110.08
1	C	114	ILE	N-CA-CB	-5.16	106.19	112.33
1	C	324	VAL	N-CA-CB	5.15	115.38	111.83
2	D	88	ARG	N-CA-C	-5.13	103.18	109.65
4	F	362	ALA	N-CA-C	-5.13	101.51	109.72
2	B	180	THR	N-CA-CB	5.12	117.60	109.71
2	D	173	PRO	N-CA-C	5.04	120.10	111.68
3	E	7	GLU	N-CA-C	5.04	116.87	107.99
2	D	115	VAL	N-CA-C	5.04	115.65	110.36
1	A	332	ILE	N-CA-C	5.01	115.73	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	MET	Peptide

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	3430	0	3340	20	0
1	C	3446	0	3354	35	0
2	B	3360	0	3242	30	0
2	D	3311	0	3192	34	1
3	E	1014	0	1029	7	0
4	F	2849	0	2796	25	1
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	1	0
8	B	6	0	8	3	0
8	C	24	0	32	9	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	24	0	26	2	0
11	B	51	0	0	0	0
12	F	31	0	14	1	0
13	A	63	0	0	1	0
13	B	66	0	0	1	0
13	C	110	0	0	2	0
13	D	19	0	0	0	0
13	E	2	0	0	0	0
13	F	37	0	0	1	0
All	All	17988	0	17105	148	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (148) 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:229:ARG:HG2	8:C:506:GOL:O2	1.50	1.09
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.36	1.02
1:C:204:VAL:HG22	1:C:302:MET:CE	1.99	0.91
1:C:204:VAL:HG13	1:C:302:MET:HE2	1.57	0.86
1:C:363:VAL:HG21	8:C:506:GOL:H2	1.62	0.80
2:D:33:THR:OG1	2:D:60:LYS:NZ	2.16	0.78
1:C:363:VAL:CG2	8:C:506:GOL:H2	2.18	0.73
2:B:31:ASP:OD1	2:B:33:THR:HB	1.89	0.72
3:E:50:ILE:O	3:E:53:LYS:HB3	1.89	0.72
2:B:278:ARG:C	2:B:280:SER:N	2.49	0.71
2:D:33:THR:CB	2:D:60:LYS:NZ	2.55	0.70
2:D:136:GLN:HA	2:D:167:ASN:O	1.92	0.68
2:D:33:THR:HB	2:D:60:LYS:NZ	2.10	0.67
1:C:229:ARG:CG	8:C:506:GOL:O2	2.38	0.64
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.80	0.63
1:C:55:GLU:HA	1:C:60:LYS:O	1.98	0.63
2:D:181:VAL:O	2:D:398:MET:HE1	2.00	0.62
1:C:204:VAL:CG2	1:C:302:MET:HE1	2.21	0.61
4:F:21:LEU:O	4:F:24:THR:OG1	2.15	0.60
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.20	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.02	0.59
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.85	0.58
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.87	0.57
2:B:323:MET:HB3	2:B:373:MET:HE1	1.87	0.56
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.40	0.56
1:C:204:VAL:CG1	1:C:302:MET:HE2	2.33	0.55
2:B:180:THR:HG22	1:C:352:LYS:NZ	2.22	0.55
4:F:74:LYS:HB3	4:F:181:VAL:HG21	1.88	0.55
2:B:401:ARG:HE	8:B:506:GOL:C1	2.20	0.55
2:B:72:PRO:O	2:B:73:GLY:C	2.50	0.55
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.89	0.55
4:F:237:THR:O	4:F:246:GLN:NE2	2.34	0.54
2:D:104:ALA:HB2	2:D:413:MET:SD	2.48	0.54
1:C:304:LYS:HG3	8:C:505:GOL:H12	1.90	0.54
2:B:399:PHE:O	2:B:402:LYS:HE2	2.09	0.53
2:D:40:SER:O	2:D:45:GLN:HB2	2.07	0.53
4:F:150:LYS:N	4:F:181:VAL:O	2.41	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.44	0.52
1:C:204:VAL:CG2	1:C:302:MET:CE	2.82	0.52
4:F:10:ASN:N	4:F:10:ASN:OD1	2.43	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.28	0.51
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:304:THR:O	4:F:310:GLN:NE2	2.42	0.51
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.11	0.50
2:B:199:ASP:OD1	10:B:504:MES:H32	2.11	0.50
2:D:393:GLU:O	2:D:396:THR:HG22	2.10	0.50
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.47	0.50
1:C:363:VAL:HG21	8:C:506:GOL:C2	2.36	0.50
2:B:199:ASP:OD2	10:B:504:MES:H52	2.12	0.49
2:B:164:ARG:HD2	13:B:649:HOH:O	2.12	0.49
1:C:1:MET:O	1:C:2:ARG:HB2	2.13	0.49
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.94	0.49
2:B:343:PHE:O	2:B:344:VAL:C	2.54	0.49
2:B:401:ARG:HH21	8:B:506:GOL:H12	1.77	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.48
2:B:401:ARG:HH21	8:B:506:GOL:C1	2.26	0.48
2:D:33:THR:HB	2:D:60:LYS:HZ2	1.78	0.48
2:D:82:PRO:O	2:D:83:PHE:HB2	2.13	0.48
2:D:118:VAL:HG11	2:D:153:LEU:HD21	1.94	0.48
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.48	0.48
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.97	0.47
2:B:180:THR:HG22	1:C:352:LYS:HZ3	1.79	0.47
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.47
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.47	0.47
1:A:183:GLU:N	1:A:184:PRO:CD	2.77	0.47
2:D:58:GLY:O	2:D:59:ASN:HB2	2.15	0.47
2:D:180:THR:O	2:D:183:GLU:HG3	2.15	0.47
8:C:507:GOL:O1	8:C:507:GOL:O3	2.28	0.46
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.46
2:B:278:ARG:O	2:B:280:SER:N	2.48	0.46
4:F:225:SER:OG	4:F:252:ASN:O	2.31	0.46
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.96	0.46
2:D:372:LYS:HE2	2:D:372:LYS:HB2	1.71	0.46
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.24	0.46
1:A:69:ASP:O	1:A:94:THR:HA	2.16	0.46
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.16	0.45
2:D:35:SER:OG	2:D:60:LYS:HE2	2.16	0.45
1:A:1:MET:C	1:A:1:MET:SD	2.99	0.45
1:C:381:THR:CG2	13:C:642:HOH:O	2.64	0.45
4:F:292:ARG:CG	4:F:378:LEU:HB3	2.46	0.45
1:C:90:GLU:HB3	1:C:121:ARG:HD2	1.99	0.45
2:D:211:ASP:O	2:D:215:ARG:HB2	2.16	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.45
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.10	0.45
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.52	0.45
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.45
1:C:270:ALA:HB3	1:C:302:MET:SD	2.57	0.45
2:D:102:ASN:OD1	2:D:102:ASN:C	2.60	0.44
4:F:28:LYS:NZ	13:F:502:HOH:O	2.50	0.44
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.18	0.44
2:D:7:ILE:O	2:D:137:LEU:HD12	2.17	0.44
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.51	0.44
2:B:56:ALA:N	2:B:60:LYS:O	2.49	0.44
1:C:381:THR:HG23	13:C:642:HOH:O	2.17	0.44
1:C:71:GLU:HG2	1:C:72:PRO:HD2	2.00	0.43
2:D:80:SER:OG	2:D:81:GLY:N	2.51	0.43
1:A:81:GLY:O	1:A:84:ARG:NH1	2.49	0.43
1:C:194:THR:O	1:C:194:THR:HG22	2.18	0.43
2:B:387:LEU:HD23	2:B:387:LEU:C	2.44	0.43
1:C:204:VAL:HG22	1:C:302:MET:HE2	1.95	0.43
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.99	0.43
4:F:247:LYS:HE3	4:F:253:TYR:CZ	2.54	0.43
4:F:275:LEU:O	4:F:276:ASN:HB3	2.18	0.43
1:A:209:ILE:HD11	1:A:302:MET:SD	2.58	0.43
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.43
2:B:284:ARG:NH2	2:B:290:GLU:OE1	2.51	0.43
1:A:2:ARG:HB3	1:A:131:GLY:O	2.18	0.43
1:C:232:SER:OG	8:C:506:GOL:C3	2.67	0.43
2:D:268:PHE:O	2:D:270:PRO:HD3	2.19	0.43
4:F:298:ILE:O	4:F:299:GLU:C	2.61	0.43
2:B:12:CYS:O	2:B:13:GLY:C	2.62	0.42
2:B:123:ARG:NH2	2:B:160:GLU:OE1	2.50	0.42
2:B:241:CYS:O	2:B:250:ALA:HA	2.19	0.42
3:E:8:VAL:C	3:E:9:ILE:HG23	2.45	0.42
8:A:504:GOL:H12	13:A:639:HOH:O	2.18	0.42
2:D:214:PHE:HD1	2:D:220:THR:HA	1.83	0.42
2:B:178:SER:OG	2:B:180:THR:HG23	2.19	0.42
1:C:10:GLY:O	1:C:11:GLN:C	2.62	0.42
2:D:401:ARG:O	2:D:403:ALA:N	2.52	0.42
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.02	0.42
4:F:226:GLU:O	4:F:238:CYS:HB2	2.19	0.42
1:C:232:SER:OG	8:C:506:GOL:H31	2.20	0.41
1:A:414:GLU:O	1:A:415:GLU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.60	0.41
3:E:8:VAL:C	3:E:9:ILE:CG2	2.93	0.41
2:B:234:THR:O	2:B:238:VAL:HG13	2.20	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.20	0.41
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.56	0.41
1:A:395:PHE:C	1:A:395:PHE:CD1	2.99	0.41
2:D:217:LEU:C	2:D:218:LYS:HG2	2.45	0.41
4:F:7:ARG:CD	4:F:40:MET:HE3	2.50	0.41
2:D:158:ARG:NH1	2:D:199:ASP:OD2	2.53	0.41
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.41
3:E:26:PRO:O	3:E:27:PRO:O	2.38	0.41
3:E:69:LEU:HD23	3:E:69:LEU:HA	1.95	0.41
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.02	0.41
2:D:12:CYS:CB	2:D:140:SER:HB3	2.50	0.41
4:F:90:SER:OG	4:F:91:CYS:N	2.53	0.41
1:A:88:HIS:O	1:A:89:PRO:C	2.64	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.41
1:C:203:MET:SD	1:C:388:TRP:CH2	3.14	0.41
2:D:294:GLN:O	2:D:297:ASP:HB2	2.21	0.41
3:E:131:GLU:OE2	3:E:131:GLU:HA	2.21	0.41
2:D:405:LEU:HD12	2:D:405:LEU:HA	1.92	0.40
4:F:3:THR:HB	4:F:30:LEU:HD21	2.03	0.40
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.23	0.40
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:ASN:OD1	4:F:384:HIS:NE2[3_555]	2.17	0.03

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%)	419 (96%)	17 (4%)	1 (0%)	43	56
1	C	439/451 (97%)	424 (97%)	14 (3%)	1 (0%)	43	56
2	B	423/445 (95%)	409 (97%)	13 (3%)	1 (0%)	43	56
2	D	418/445 (94%)	401 (96%)	14 (3%)	3 (1%)	18	25
3	E	119/143 (83%)	112 (94%)	6 (5%)	1 (1%)	16	22
4	F	336/384 (88%)	308 (92%)	24 (7%)	4 (1%)	10	13
All	All	2172/2319 (94%)	2073 (95%)	88 (4%)	11 (0%)	24	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	402	LYS
3	E	27	PRO
4	F	91	CYS
4	F	142	ARG
2	B	73	GLY
2	D	81	GLY
1	C	2	ARG
4	F	248	GLU
1	A	89	PRO
4	F	227	PRO
2	D	143	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/379 (98%)	353 (95%)	17 (5%)	24	36
1	C	372/379 (98%)	360 (97%)	12 (3%)	34	51
2	B	368/381 (97%)	351 (95%)	17 (5%)	24	36
2	D	363/381 (95%)	343 (94%)	20 (6%)	19	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	110/127 (87%)	103 (94%)	7 (6%)	16	23
4	F	312/342 (91%)	291 (93%)	21 (7%)	15	21
All	All	1895/1989 (95%)	1801 (95%)	94 (5%)	22	33

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	62	VAL
1	A	63	PRO
1	A	68	VAL
1	A	71	GLU
1	A	163	LYS
1	A	179	THR
1	A	181	VAL
1	A	188	ILE
1	A	214	ARG
1	A	298	PRO
1	A	334	THR
1	A	338	LYS
1	A	340	SER
1	A	372	GLN
1	A	381	THR
1	A	437	VAL
2	B	33	THR
2	B	80	SER
2	B	90	ASP
2	B	117	SER
2	B	147	SER
2	B	180	THR
2	B	181	VAL
2	B	217	LEU
2	B	280	SER
2	B	281	GLN
2	B	322	ARG
2	B	369	ARG
2	B	373	MET
2	B	400	ARG
2	B	402	LYS
2	B	405	LEU
2	B	423	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	48	SER
1	C	114	ILE
1	C	120	ASP
1	C	164	LYS
1	C	196	GLU
1	C	318	LEU
1	C	325	PRO
1	C	335	ILE
1	C	342	GLN
1	C	361	THR
1	C	381	THR
1	C	440	VAL
2	D	49	ILE
2	D	50	ASN
2	D	74	THR
2	D	88	ARG
2	D	96	GLN
2	D	124	LYS
2	D	133	GLN
2	D	179	ASP
2	D	181	VAL
2	D	204	ILE
2	D	221	THR
2	D	269	MET
2	D	299	LYS
2	D	345	GLU
2	D	357	ASP
2	D	372	LYS
2	D	400	ARG
2	D	405	LEU
2	D	407	TRP
2	D	409	THR
3	E	25	LYS
3	E	44	ASP
3	E	53	LYS
3	E	59	GLU
3	E	92	ASN
3	E	95	LYS
3	E	100	LYS
4	F	10	ASN
4	F	12	SER
4	F	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	33	ASP
4	F	87	LEU
4	F	103	THR
4	F	125	THR
4	F	148	ILE
4	F	167	SER
4	F	180	HIS
4	F	182	ILE
4	F	203	SER
4	F	238	CYS
4	F	248	GLU
4	F	255	ARG
4	F	305	LYS
4	F	324	GLU
4	F	326	LYS
4	F	331	GLU
4	F	361	LEU
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	309	HIS
1	A	358	GLN
1	A	372	GLN
1	A	393	HIS
2	B	101	ASN
2	B	167	ASN
2	B	300	ASN
2	B	349	ASN
2	B	436	GLN
1	C	11	GLN
1	C	31	GLN
1	C	85	GLN
1	C	393	HIS
2	D	37	HIS
2	D	247	GLN
2	D	433	GLN
3	E	12	ASN
3	E	78	HIS
3	E	115	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	136	ASN
4	F	183	GLN
4	F	333	ASN
4	F	383	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	6	33,34,34	1.35	6 (18%)	50,54,54	1.78	13 (26%)
5	GTP	C	501	6	33,34,34	1.22	4 (12%)	50,54,54	1.93	14 (28%)
8	GOL	B	506	-	5,5,5	0.90	0	5,5,5	0.88	0
9	GDP	D	501	6	29,30,30	1.28	5 (17%)	45,47,47	1.88	9 (20%)
8	GOL	A	504	-	5,5,5	0.50	0	5,5,5	0.56	0
8	GOL	C	506	-	5,5,5	0.66	0	5,5,5	1.00	0
12	ACP	F	401	-	31,33,33	2.46	11 (35%)	47,52,52	1.74	9 (19%)
8	GOL	C	503	-	5,5,5	0.59	0	5,5,5	0.92	0
10	MES	B	505	-	12,12,12	2.34	2 (16%)	15,16,16	1.71	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	4Q5	B	507	-	52,52,52	1.37	6 (11%)	56,72,72	1.80	13 (23%)
9	GDP	B	501	6	29,30,30	1.24	4 (13%)	45,47,47	1.83	9 (20%)
8	GOL	C	507	-	5,5,5	0.36	0	5,5,5	0.76	0
8	GOL	A	506	-	5,5,5	0.57	0	5,5,5	0.30	0
8	GOL	C	505	-	5,5,5	0.69	0	5,5,5	0.92	0
10	MES	B	504	-	12,12,12	2.10	3 (25%)	15,16,16	5.58	8 (53%)
8	GOL	A	505	-	5,5,5	0.46	0	5,5,5	1.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
8	GOL	B	506	-	-	2/4/4/4	-
9	GDP	D	501	6	-	5/16/32/32	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
8	GOL	C	506	-	-	1/4/4/4	-
12	ACP	F	401	-	-	4/19/38/38	0/3/3/3
8	GOL	C	503	-	-	2/4/4/4	-
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
11	4Q5	B	507	-	-	11/76/86/86	0/2/2/2
9	GDP	B	501	6	-	4/16/32/32	0/3/3/3
8	GOL	C	507	-	-	2/4/4/4	-
8	GOL	A	506	-	-	1/4/4/4	-
8	GOL	C	505	-	-	2/4/4/4	-
10	MES	B	504	-	-	5/6/14/14	0/1/1/1
8	GOL	A	505	-	-	3/4/4/4	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-7.52	1.67	1.77
12	F	401	ACP	PG-O1G	6.28	1.62	1.50
12	F	401	ACP	PB-O3A	6.14	1.65	1.58
10	B	504	MES	C8-S	-5.98	1.69	1.77
12	F	401	ACP	PA-O3A	5.32	1.65	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	C5-C4	5.22	1.48	1.39
11	B	507	4Q5	CBN-CBM	-5.18	1.44	1.51
5	A	501	GTP	PB-O3B	3.42	1.63	1.59
12	F	401	ACP	PG-O3G	3.33	1.62	1.55
11	B	507	4Q5	CBY-CBN	3.16	1.44	1.39
9	D	501	GDP	C5-C4	2.82	1.46	1.38
9	B	501	GDP	PA-O3A	2.81	1.62	1.59
5	A	501	GTP	C5-N7	-2.79	1.33	1.39
5	C	501	GTP	C5-N7	-2.78	1.33	1.39
5	A	501	GTP	C6-N1	-2.77	1.33	1.38
9	D	501	GDP	C5-N7	-2.76	1.33	1.39
12	F	401	ACP	C5-C6	2.71	1.48	1.41
5	C	501	GTP	PA-O3A	2.66	1.62	1.59
10	B	504	MES	O2S-S	2.63	1.52	1.45
9	B	501	GDP	C6-N1	-2.62	1.33	1.38
12	F	401	ACP	C8-N7	2.60	1.36	1.31
12	F	401	ACP	PG-O2G	-2.53	1.49	1.55
9	B	501	GDP	C5-C4	2.45	1.45	1.38
5	C	501	GTP	PB-O3B	2.41	1.62	1.59
12	F	401	ACP	PB-O2B	2.38	1.62	1.56
10	B	505	MES	O1S-S	2.29	1.51	1.45
5	A	501	GTP	C8-N9	-2.23	1.32	1.37
11	B	507	4Q5	OBO-CBH	2.21	1.48	1.42
9	B	501	GDP	C5-N7	-2.21	1.34	1.39
9	D	501	GDP	C6-N1	-2.21	1.34	1.38
5	A	501	GTP	C5-C4	2.20	1.44	1.38
10	B	504	MES	O1S-S	2.16	1.51	1.45
9	D	501	GDP	PA-O3A	2.16	1.61	1.59
11	B	507	4Q5	CBV-CBU	2.12	1.42	1.38
5	C	501	GTP	C5-C4	2.11	1.44	1.38
5	A	501	GTP	C4-N9	-2.08	1.32	1.38
12	F	401	ACP	C4-N9	-2.08	1.33	1.37
11	B	507	4Q5	CBM-CBL	2.07	1.55	1.54
12	F	401	ACP	C5-N7	-2.06	1.35	1.39
9	D	501	GDP	C2-N3	2.04	1.38	1.33
11	B	507	4Q5	CAE-CAF	2.00	1.58	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O3S-S-O2S	-11.46	82.73	111.40
10	B	504	MES	O3S-S-O1S	-10.74	84.53	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O1S-S-C8	9.16	120.57	106.73
10	B	504	MES	O3S-S-C8	-8.19	89.98	106.00
10	B	504	MES	O2S-S-C8	6.21	116.11	106.73
9	D	501	GDP	C5-C4-N3	-5.83	119.11	128.39
9	B	501	GDP	C5-C4-N3	-5.69	119.33	128.39
11	B	507	4Q5	CB-CA-C	-5.63	97.65	111.38
12	F	401	ACP	C5-C4-N3	-5.46	119.20	126.72
5	C	501	GTP	C5-C4-N3	-5.22	120.08	128.39
5	C	501	GTP	C2-N3-C4	5.17	121.21	112.30
9	B	501	GDP	C2-N3-C4	4.96	120.84	112.30
5	A	501	GTP	C5-C4-N3	-4.90	120.59	128.39
9	D	501	GDP	C2-N3-C4	4.84	120.64	112.30
10	B	505	MES	O1S-S-C8	4.75	113.91	106.73
12	F	401	ACP	N3-C4-N9	4.54	134.90	127.17
9	D	501	GDP	N9-C4-N3	4.48	134.92	125.95
9	B	501	GDP	N9-C4-N3	4.39	134.72	125.95
11	B	507	4Q5	CAW-CAX-CAY	-4.18	106.19	112.38
5	A	501	GTP	N9-C4-N3	4.05	134.05	125.95
5	C	501	GTP	N9-C4-N3	3.88	133.72	125.95
11	B	507	4Q5	CBI-CBJ-NBK	-3.87	110.62	116.35
5	C	501	GTP	O2A-PA-O3A	3.68	117.22	107.27
9	D	501	GDP	C6-C5-N7	3.47	136.60	130.29
5	C	501	GTP	C6-C5-N7	3.41	136.49	130.29
10	B	504	MES	C6-C5-N4	3.38	115.25	110.12
12	F	401	ACP	C2-N3-C4	3.38	120.08	111.83
5	A	501	GTP	C2-N3-C4	3.34	118.05	112.30
11	B	507	4Q5	CBS-CBL-CBM	-3.28	109.57	112.67
9	B	501	GDP	O6-C6-C5	-3.25	117.95	126.53
11	B	507	4Q5	CBW-CBV-CBU	3.23	124.22	120.24
9	B	501	GDP	C6-C5-N7	3.19	136.10	130.29
10	B	505	MES	O3S-S-O1S	-3.14	103.53	111.40
11	B	507	4Q5	OAP-CAF-CAE	3.12	125.83	119.96
5	A	501	GTP	C6-C5-N7	3.06	135.87	130.29
12	F	401	ACP	N3-C2-N1	-3.02	124.01	128.58
12	F	401	ACP	C4-N9-C8	2.98	108.87	105.74
12	F	401	ACP	C4-C5-N7	-2.96	107.20	110.58
5	C	501	GTP	O6-C6-C5	-2.96	118.72	126.53
11	B	507	4Q5	CAM-CAE-CAF	2.93	116.44	110.71
9	D	501	GDP	C4-C5-N7	-2.89	106.09	110.67
5	A	501	GTP	O6-C6-C5	-2.74	119.30	126.53
9	D	501	GDP	O3B-PB-O1B	2.72	121.45	110.83
9	D	501	GDP	C8-N7-C5	2.72	109.10	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	507	4Q5	CAM-CAE-NAD	2.70	117.97	111.44
5	A	501	GTP	N9-C8-N7	-2.69	108.42	113.40
5	A	501	GTP	C8-N9-C4	2.64	110.97	106.03
5	A	501	GTP	C4-C5-N7	-2.62	106.52	110.67
5	C	501	GTP	C4-C5-N7	-2.59	106.56	110.67
5	A	501	GTP	C8-N7-C5	2.51	108.74	104.26
11	B	507	4Q5	CBP-OBO-CBH	-2.49	108.07	114.47
5	C	501	GTP	N9-C8-N7	-2.46	108.84	113.40
9	D	501	GDP	N9-C8-N7	-2.44	108.88	113.40
5	C	501	GTP	O3B-PB-O1B	2.42	117.99	110.70
10	B	504	MES	O2S-S-O1S	2.41	121.64	113.82
5	C	501	GTP	C8-N7-C5	2.40	108.54	104.26
5	A	501	GTP	O3G-PG-O1G	2.40	120.18	110.83
12	F	401	ACP	C2'-C1'-N9	-2.34	107.48	113.30
11	B	507	4Q5	OBR-CBJ-NBK	2.33	127.13	122.96
9	B	501	GDP	C4-C5-N7	-2.29	107.05	110.67
5	A	501	GTP	C3'-C2'-C1'	-2.28	97.15	101.46
10	B	504	MES	C2-C3-N4	2.24	113.53	110.12
11	B	507	4Q5	OAP-CAF-NAG	-2.18	118.19	121.76
12	F	401	ACP	C5-N7-C8	2.18	106.87	103.45
11	B	507	4Q5	O-C-CA	-2.17	116.34	120.75
5	C	501	GTP	C5-C6-N1	2.15	118.74	113.25
9	B	501	GDP	C2-N1-C6	-2.14	121.23	125.11
11	B	507	4Q5	CAQ-NAG-CAR	2.14	123.70	119.48
5	C	501	GTP	O2B-PB-O3A	2.10	112.96	107.27
5	C	501	GTP	O3'-C3'-C4'	-2.09	105.06	111.08
5	C	501	GTP	O3A-PB-O1B	-2.09	104.41	110.70
9	D	501	GDP	C8-N9-C4	2.09	109.95	106.03
9	B	501	GDP	C5-C6-N1	2.09	118.58	113.25
12	F	401	ACP	O4'-C1'-N9	2.04	112.02	108.09
5	A	501	GTP	C1'-N9-C4	-2.03	120.49	126.49
5	A	501	GTP	O2B-PB-O3A	-2.03	101.79	107.27
9	B	501	GDP	C8-N7-C5	2.03	107.87	104.26
10	B	505	MES	O3S-S-C8	2.01	109.94	106.00

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O3G
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	A	504	GOL	O1-C1-C2-C3
8	B	506	GOL	O1-C1-C2-C3
8	C	507	GOL	C1-C2-C3-O3
8	C	507	GOL	O2-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O2S
11	B	507	4Q5	C-CA-CB-CG1
11	B	507	4Q5	C-CA-CB-CG2
11	B	507	4Q5	CAF-CAE-CAM-CAN
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
11	B	507	4Q5	N-CA-CB-CG1
11	B	507	4Q5	N-CA-CB-CG2
11	B	507	4Q5	NAD-CAE-CAM-CAN
11	B	507	4Q5	NAD-CAE-CAM-CAO
11	B	507	4Q5	CAF-CAE-CAM-CAO
8	A	505	GOL	O1-C1-C2-C3
8	C	503	GOL	C1-C2-C3-O3
8	C	505	GOL	O1-C1-C2-C3
8	B	506	GOL	O1-C1-C2-O2
8	C	505	GOL	O1-C1-C2-O2
8	A	504	GOL	O1-C1-C2-O2
11	B	507	4Q5	CAV-CAS-CAT-CAU
8	A	505	GOL	O1-C1-C2-O2
8	A	505	GOL	O2-C2-C3-O3
8	C	506	GOL	O1-C1-C2-O2
11	B	507	4Q5	CAR-CAS-CAT-CAU
8	C	503	GOL	O2-C2-C3-O3
10	B	504	MES	C7-C8-S-O1S
11	B	507	4Q5	CBS-CBL-CBM-CBN
8	A	506	GOL	O1-C1-C2-C3
10	B	504	MES	N4-C7-C8-S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C3
9	D	501	GDP	C4'-C5'-O5'-PA
12	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
9	B	501	GDP	PB-O3A-PA-O1A
9	D	501	GDP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A

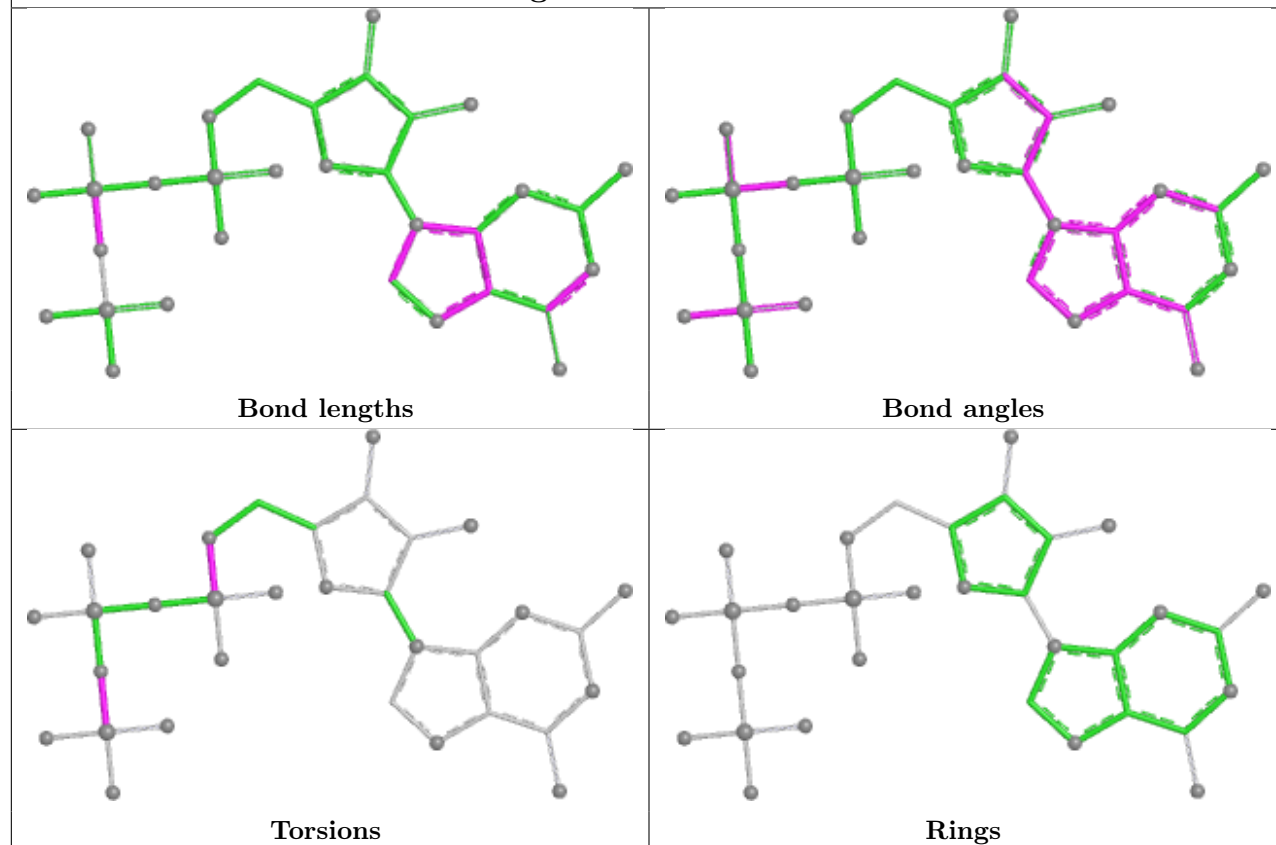
There are no ring outliers.

8 monomers are involved in 17 short contacts:

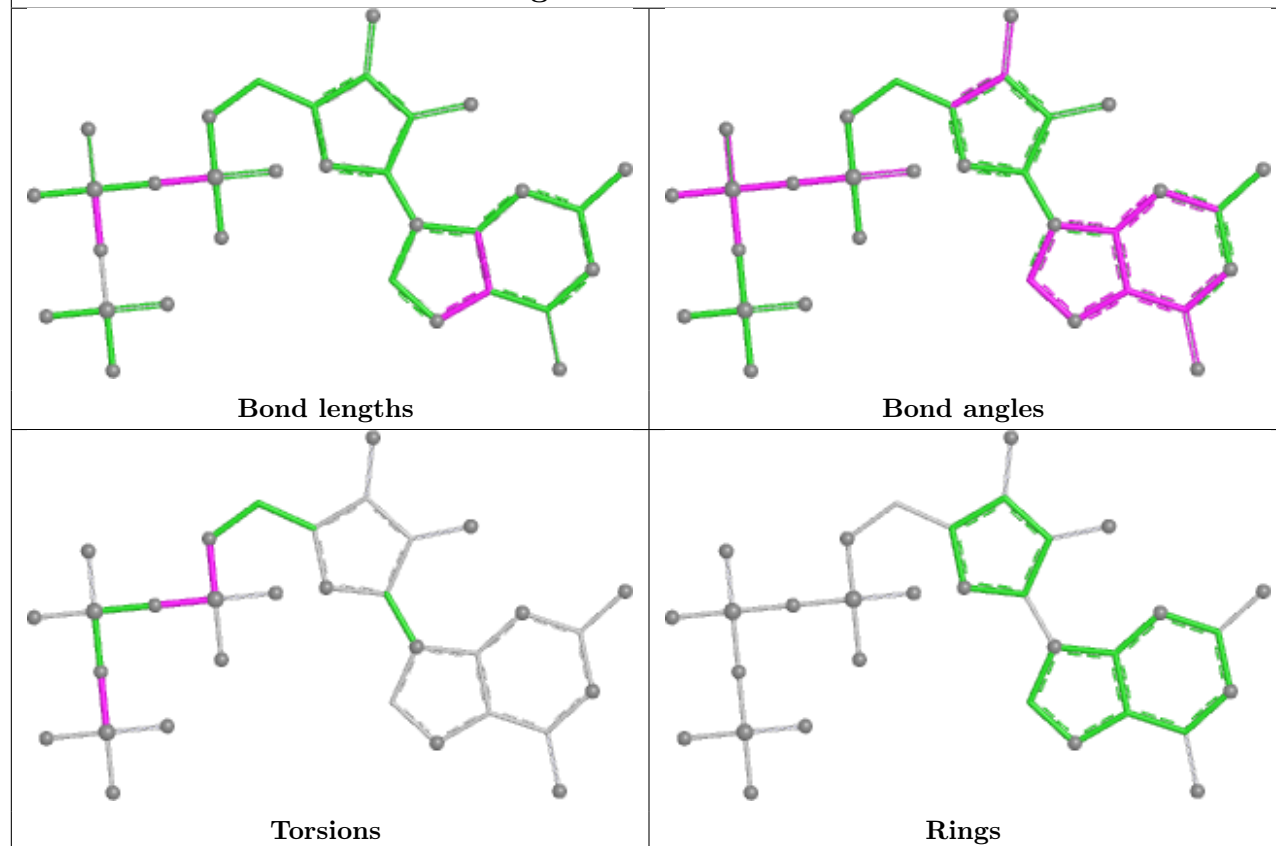
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	B	506	GOL	3	0
8	A	504	GOL	1	0
8	C	506	GOL	7	0
12	F	401	ACP	1	0
8	C	507	GOL	1	0
8	C	505	GOL	1	0
10	B	504	MES	2	0

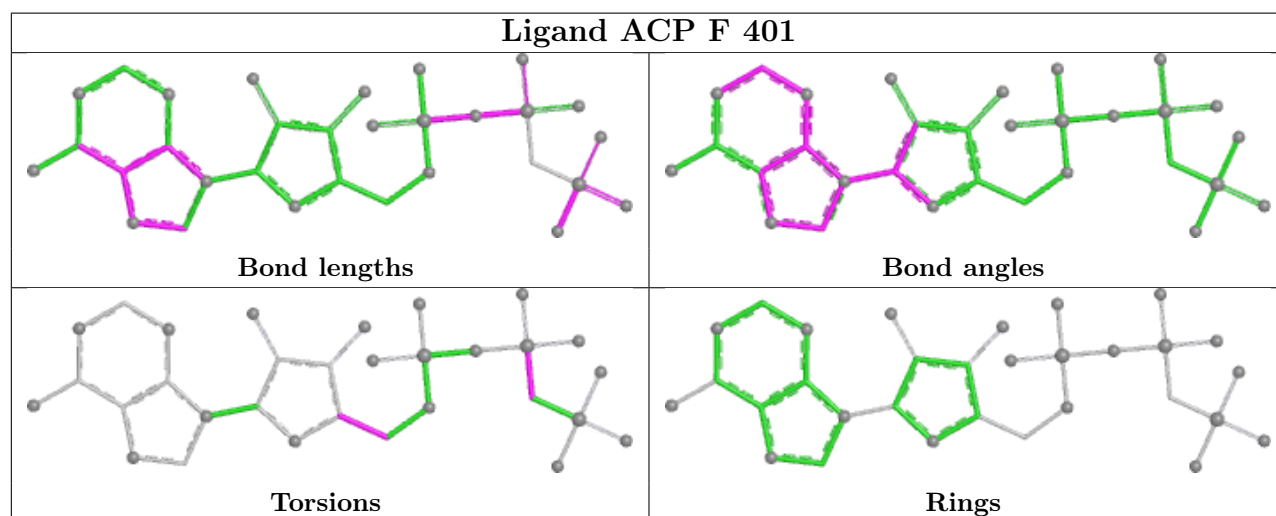
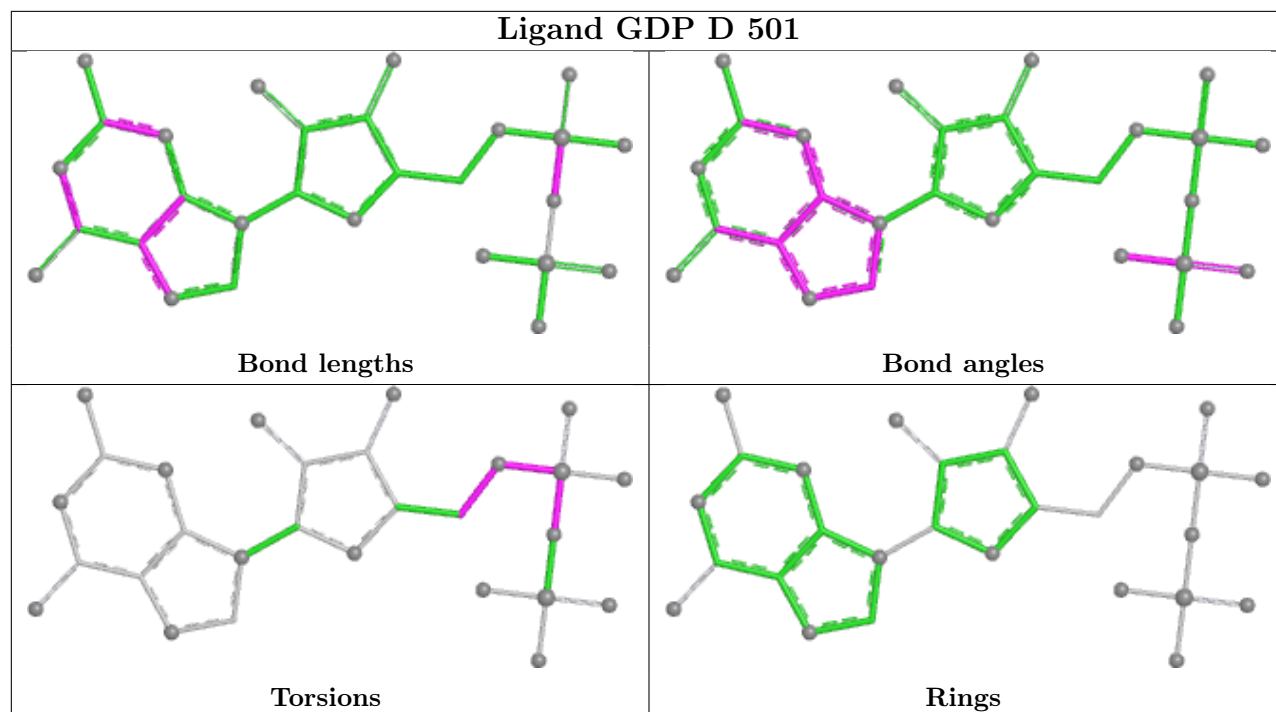
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 501

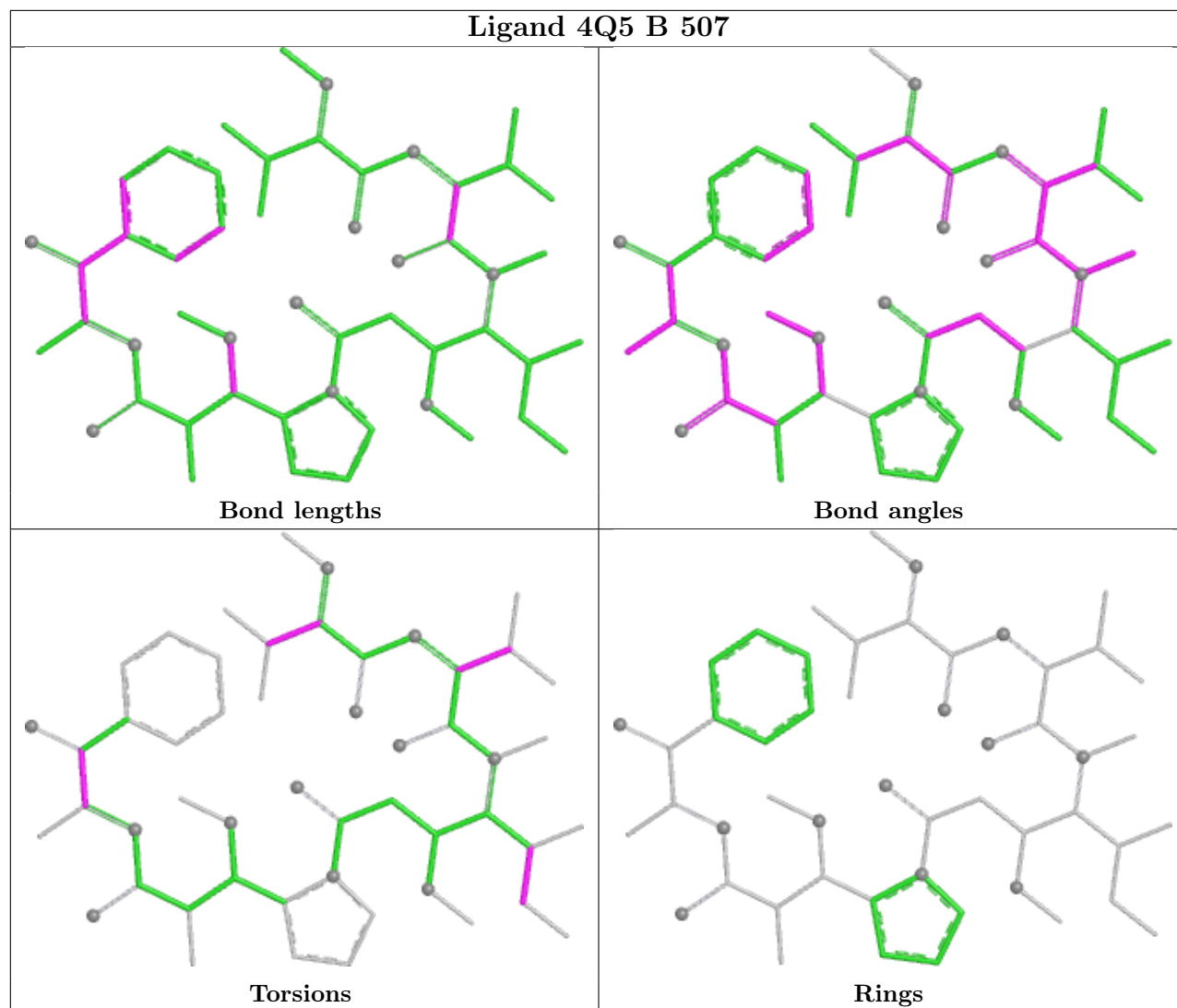


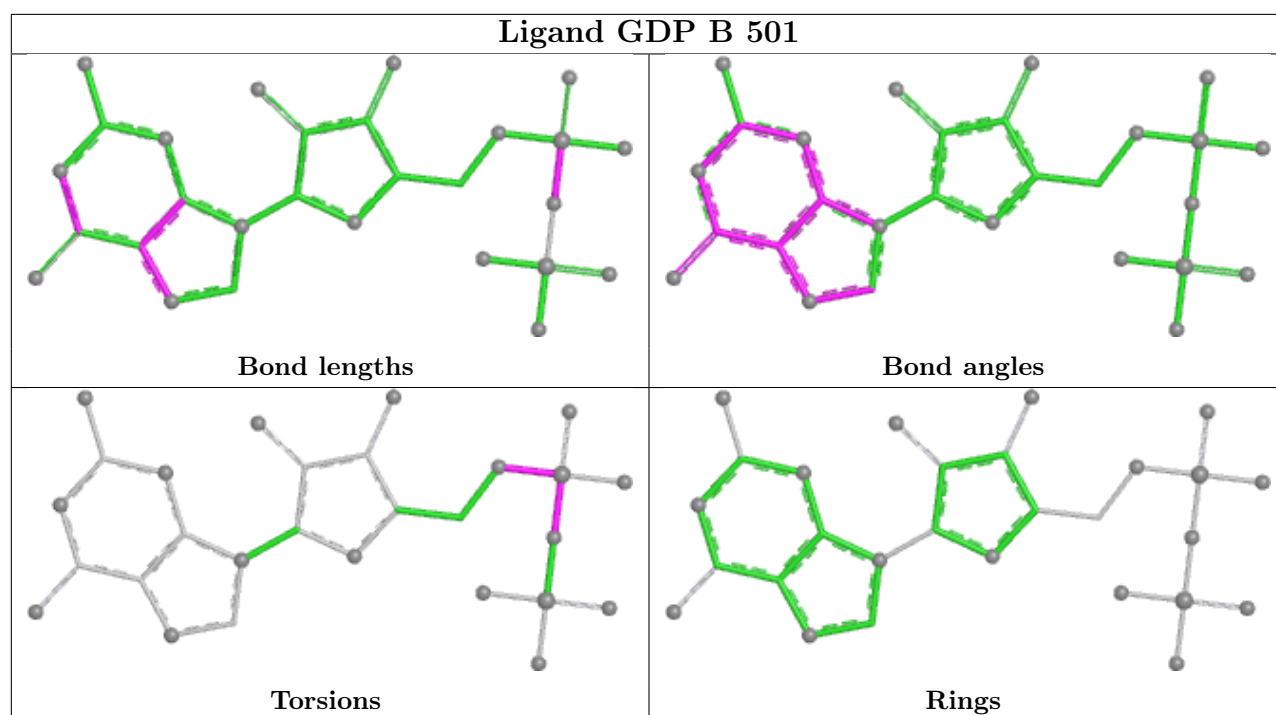
Ligand GTP C 501





Ligand 4Q5 B 507





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	439/451 (97%)	-0.21	2 (0%)	87 89	18, 35, 61, 98	0
1	C	440/451 (97%)	-0.44	4 (0%)	81 83	16, 28, 51, 79	1 (0%)
2	B	427/445 (95%)	-0.32	8 (1%)	66 66	16, 30, 61, 101	0
2	D	422/445 (94%)	0.24	21 (4%)	34 33	25, 47, 80, 93	0
3	E	123/143 (86%)	0.48	6 (4%)	35 34	29, 51, 85, 109	0
4	F	346/384 (90%)	0.71	44 (12%)	8 7	27, 59, 116, 135	0
All	All	2197/2319 (94%)	-0.01	85 (3%)	43 44	16, 39, 85, 135	1 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	4.8
4	F	161	LEU	4.5
4	F	125	THR	4.3
2	D	1	MET	4.1
4	F	362	ALA	4.0
2	B	1	MET	4.0
4	F	233	PHE	3.8
4	F	169	LEU	3.7
4	F	150	LYS	3.6
3	E	6	MET	3.6
2	D	407	TRP	3.6
1	C	357	TYR	3.6
2	D	276	THR	3.6
4	F	372	THR	3.5
2	B	282	GLN	3.5
4	F	245	ILE	3.3
2	D	286	LEU	3.3
4	F	182	ILE	3.3
1	A	262	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	133	ALA	3.2
4	F	159	GLY	3.2
3	E	139	LEU	3.2
4	F	130	VAL	3.1
2	D	74	THR	3.0
4	F	249	TYR	3.0
4	F	243	HIS	3.0
4	F	363	ASP	3.0
1	C	440	VAL	3.0
4	F	225	SER	3.0
4	F	132	LEU	2.9
2	D	98	GLY	2.9
4	F	149	ALA	2.9
4	F	237	THR	2.8
2	B	57	ALA	2.8
2	D	94	PHE	2.8
4	F	172	PHE	2.8
1	A	439	SER	2.8
4	F	104	ASN	2.8
2	D	404	PHE	2.8
4	F	179	VAL	2.7
2	D	57	ALA	2.7
4	F	103	THR	2.7
2	D	82	PRO	2.6
2	D	75	MET	2.6
2	D	37	HIS	2.6
4	F	381	HIS	2.6
4	F	160	ILE	2.5
2	B	82	PRO	2.5
4	F	227	PRO	2.5
4	F	181	VAL	2.5
4	F	186	LEU	2.4
4	F	90	SER	2.4
3	E	53	LYS	2.4
4	F	244	CYS	2.4
4	F	142	ARG	2.4
2	D	99	ALA	2.4
2	B	281	GLN	2.4
4	F	131	PHE	2.4
2	B	284	ARG	2.3
2	D	83	PHE	2.3
2	B	283	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	135	LYS	2.3
2	B	56	ALA	2.2
2	D	370	GLY	2.2
1	C	340	SER	2.2
4	F	341	LYS	2.2
4	F	147	TRP	2.2
4	F	384	HIS	2.1
4	F	146	VAL	2.1
4	F	239	HIS	2.1
3	E	124	GLN	2.1
2	D	372	LYS	2.1
4	F	166	ALA	2.1
4	F	254	GLY	2.1
4	F	173	ILE	2.1
4	F	167	SER	2.1
2	D	56	ALA	2.1
2	D	405	LEU	2.1
1	C	163	LYS	2.0
4	F	253	TYR	2.0
4	F	134	ALA	2.0
4	F	236	LYS	2.0
2	D	220	THR	2.0
2	D	221	THR	2.0
2	D	416	MET	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](#)

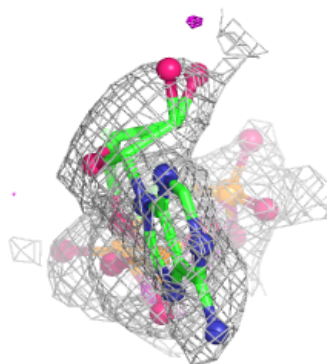
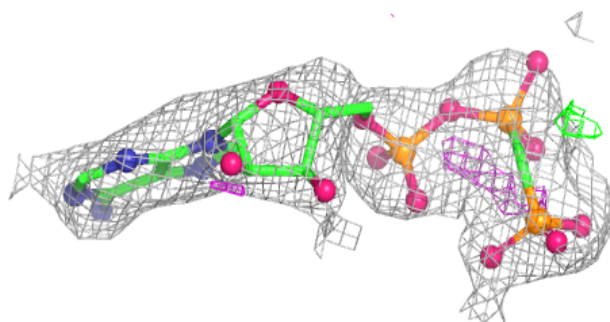
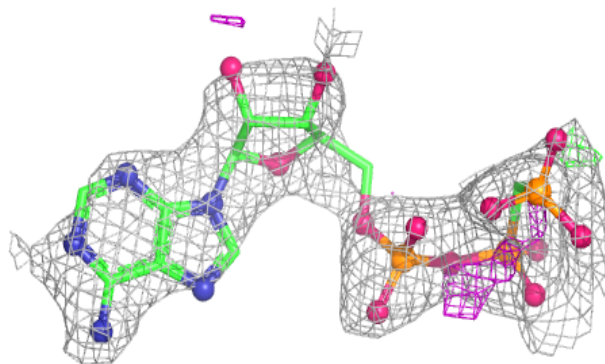
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
8	GOL	A	504	6/6	0.79	0.20	63,69,72,81	0
8	GOL	B	506	6/6	0.84	0.14	49,51,54,55	0
12	ACP	F	401	31/31	0.84	0.13	66,83,96,109	0
8	GOL	C	506	6/6	0.85	0.28	50,68,69,82	0
8	GOL	A	505	6/6	0.86	0.17	46,59,60,67	0
8	GOL	A	506	6/6	0.87	0.15	54,61,65,67	0
7	CA	B	503	1/1	0.89	0.19	82,82,82,82	0
8	GOL	C	503	6/6	0.89	0.21	54,69,72,77	0
8	GOL	C	505	6/6	0.90	0.15	44,53,55,63	0
10	MES	B	504	12/12	0.93	0.11	45,49,56,60	0
6	MG	D	502	1/1	0.93	0.13	46,46,46,46	0
10	MES	B	505	12/12	0.94	0.11	49,52,53,55	0
9	GDP	D	501	28/28	0.94	0.08	34,38,48,60	0
6	MG	B	502	1/1	0.95	0.07	63,63,63,63	0
8	GOL	C	507	6/6	0.95	0.10	45,51,53,55	0
11	4Q5	B	507	51/51	0.96	0.07	18,22,25,25	0
7	CA	A	503	1/1	0.97	0.04	57,57,57,57	0
5	GTP	C	501	32/32	0.99	0.04	17,20,23,23	0
6	MG	A	502	1/1	0.99	0.04	25,25,25,25	0
5	GTP	A	501	32/32	0.99	0.04	18,22,25,26	0
7	CA	C	504	1/1	0.99	0.05	35,35,35,35	0
9	GDP	B	501	28/28	0.99	0.04	15,18,19,20	0
6	MG	C	502	1/1	1.00	0.02	23,23,23,23	0

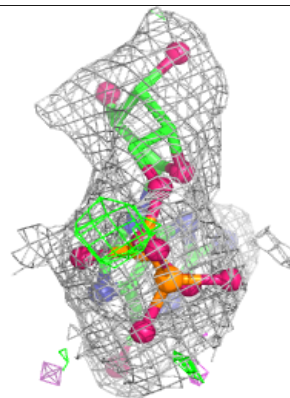
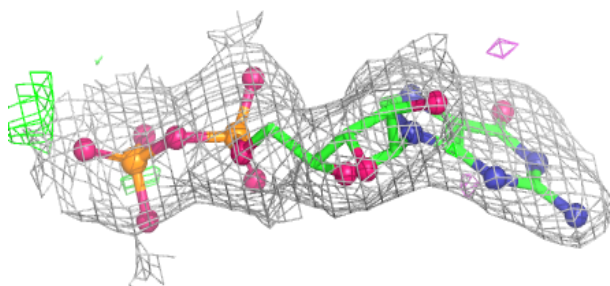
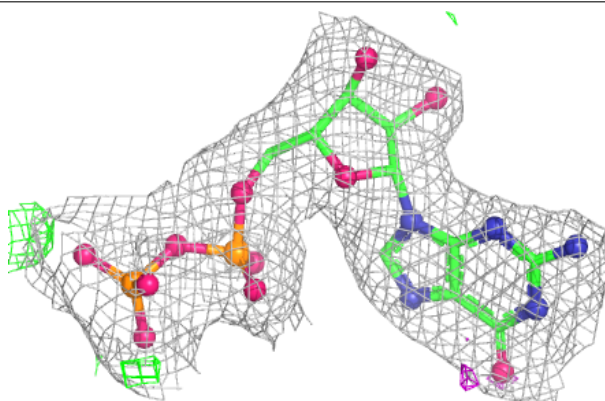
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

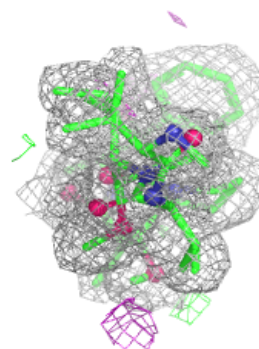
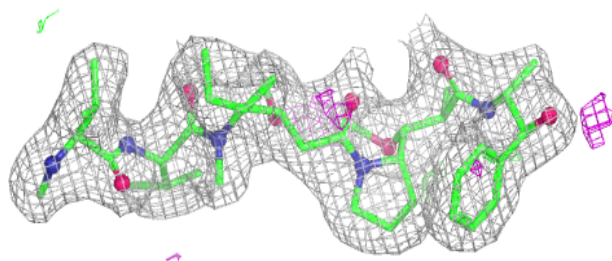
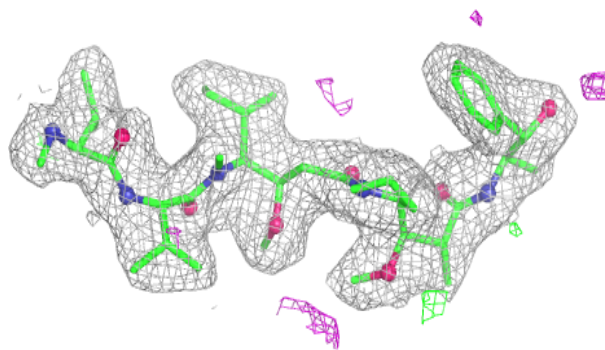
**Electron density around GDP D 501:**

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

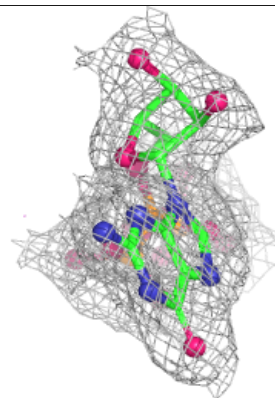
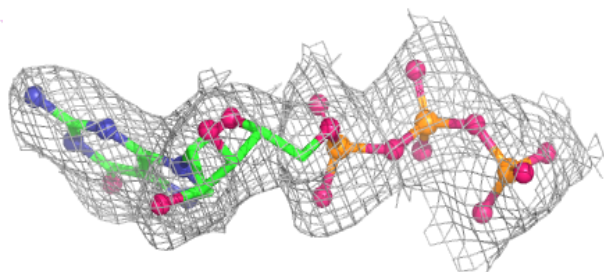
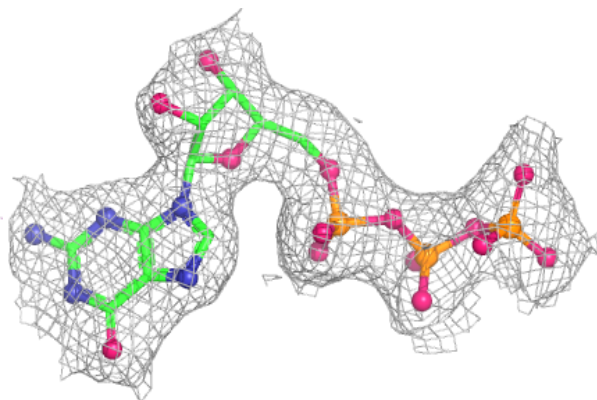


Electron density around 4Q5 B 507:

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

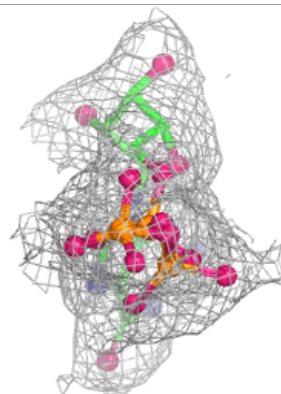
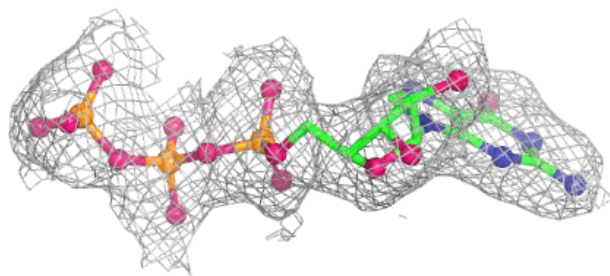
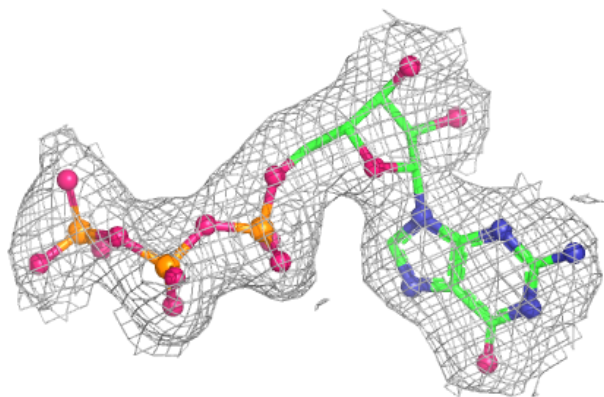
**Electron density around GTP C 501:**

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



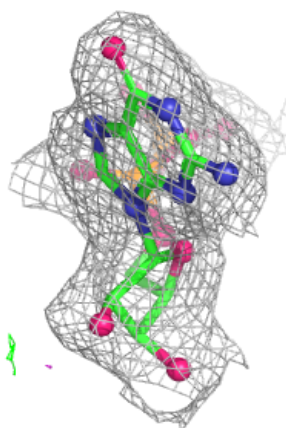
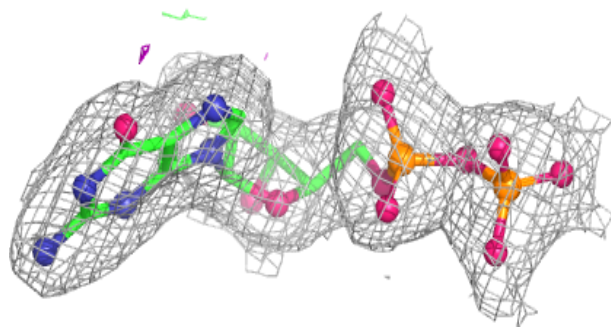
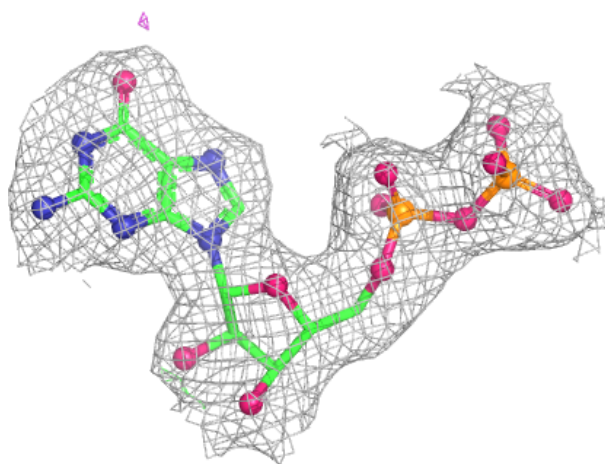
Electron density around GTP A 501:

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



Electron density around 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.