



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:08 AM UTC

PDB ID : 7DP8 / pdb_00007dp8
Title : Crystal structure of T2R-TTL-Cevipabulin-eribulin complex
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on : 2020-12-18
Resolution : 2.45 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

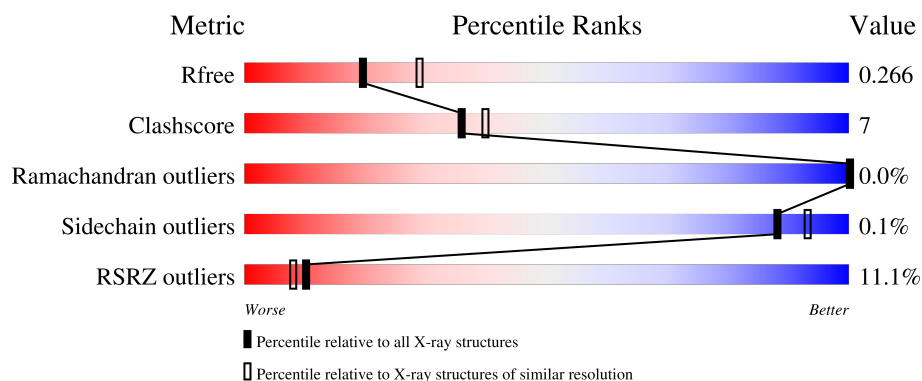
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	450	5% 82% 15% .
1	C	450	2% 87% 10% .
2	B	445	8% 78% 16% 6%
2	D	445	14% 82% 14% .
3	E	143	17% 70% 15% . 14%

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (23%), green (69%), yellow (22%), and grey (9%). The percentages are labeled above or below the segments.

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 35012 atoms, of which 17101 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	438	Total	C	H	N	O	S	0	4	0
			6802	2182	3351	588	657	24			
1	C	440	Total	C	H	N	O	S	0	8	0
			6844	2201	3369	589	662	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	418	Total	C	H	N	O	S	0	4	0
			6498	2080	3185	565	639	29			
2	D	426	Total	C	H	N	O	S	0	1	0
			6563	2100	3217	570	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	2	0
			2069	635	1037	188	204	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	351	Total	C	H	N	O	S	0	1	0
			5696	1838	2824	491	528	15			

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	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	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		

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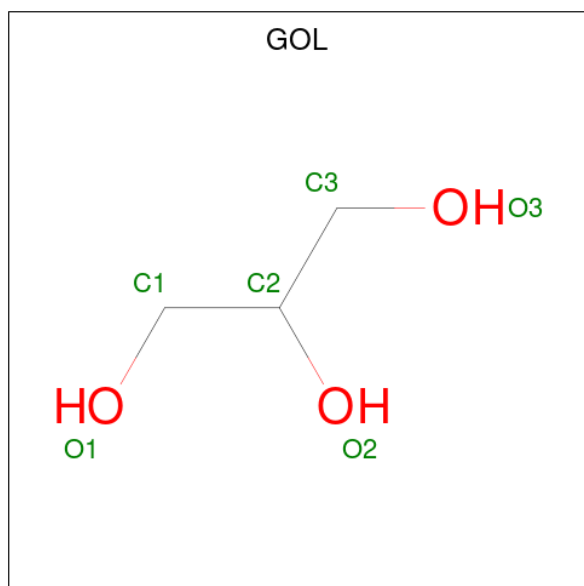
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

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

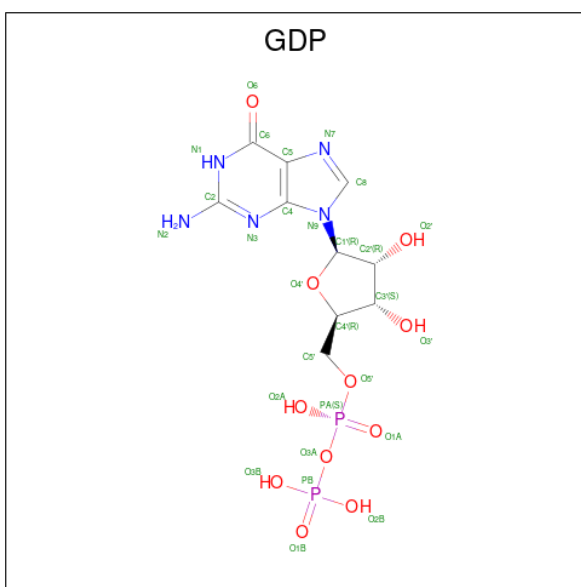
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		
7	C	2	Total	Ca	0	0
			2	2		

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



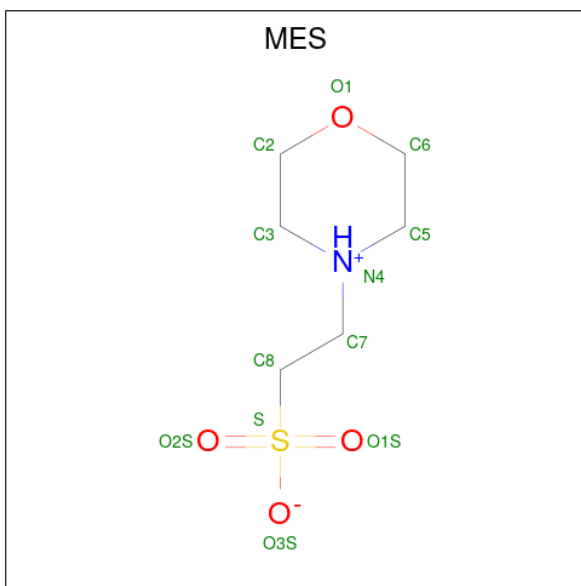
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	

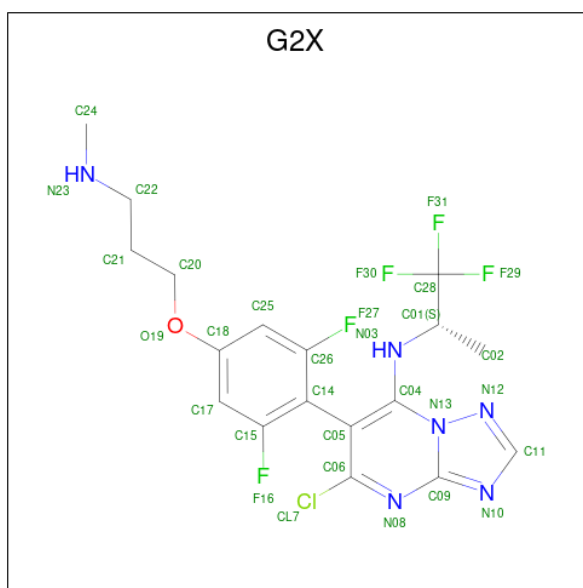
- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			24	6	12	1	4	1	

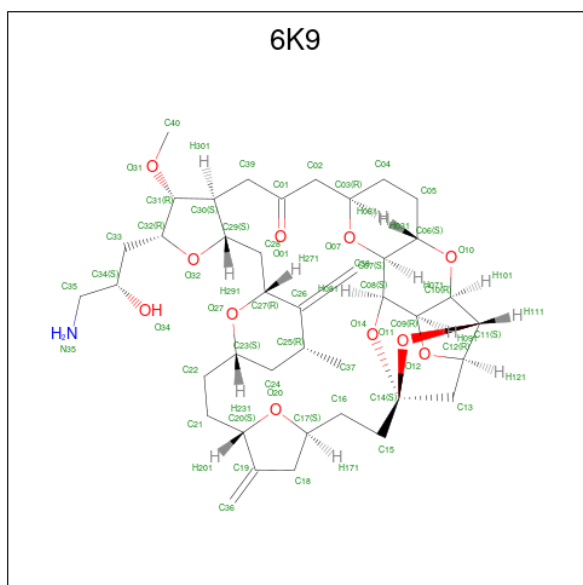
- Molecule 11 is 6-[2,6-bis(fluoranyl)-4-[3-(methylamino)propoxy]phenyl]-5-chloranyl-N-[(2S)-1,1,1-tris(fluoranyl)propan-2-yl]-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (CCD ID: G2X)

(formula: $C_{18}H_{18}ClF_5N_6O$) (labeled as "Ligand of Interest" by depositor).



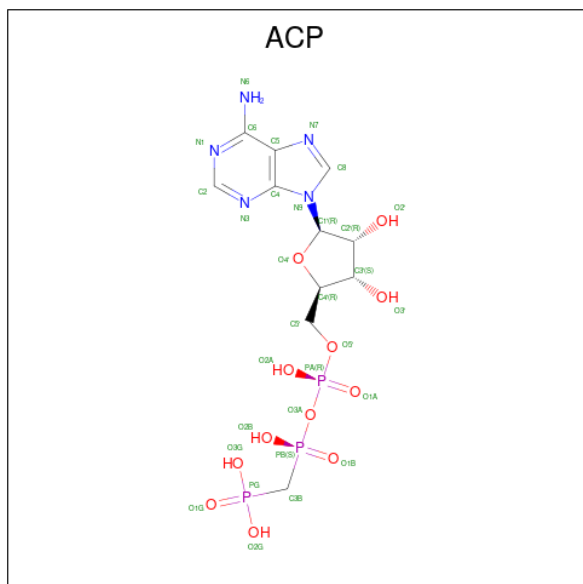
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
11	C	1	Total	C	Cl	F	H	N	O	0	0
			49	18	1	5	18	6	1		
11	C	1	Total	C	Cl	F	H	N	O	0	0
			49	18	1	5	18	6	1		

- Molecule 12 is (1S,3S,6S,9S,12S,14R,16R,18S,20R,21R,22S,26R,29S,31R,32S,33R,35R,36S)-20-[(2S)-3-amino-2-hydroxypropyl]-21-methoxy-14-methyl-8,15-dimethylidene-2,19,30,34,37,39,40,41-octaoxanonacyclo[24.9.2.1^{3,32}.1^{3,33}.1^{6,9}.1^{12,16}.0^{18,22}.0^{29,36}.0^{31,35}]hen tetracontan-24-one (non-preferred name) (CCD ID: 6K9) (formula: $C_{40}H_{59}NO_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	N	O	0	0
			52	40	1	11		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



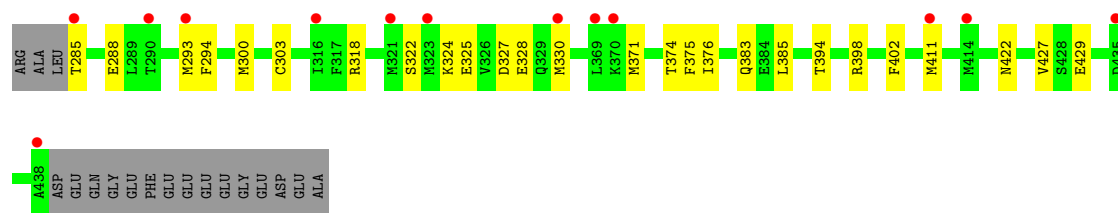
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 14 is water.

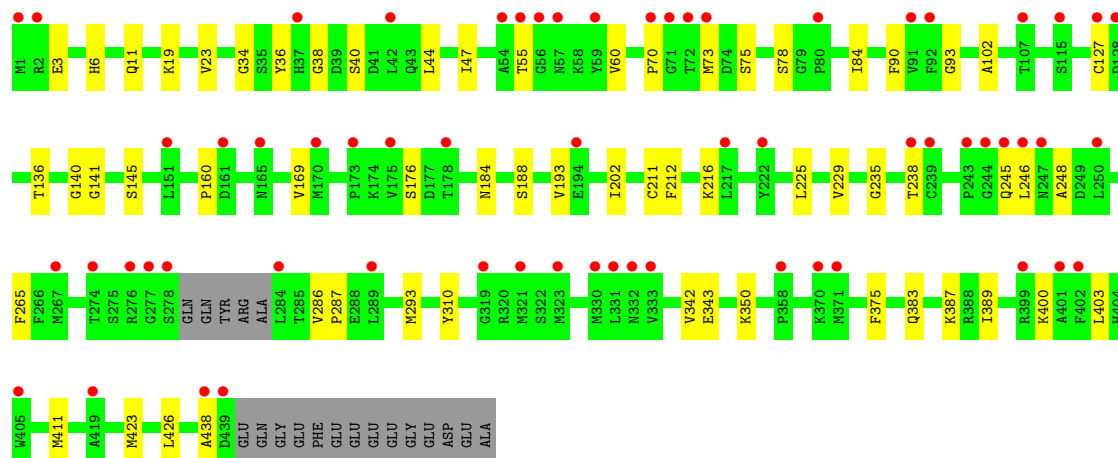
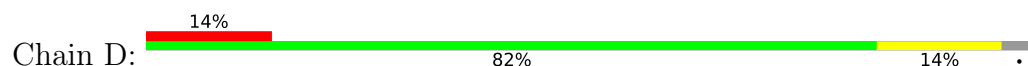
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	18	Total	O	0	0
			18	18		
14	B	29	Total	O	0	0
			29	29		
14	C	57	Total	O	0	0
			57	57		
14	D	7	Total	O	0	0
			7	7		
14	E	4	Total	O	0	0
			4	4		
14	F	3	Total	O	0	0
			3	3		

- Molecule 1: Tubulin alpha-1B chain

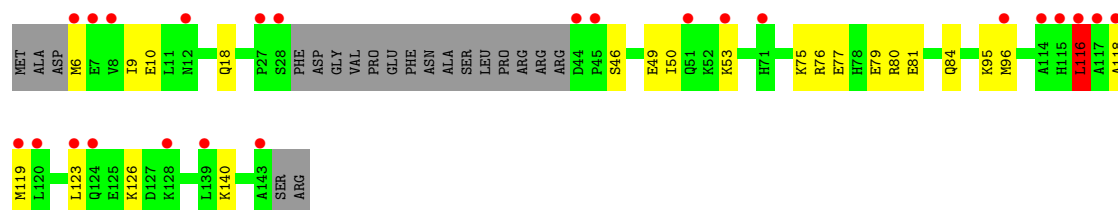




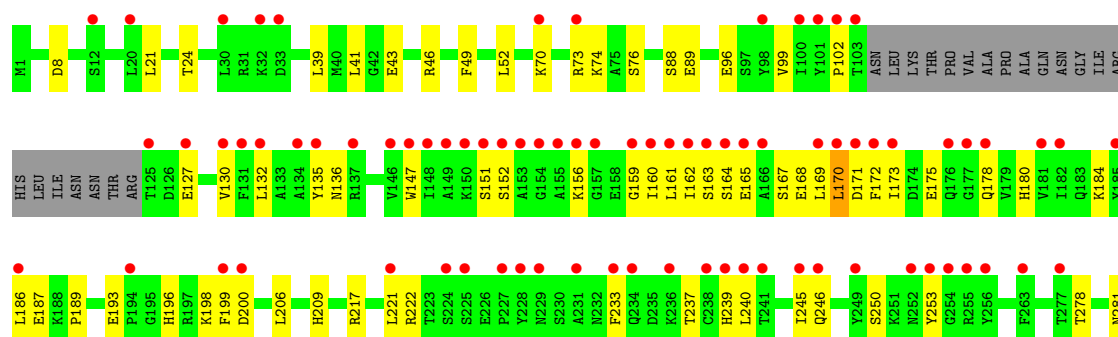
• Molecule 2: Tubulin beta chain

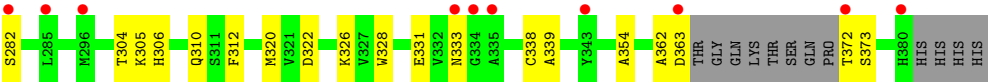


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.94Å 159.07Å 176.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.46 – 2.45 59.46 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.0 (59.46-2.45) 95.0 (59.46-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.227 , 0.264 0.230 , 0.266	Depositor DCC
R_{free} test set	5153 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35012	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: MES, G2X, CA, MG, ACP, GTP, GOL, 6K9, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.28	2/3532 (0.1%)	0.45	2/4794 (0.0%)
1	C	0.26	2/3577 (0.1%)	0.55	6/4859 (0.1%)
2	B	0.18	0/3389	0.37	0/4588
2	D	0.18	0/3422	0.40	0/4634
3	E	0.22	0/1041	0.45	1/1382 (0.1%)
4	F	0.17	0/2937	0.45	0/3967
All	All	0.22	4/17898 (0.0%)	0.45	9/24224 (0.0%)

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
1	A	0	1
1	C	0	1
2	D	0	1
3	E	0	1
4	F	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	339	ARG	C-N	7.36	1.44	1.33
1	A	285	GLN	CB-CG	-6.62	1.32	1.52
1	C	340	SER	CB-OG	5.79	1.53	1.42
1	A	285	GLN	CA-CB	-5.42	1.44	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	SER	CA-CB-OG	19.10	149.30	111.10
1	C	340	SER	N-CA-C	-10.38	100.03	112.89
1	A	285	GLN	CB-CG-CD	-9.75	96.02	112.60
1	C	340	SER	CA-C-O	7.02	128.02	119.31
1	C	340	SER	CB-CA-C	-6.88	95.61	109.99
1	C	340	SER	N-CA-CB	6.44	120.90	110.40
1	A	285	GLN	CG-CD-OE1	-6.38	108.04	120.80
3	E	116	LEU	CA-CB-CG	5.66	136.10	116.30
1	C	339	ARG	O-C-N	5.07	128.68	122.34

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	GLN	Sidechain
1	C	340	SER	Mainchain
2	D	55	THR	Peptide
3	E	116	LEU	Peptide
4	F	170	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3451	3351	3362	46	1
1	C	3475	3369	3384	31	1
2	B	3313	3185	3192	54	0
2	D	3346	3217	3227	43	0
3	E	1032	1037	1040	25	0
4	F	2872	2824	2835	65	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	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
6	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
8	A	12	16	16	1	0
9	B	28	10	12	2	0
10	B	12	12	12	0	0
11	C	62	36	0	0	0
12	D	52	0	0	2	0
13	F	31	14	14	1	0
14	A	18	0	0	1	0
14	B	29	0	0	4	0
14	C	57	0	0	3	0
14	D	7	0	0	0	0
14	E	4	0	0	2	0
14	F	3	0	0	0	0
All	All	17911	17101	17130	256	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 7.

All (256) 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:162:ARG:NH1	14:B:601:HOH:O	1.93	1.00
3:E:116:LEU:HA	3:E:119:MET:H	1.47	0.80
2:D:75:SER:O	2:D:78:SER:OG	1.99	0.79
1:A:276:ILE:HG21	1:A:283:HIS:CE1	2.19	0.77
4:F:168:GLU:HA	4:F:171:ASP:HB3	1.68	0.76
1:C:439:SER:O	14:C:701:HOH:O	2.05	0.74
1:C:218:ASP:OD2	14:C:702:HOH:O	2.10	0.69
2:D:73:MET:HG3	2:D:90:PHE:HD2	1.59	0.68
2:D:60:VAL:HG23	2:D:84:ILE:O	1.93	0.68
2:B:145[A]:SER:HG	2:B:188:SER:HG	1.34	0.67
4:F:168:GLU:HA	4:F:171:ASP:CB	2.24	0.67
4:F:304:THR:OG1	4:F:310:GLN:OE1	2.11	0.67
1:A:250:VAL:HG22	1:A:254:GLU:OE2	1.96	0.66
2:B:262:ARG:NH1	2:B:429:GLU:OE2	2.28	0.66
2:B:11:GLN:NE2	14:B:605:HOH:O	2.29	0.65
3:E:75:LYS:HD3	3:E:76:ARG:NH2	2.10	0.65
9:B:501:GDP:O1A	14:B:602:HOH:O	2.14	0.65
2:D:44:LEU:HD22	2:D:47:ILE:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:ASN:OD1	14:B:603:HOH:O	2.14	0.64
2:B:322:SER:HG	2:B:325:GLU:HB2	1.63	0.64
8:A:504:GOL:O1	8:A:504:GOL:O3	2.13	0.63
4:F:217:ARG:NH2	4:F:373:SER:O	2.32	0.63
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.81	0.62
2:D:343:GLU:HG3	2:D:438:ALA:HB2	1.81	0.62
1:A:276:ILE:HG21	1:A:283:HIS:ND1	2.18	0.59
2:D:245:GLN:HA	2:D:248:ALA:HB2	1.85	0.58
2:B:322:SER:OG	2:B:325:GLU:HB2	2.03	0.58
1:A:265:ILE:O	1:A:265:ILE:HG22	2.02	0.58
1:C:178:SER:OG	2:D:350:LYS:NZ	2.37	0.58
2:B:112:LEU:HD23	2:B:147:MET:HE1	1.86	0.58
4:F:170:LEU:HA	4:F:173:ILE:HG12	1.86	0.58
1:A:327:ASP:OD2	14:A:601:HOH:O	2.17	0.57
4:F:278:THR:OG1	4:F:281:ASN:N	2.36	0.57
2:B:70:PRO:HG2	1:C:1:MET:HE2	1.86	0.57
2:D:36:TYR:OH	2:D:40:SER:O	2.21	0.57
1:A:203:MET:HE1	1:A:388:TRP:CH2	2.39	0.57
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.38	0.56
3:E:53:LYS:O	14:E:201:HOH:O	2.18	0.56
4:F:198:LYS:HE2	4:F:320:MET:HE1	1.88	0.56
1:A:221:ARG:NH1	2:B:327:ASP:OD2	2.39	0.55
2:D:141:GLY:O	2:D:184:ASN:ND2	2.39	0.55
4:F:278:THR:O	4:F:282:SER:OG	2.16	0.55
2:B:215:LEU:HD12	2:B:215:LEU:H	1.71	0.55
3:E:116:LEU:HB2	3:E:119:MET:HB3	1.88	0.55
2:B:126:SER:O	2:B:126:SER:OG	2.25	0.54
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.89	0.54
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.42	0.54
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.88	0.54
2:B:131:GLN:OE1	2:B:250:LEU:N	2.37	0.53
3:E:140:LYS:NZ	14:E:202:HOH:O	2.32	0.53
3:E:116:LEU:CB	3:E:119:MET:HB3	2.39	0.53
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.90	0.53
4:F:151:SER:HB3	4:F:180:HIS:CG	2.44	0.53
4:F:246:GLN:O	4:F:250:SER:HB3	2.08	0.53
1:A:71:GLU:OE1	1:A:73:THR:HG23	2.08	0.53
1:A:281:ALA:O	1:A:282:TYR:HB2	2.09	0.53
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.91	0.52
2:B:262:ARG:NH2	2:B:422:ASN:OD1	2.43	0.52
1:C:160:ASP:OD2	14:C:703:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:MET:HG2	2:D:375:PHE:HB2	1.92	0.52
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.92	0.52
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.93	0.51
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.44	0.51
1:A:276:ILE:CG2	1:A:283:HIS:CE1	2.91	0.51
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.46	0.51
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.46	0.51
4:F:89:GLU:CD	4:F:89:GLU:H	2.19	0.51
1:A:209:ILE:HD11	1:A:302:MET:SD	2.50	0.51
2:D:212:PHE:O	2:D:216:LYS:HA	2.10	0.51
3:E:116:LEU:HB3	3:E:119:MET:HB2	1.93	0.50
4:F:200:ASP:OD2	4:F:222:ARG:HB2	2.11	0.50
2:D:34:GLY:HA2	2:D:84:ILE:HD11	1.94	0.50
4:F:46:ARG:NH1	4:F:46:ARG:HG2	2.27	0.50
4:F:193:GLU:OE1	4:F:196:HIS:ND1	2.35	0.50
2:D:193:VAL:HG22	2:D:265:PHE:HE2	1.77	0.49
1:A:71:GLU:CD	1:A:73:THR:HG1	2.21	0.49
4:F:233:PHE:HA	4:F:239:HIS:NE2	2.27	0.49
1:A:251:ASP:OD1	1:A:252:LEU:N	2.45	0.49
4:F:178:GLN:HA	4:F:178:GLN:OE1	2.13	0.49
4:F:239:HIS:C	4:F:240:LEU:HD23	2.38	0.49
2:B:35:SER:OG	2:B:58:LYS:HE3	2.12	0.49
2:D:193:VAL:HG22	2:D:265:PHE:CE2	2.48	0.49
4:F:73:ARG:HE	4:F:152:SER:HB3	1.77	0.49
4:F:46:ARG:HG2	4:F:46:ARG:HH11	1.78	0.48
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.46	0.48
4:F:170:LEU:HA	4:F:173:ILE:CG1	2.43	0.48
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.48	0.48
1:A:287:SER:OG	1:A:290:GLU:N	2.42	0.48
3:E:116:LEU:HB3	3:E:119:MET:CB	2.44	0.48
4:F:8:ASP:HB2	4:F:43:GLU:HA	1.95	0.48
2:B:136:THR:HG21	2:B:233:MET:HE1	1.96	0.48
2:D:19:LYS:O	2:D:23:VAL:HG23	2.14	0.48
4:F:127:GLU:HA	4:F:130:VAL:HG23	1.95	0.48
3:E:123:LEU:HD22	3:E:126:LYS:HD3	1.94	0.48
4:F:96:GLU:HG2	4:F:147:TRP:CH2	2.49	0.48
4:F:135:TYR:HD1	4:F:136:ASN:OD1	1.97	0.48
2:B:267:MET:HE3	2:B:303:CYS:HB2	1.96	0.48
1:A:261:PRO:HG2	1:A:313:MET:HE2	1.96	0.48
2:D:160:PRO:HB2	3:E:119:MET:HE2	1.95	0.48
4:F:127:GLU:HB3	4:F:130:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:163:SER:OG	4:F:164:SER:N	2.46	0.48
2:D:235:GLY:O	2:D:238:THR:HG22	2.14	0.47
4:F:233:PHE:HA	4:F:239:HIS:CE1	2.50	0.47
4:F:372:THR:OG1	4:F:373:SER:N	2.47	0.47
2:D:140:GLY:O	2:D:184:ASN:ND2	2.42	0.47
2:D:202:ILE:HG21	2:D:229:VAL:HG22	1.96	0.47
1:A:265:ILE:HD12	1:A:265:ILE:N	2.28	0.47
4:F:70:LYS:HA	4:F:76:SER:HB3	1.97	0.47
2:B:294:PHE:HE2	2:B:330:MET:HE1	1.79	0.47
1:C:2:ARG:HA	1:C:131:GLY:O	2.15	0.47
4:F:189:PRO:HA	4:F:322:ASP:HA	1.96	0.47
2:B:40:SER:OG	2:B:41:ASP:N	2.47	0.47
2:D:169:VAL:HA	2:D:202:ILE:O	2.15	0.47
4:F:156:LYS:C	4:F:245:ILE:HD11	2.39	0.47
2:B:324:LYS:C	2:B:324:LYS:HE2	2.40	0.47
2:D:389:ILE:CG2	2:D:423:MET:HE1	2.45	0.46
4:F:161:LEU:HD23	4:F:169:LEU:HD13	1.97	0.46
2:B:383:GLN:HG3	2:B:427:VAL:HG13	1.97	0.46
1:A:79:ARG:NH2	1:A:94:THR:HG23	2.31	0.46
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.98	0.46
1:C:172:TYR:HB2	1:C:203:MET:HE3	1.96	0.46
2:D:193:VAL:CG2	2:D:426:LEU:HD22	2.46	0.46
4:F:338:CYS:SG	4:F:339:ALA:N	2.89	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.46
4:F:362:ALA:O	4:F:363:ASP:HB2	2.16	0.46
2:B:210:ILE:HG22	2:B:215:LEU:CD1	2.46	0.46
2:B:285:THR:N	2:B:288:GLU:OE1	2.48	0.46
4:F:237:THR:O	4:F:246:GLN:NE2	2.49	0.46
2:B:318:ARG:O	2:B:371:MET:HA	2.16	0.46
1:C:133:GLN:OE1	1:C:251:ASP:HB2	2.16	0.45
3:E:116:LEU:HA	3:E:119:MET:N	2.23	0.45
1:C:115:ILE:O	1:C:119:LEU:HD23	2.17	0.45
4:F:246:GLN:O	4:F:253:TYR:HB2	2.17	0.45
2:B:105:HIS:HE1	3:E:75:LYS:NZ	2.14	0.45
2:B:170:MET:SD	2:B:385:LEU:HD21	2.55	0.45
3:E:116:LEU:CA	3:E:119:MET:H	2.23	0.45
2:B:39:ASP:OD1	2:B:39:ASP:N	2.44	0.45
2:D:176:SER:HA	12:D:503:6K9:O01	2.16	0.45
1:A:68:VAL:HG12	1:A:93:ILE:HD12	1.99	0.45
2:D:193:VAL:HG21	2:D:426:LEU:HD22	1.98	0.45
3:E:50:ILE:O	3:E:53:LYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:99:VAL:HG12	4:F:127:GLU:OE1	2.16	0.45
2:D:73:MET:CA	2:D:73:MET:HE2	2.46	0.45
1:A:210:TYR:OH	1:A:221:ARG:CD	2.65	0.44
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.44
2:B:162:ARG:HG2	2:B:162:ARG:HH11	1.81	0.44
2:B:207:LEU:HD21	2:B:300:MET:HB3	1.98	0.44
4:F:333:ASN:ND2	13:F:402:ACP:O3G	2.51	0.44
2:D:70:PRO:HG3	2:D:93:GLY:O	2.18	0.44
1:C:265:ILE:HG21	1:C:313:MET:HE1	2.00	0.44
3:E:116:LEU:C	3:E:118:ALA:N	2.73	0.44
4:F:186:LEU:HD12	4:F:320:MET:HE2	1.99	0.44
1:A:90:GLU:HG2	1:A:121:ARG:HD2	1.99	0.44
4:F:161:LEU:HD23	4:F:169:LEU:CD1	2.48	0.44
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.44
4:F:305:LYS:HD3	4:F:306:HIS:NE2	2.33	0.44
2:B:294:PHE:CE2	2:B:330:MET:HE1	2.52	0.44
3:E:116:LEU:CB	3:E:119:MET:CB	2.95	0.44
2:B:91:VAL:HG12	2:B:112:LEU:HD11	2.00	0.44
2:B:383:GLN:CG	2:B:427:VAL:HG13	2.48	0.44
2:B:219:THR:HG22	1:C:326:LYS:HE3	1.99	0.43
4:F:326:LYS:HE3	4:F:328:TRP:CZ2	2.53	0.43
2:B:394:THR:O	2:B:398:ARG:HG3	2.18	0.43
2:B:36:TYR:CE1	2:B:44:LEU:HD11	2.53	0.43
1:C:154:MET:HE3	1:C:166:LYS:HE2	1.99	0.43
2:D:3:GLU:CD	2:D:127:CYS:HB3	2.43	0.43
2:D:383:GLN:O	2:D:387:LYS:HG3	2.18	0.43
1:A:88:HIS:NE2	1:A:90:GLU:HB2	2.33	0.43
1:A:280:LYS:HZ2	1:A:280:LYS:HB3	1.84	0.43
2:B:139:LEU:HD11	2:B:170:MET:HE2	2.00	0.43
9:B:501:GDP:H8	9:B:501:GDP:H5''	1.83	0.43
1:C:270:ALA:O	1:C:302:MET:HB2	2.19	0.43
1:C:296:PHE:CE1	1:C:377:MET:HE1	2.53	0.43
2:B:165:ASN:ND2	2:B:198:GLU:HB2	2.34	0.43
2:B:293[B]:MET:CG	2:B:375:PHE:HB2	2.48	0.43
4:F:209:HIS:H	4:F:209:HIS:CD2	2.37	0.43
2:B:269:GLY:O	2:B:374:THR:HG23	2.19	0.43
4:F:21:LEU:O	4:F:24:THR:OG1	2.31	0.43
4:F:167:SER:CB	4:F:168:GLU:OE1	2.67	0.43
1:A:33:ASP:HA	1:A:85:GLN:HG3	2.00	0.43
4:F:172:PHE:O	4:F:175:GLU:HB3	2.18	0.43
1:A:223:THR:O	1:A:227:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	2.01	0.43
1:A:191:THR:HG21	1:A:425:MET:HE1	2.00	0.42
4:F:184:LYS:NZ	4:F:187:GLU:OE2	2.51	0.42
1:C:11:GLN:HG3	1:C:74:VAL:HG21	2.01	0.42
2:D:11:GLN:OE1	12:D:503:6K9:C13	2.67	0.42
2:D:44:LEU:HA	2:D:47:ILE:HB	2.00	0.42
2:B:208:TYR:OH	1:C:326:LYS:HG3	2.20	0.42
1:C:384:ILE:HG12	1:C:384:ILE:O	2.19	0.42
3:E:80:ARG:O	3:E:84:GLN:HG3	2.20	0.42
2:B:73:MET:HA	2:B:76:VAL:HG22	2.00	0.42
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.01	0.42
1:A:333:ALA:O	1:A:337:THR:HG23	2.19	0.42
2:D:6:HIS:HE1	2:D:136:THR:HG21	1.83	0.42
2:D:102:ALA:HB2	2:D:411:MET:SD	2.60	0.42
3:E:9:ILE:HB	3:E:10:GLU:OE1	2.19	0.42
2:B:257:MET:HE2	2:B:376:ILE:HG22	2.01	0.42
1:C:272:TYR:HB3	1:C:302:MET:HE1	2.01	0.42
2:B:27:GLU:OE2	2:B:234:SER:OG	2.33	0.42
3:E:77:GLU:O	3:E:81:GLU:HG3	2.20	0.42
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.01	0.42
1:A:334:THR:O	1:A:337:THR:OG1	2.27	0.42
2:D:145:SER:HG	2:D:188:SER:HG	1.66	0.42
2:D:343:GLU:CG	2:D:438:ALA:HB2	2.47	0.42
4:F:135:TYR:OH	4:F:165:GLU:HA	2.20	0.42
4:F:278:THR:OG1	4:F:281:ASN:HB2	2.20	0.42
2:D:6:HIS:CE1	2:D:136:THR:HG21	2.55	0.42
1:A:63:PRO:HG2	1:A:86:LEU:HD23	2.02	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.03	0.41
1:A:134:GLY:HA2	1:A:164:LYS:HB3	2.01	0.41
1:A:333:ALA:HB2	3:E:6:MET:SD	2.60	0.41
2:B:102:ALA:HB2	2:B:411:MET:SD	2.60	0.41
2:B:232:THR:HG21	2:B:300:MET:SD	2.60	0.41
1:A:100:ALA:HA	2:B:252:LYS:HG3	2.02	0.41
1:A:357:TYR:OH	3:E:18:GLN:HG3	2.20	0.41
2:B:181:GLU:CG	2:B:182:PRO:HD3	2.50	0.41
2:B:179:VAL:HG11	2:B:402:PHE:CZ	2.55	0.41
1:C:172:TYR:CE2	1:C:387:ALA:HB1	2.56	0.41
2:D:400:LYS:HB3	2:D:403:LEU:HD12	2.02	0.41
1:A:88:HIS:ND1	1:A:89:PRO:HD2	2.35	0.41
2:B:81:PHE:O	2:B:84:ILE:HG22	2.20	0.41
2:D:44:LEU:CD2	2:D:47:ILE:HD13	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:198:LYS:HE2	4:F:320:MET:CE	2.49	0.41
4:F:250:SER:OG	4:F:253:TYR:HB2	2.20	0.41
1:A:172:TYR:OH	1:A:391:LEU:HG	2.21	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.03	0.41
2:D:211:CYS:SG	2:D:225:LEU:HD23	2.60	0.41
2:B:179:VAL:O	1:C:349:THR:OG1	2.39	0.41
2:B:324:LYS:HE3	2:B:328:GLU:OE1	2.20	0.41
2:D:389:ILE:HG22	2:D:423:MET:HE1	2.03	0.41
1:A:72:PRO:HB2	1:A:76:ASP:OD2	2.20	0.41
1:A:132:LEU:O	1:A:164:LYS:NZ	2.42	0.41
1:A:284:GLU:O	1:A:285:GLN:C	2.63	0.41
1:C:205:ASP:OD1	1:C:205:ASP:C	2.64	0.41
2:D:310:TYR:O	2:D:342:VAL:HG22	2.21	0.41
4:F:163:SER:HA	4:F:233:PHE:CD1	2.56	0.41
2:D:246:LEU:HD21	2:D:350:LYS:HB3	2.02	0.41
3:E:75:LYS:CE	3:E:79:GLU:OE2	2.69	0.41
4:F:304:THR:HG1	4:F:310:GLN:CD	2.27	0.41
3:E:46:SER:HB3	3:E:49:GLU:HG3	2.02	0.40
2:B:285:THR:HG23	2:B:288:GLU:CD	2.46	0.40
1:C:234:ILE:HD11	1:C:302:MET:HE1	2.02	0.40
4:F:159:GLY:O	4:F:160:ILE:HG12	2.21	0.40
4:F:162:ILE:HD11	4:F:240:LEU:HD21	2.03	0.40
1:A:166:LYS:HE2	1:A:197:HIS:O	2.20	0.40
1:C:333:ALA:O	1:C:337:THR:HG23	2.21	0.40
1:A:194:THR:O	1:A:194:THR:HG22	2.21	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.22	0.40
3:E:95:LYS:O	3:E:96:MET:C	2.65	0.40
4:F:312:PHE:CG	4:F:354:ALA:HB1	2.57	0.40
1:C:139:HIS:O	1:C:170:SER:HA	2.21	0.40
1:C:154:MET:HE1	1:C:166:LYS:HB3	2.02	0.40
4:F:102:PRO:HB3	4:F:173:ILE:O	2.21	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)
1:A:245:ASP:OD1	1:C:57:GLY:H[2_565]	1.50	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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	440/450 (98%)	426 (97%)	14 (3%)	0	100	100
1	C	446/450 (99%)	431 (97%)	15 (3%)	0	100	100
2	B	418/445 (94%)	402 (96%)	16 (4%)	0	100	100
2	D	423/445 (95%)	409 (97%)	14 (3%)	0	100	100
3	E	121/143 (85%)	118 (98%)	3 (2%)	0	100	100
4	F	346/384 (90%)	329 (95%)	16 (5%)	1 (0%)	36	44
All	All	2194/2317 (95%)	2115 (96%)	78 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	88	SER

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	373/378 (99%)	373 (100%)	0	100	100
1	C	379/378 (100%)	378 (100%)	1 (0%)	86	91
2	B	365/383 (95%)	365 (100%)	0	100	100
2	D	369/383 (96%)	369 (100%)	0	100	100
3	E	112/127 (88%)	112 (100%)	0	100	100
4	F	314/342 (92%)	314 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1912/1991 (96%)	1911 (100%)	1 (0%)	88 93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	18	ASN
1	A	107	HIS
1	A	176	GLN
1	A	285	GLN
2	B	105	HIS
2	B	134	GLN
2	B	165	ASN
2	B	337	ASN
2	B	383	GLN
1	C	15	GLN
1	C	18	ASN
1	C	31	GLN
1	C	101	ASN
1	C	128	GLN
1	C	197	HIS
1	C	216	ASN
1	C	356	ASN
2	D	37	HIS
2	D	43	GLN
2	D	245	GLN
2	D	292	GLN
2	D	329	GLN
2	D	334	GLN
3	E	18	GLN
3	E	78	HIS
3	E	136	ASN
4	F	180	HIS
4	F	239	HIS
4	F	242	ASN
4	F	243	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 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 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	D	502	6	33,34,34	0.85	1 (3%)	50,54,54	1.63	11 (22%)
5	GTP	C	602	6	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
13	ACP	F	402	6	31,33,33	2.52	9 (29%)	47,52,52	2.51	16 (34%)
5	GTP	A	501	6	33,34,34	0.90	2 (6%)	50,54,54	1.58	10 (20%)
9	GDP	B	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	10 (22%)
11	G2X	C	601	-	30,33,33	2.22	13 (43%)	37,48,48	1.99	10 (27%)
8	GOL	A	504	-	5,5,5	0.82	0	5,5,5	0.82	0
11	G2X	C	605	-	30,33,33	2.40	16 (53%)	37,48,48	1.86	10 (27%)
10	MES	B	503	-	12,12,12	2.08	1 (8%)	15,16,16	1.66	3 (20%)
12	6K9	D	503	-	57,60,60	2.22	14 (24%)	61,92,92	1.74	15 (24%)
8	GOL	A	505	-	5,5,5	0.54	0	5,5,5	0.80	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	D	502	6	-	5/22/38/38	0/3/3/3
5	GTP	C	602	6	-	7/22/38/38	0/3/3/3
13	ACP	F	402	6	-	1/19/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
9	GDP	B	501	-	-	3/16/32/32	0/3/3/3
11	G2X	C	601	-	-	3/20/20/20	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
11	G2X	C	605	-	-	4/20/20/20	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
12	6K9	D	503	-	-	3/31/131/131	-
8	GOL	A	505	-	-	4/4/4/4	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	6K9	C18-C19	-7.35	1.40	1.51
12	D	503	6K9	C02-C01	-7.07	1.41	1.51
10	B	503	MES	C8-S	-6.86	1.68	1.77
13	F	402	ACP	PB-O3A	5.74	1.64	1.58
12	D	503	6K9	C39-C01	-5.54	1.43	1.51
13	F	402	ACP	PA-O3A	5.30	1.65	1.59
11	C	605	G2X	C09-N10	4.67	1.40	1.33
12	D	503	6K9	O11-C11	4.42	1.50	1.43
13	F	402	ACP	C6-N6	4.33	1.45	1.34
13	F	402	ACP	O4'-C1'	4.31	1.52	1.42
12	D	503	6K9	C38-C26	4.29	1.39	1.32
11	C	605	G2X	C11-N10	4.12	1.43	1.36
11	C	601	G2X	C09-N10	4.08	1.39	1.33
13	F	402	ACP	C5-N7	3.97	1.46	1.39
11	C	605	G2X	C25-C26	3.82	1.44	1.37
11	C	601	G2X	C11-N10	3.73	1.42	1.36
12	D	503	6K9	C20-C19	-3.47	1.43	1.51
11	C	605	G2X	C11-N12	3.45	1.38	1.32
12	D	503	6K9	C33-C32	3.39	1.58	1.52
11	C	601	G2X	C17-C15	3.34	1.43	1.37
11	C	605	G2X	C14-C15	3.32	1.44	1.39
11	C	605	G2X	C06-N08	3.24	1.36	1.30
11	C	601	G2X	C25-C26	3.22	1.43	1.37
11	C	601	G2X	C06-N08	3.21	1.36	1.30
11	C	601	G2X	C11-N12	3.15	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	402	ACP	C8-N9	-3.08	1.32	1.37
11	C	601	G2X	C04-N13	3.08	1.43	1.36
9	B	501	GDP	C5-C4	3.07	1.47	1.38
13	F	402	ACP	O4'-C4'	3.04	1.51	1.45
13	F	402	ACP	C5-C4	3.00	1.44	1.39
11	C	605	G2X	C17-C15	2.99	1.42	1.37
11	C	601	G2X	C06-CL7	2.95	1.78	1.72
12	D	503	6K9	C30-C29	2.94	1.59	1.53
12	D	503	6K9	C27-C26	-2.92	1.43	1.52
13	F	402	ACP	C2'-C3'	-2.89	1.45	1.53
12	D	503	6K9	C08-C07	-2.88	1.46	1.52
11	C	605	G2X	C06-CL7	2.88	1.78	1.72
11	C	605	G2X	C09-N08	2.81	1.40	1.34
11	C	605	G2X	C14-C26	2.74	1.43	1.39
11	C	605	G2X	N13-N12	2.71	1.42	1.37
11	C	601	G2X	N13-N12	2.71	1.42	1.37
11	C	601	G2X	C09-N08	2.71	1.40	1.34
11	C	605	G2X	C04-N13	2.67	1.42	1.36
12	D	503	6K9	C33-C34	2.64	1.58	1.52
9	B	501	GDP	C6-N1	-2.54	1.34	1.38
11	C	601	G2X	C14-C15	2.53	1.43	1.39
11	C	601	G2X	C09-N13	2.49	1.41	1.38
11	C	605	G2X	C04-N03	2.48	1.45	1.38
12	D	503	6K9	C24-C25	2.42	1.57	1.53
12	D	503	6K9	O07-C03	2.36	1.48	1.44
11	C	605	G2X	C14-C05	2.21	1.54	1.50
5	A	501	GTP	PA-O3A	2.21	1.61	1.59
11	C	605	G2X	C21-C22	2.17	1.60	1.51
5	D	502	GTP	C2-N3	2.13	1.38	1.33
5	A	501	GTP	C2-N3	2.12	1.38	1.33
12	D	503	6K9	C05-C04	2.10	1.58	1.52
11	C	601	G2X	C21-C22	2.09	1.59	1.51
11	C	605	G2X	C09-N13	2.05	1.40	1.38
9	B	501	GDP	C5-N7	-2.01	1.35	1.39
5	C	602	GTP	C2-N3	2.00	1.38	1.33

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	402	ACP	C4-N9-C8	9.16	115.36	105.74
11	C	601	G2X	C11-N12-N13	6.24	105.95	100.86
9	B	501	GDP	C5-C4-N3	-5.98	118.86	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	605	G2X	C11-N12-N13	5.89	105.66	100.86
13	F	402	ACP	N3-C4-N9	5.11	135.85	127.17
13	F	402	ACP	C5-C4-N3	-4.85	120.04	126.72
5	A	501	GTP	C5-C4-N3	-4.79	120.77	128.39
5	C	602	GTP	C5-C4-N3	-4.71	120.89	128.39
5	D	502	GTP	C5-C4-N3	-4.67	120.96	128.39
13	F	402	ACP	C4-C5-N7	-4.67	105.25	110.58
13	F	402	ACP	N3-C2-N1	-4.62	121.59	128.58
5	D	502	GTP	C2-N3-C4	4.57	120.17	112.30
5	A	501	GTP	C2-N3-C4	4.56	120.16	112.30
5	C	602	GTP	C2-N3-C4	4.56	120.15	112.30
9	B	501	GDP	C2-N3-C4	4.54	120.13	112.30
9	B	501	GDP	N9-C4-N3	4.40	134.76	125.95
13	F	402	ACP	N9-C8-N7	-4.22	107.95	113.94
10	B	503	MES	C5-N4-C3	4.06	117.59	108.84
12	D	503	6K9	C16-C15-C14	-3.94	108.98	114.43
11	C	601	G2X	C11-N10-C09	3.63	104.78	102.36
11	C	605	G2X	C11-N10-C09	3.57	104.74	102.36
12	D	503	6K9	O27-C23-C24	-3.54	104.74	110.14
11	C	601	G2X	C04-N13-N12	3.46	130.76	124.82
12	D	503	6K9	C33-C34-C35	3.45	114.86	111.87
12	D	503	6K9	C10-O10-C06	3.45	121.70	113.83
9	B	501	GDP	C6-C5-N7	3.43	136.52	130.29
11	C	601	G2X	C09-N13-N12	-3.42	107.81	110.11
12	D	503	6K9	C18-C19-C36	-3.41	120.16	126.31
13	F	402	ACP	C3'-C2'-C1'	3.38	107.85	101.46
11	C	605	G2X	N12-C11-N10	-3.33	111.50	116.78
12	D	503	6K9	C04-C03-C02	-3.30	106.65	113.11
11	C	601	G2X	N12-C11-N10	-3.23	111.66	116.78
13	F	402	ACP	C2-N3-C4	3.23	119.72	111.83
11	C	601	G2X	N13-C09-N08	-3.22	119.81	122.61
11	C	605	G2X	N13-C09-N08	-3.12	119.89	122.61
13	F	402	ACP	PB-O3A-PA	-3.07	122.34	132.37
12	D	503	6K9	C23-O27-C27	3.07	117.26	112.39
11	C	605	G2X	C25-C26-C14	-3.06	121.03	123.96
5	A	501	GTP	N9-C4-N3	3.05	132.06	125.95
5	C	602	GTP	N9-C8-N7	-3.02	107.79	113.40
5	D	502	GTP	N9-C8-N7	-3.01	107.81	113.40
5	C	602	GTP	N9-C4-N3	2.99	131.92	125.95
5	A	501	GTP	N9-C8-N7	-2.85	108.12	113.40
5	D	502	GTP	N9-C4-N3	2.84	131.62	125.95
11	C	601	G2X	C09-N13-C04	-2.80	121.42	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	GTP	C2-N1-C6	-2.80	120.04	125.11
5	D	502	GTP	C8-N7-C5	2.79	109.23	104.26
9	B	501	GDP	C4-C5-N7	-2.78	106.26	110.67
5	C	602	GTP	C2-N1-C6	-2.78	120.07	125.11
13	F	402	ACP	C2-N1-C6	2.76	123.27	118.73
5	A	501	GTP	C2-N1-C6	-2.76	120.11	125.11
5	C	602	GTP	C8-N7-C5	2.73	109.13	104.26
11	C	601	G2X	C17-C15-C14	-2.73	121.35	123.96
13	F	402	ACP	C6-C5-N7	2.71	137.32	132.09
13	F	402	ACP	C2'-C3'-C4'	2.68	107.79	102.61
5	A	501	GTP	C8-N7-C5	2.66	109.00	104.26
12	D	503	6K9	C37-C25-C24	-2.60	107.33	111.51
11	C	601	G2X	C25-C26-C14	-2.58	121.49	123.96
5	C	602	GTP	C5-C6-N1	2.57	119.80	113.25
11	C	605	G2X	C04-N13-N12	2.53	129.16	124.82
10	B	503	MES	C7-N4-C5	2.51	117.94	111.24
13	F	402	ACP	O2A-PA-O1A	-2.51	100.79	112.44
5	D	502	GTP	C5-C6-N1	2.50	119.62	113.25
12	D	503	6K9	O12-C12-C11	-2.48	99.68	104.92
13	F	402	ACP	C4-N9-C1'	-2.47	120.84	126.63
13	F	402	ACP	C5-N7-C8	2.47	107.33	103.45
12	D	503	6K9	O20-C17-C16	2.47	112.76	109.17
11	C	601	G2X	C25-C18-C17	-2.43	117.30	120.98
5	C	602	GTP	O6-C6-C5	-2.42	120.16	126.53
5	A	501	GTP	C5-C6-N1	2.39	119.33	113.25
12	D	503	6K9	C10-C11-C12	2.32	109.16	103.78
5	A	501	GTP	O2G-PG-O3B	2.30	112.33	104.64
11	C	605	G2X	C25-C18-C17	-2.27	117.53	120.98
5	A	501	GTP	O6-C6-C5	-2.27	120.54	126.53
13	F	402	ACP	C4'-O4'-C1'	-2.27	104.46	109.47
12	D	503	6K9	O07-C03-C04	2.24	112.27	109.91
11	C	605	G2X	C09-N13-N12	-2.24	108.61	110.11
12	D	503	6K9	C32-C33-C34	-2.23	109.52	114.49
12	D	503	6K9	C40-O31-C31	-2.22	108.79	114.47
5	D	502	GTP	O6-C6-C5	-2.19	120.75	126.53
5	D	502	GTP	C2'-C3'-C4'	2.13	106.73	102.61
11	C	605	G2X	C18-C25-C26	2.11	122.09	118.07
5	D	502	GTP	O2B-PB-O3B	2.11	112.98	107.27
9	B	501	GDP	C8-N7-C5	2.08	107.97	104.26
9	B	501	GDP	C2'-C3'-C4'	2.06	106.60	102.61
12	D	503	6K9	C05-C06-C07	-2.06	106.81	110.87
9	B	501	GDP	C2-N1-C6	-2.06	121.38	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	GTP	C4-C5-N7	-2.05	107.42	110.67
5	A	501	GTP	O2A-PA-O3A	2.04	112.79	107.27
9	B	501	GDP	O6-C6-C5	-2.02	121.19	126.53
10	B	503	MES	O3S-S-C8	2.01	109.93	106.00
9	B	501	GDP	C5-C6-N1	2.00	118.35	113.25
11	C	605	G2X	N10-C09-N08	2.00	130.62	127.95

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
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	602	GTP	PB-O3B-PG-O2G
5	C	602	GTP	C5'-O5'-PA-O3A
5	C	602	GTP	C5'-O5'-PA-O1A
5	C	602	GTP	C5'-O5'-PA-O2A
5	D	502	GTP	C5'-O5'-PA-O3A
5	D	502	GTP	C5'-O5'-PA-O1A
5	D	502	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
8	A	505	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
11	C	601	G2X	C21-C22-N23-C24
11	C	605	G2X	C02-C01-C28-F29
11	C	605	G2X	C02-C01-C28-F30
11	C	605	G2X	C02-C01-C28-F31
12	D	503	6K9	C33-C34-C35-N35
12	D	503	6K9	O34-C34-C35-N35
13	F	402	ACP	C5'-O5'-PA-O1A
8	A	505	GOL	O1-C1-C2-O2
8	A	505	GOL	C1-C2-C3-O3
8	A	504	GOL	O1-C1-C2-O2
8	A	505	GOL	O2-C2-C3-O3
5	D	502	GTP	PB-O3B-PG-O1G
5	D	502	GTP	PB-O3B-PG-O2G
11	C	601	G2X	O19-C20-C21-C22
5	A	501	GTP	PB-O3A-PA-O2A

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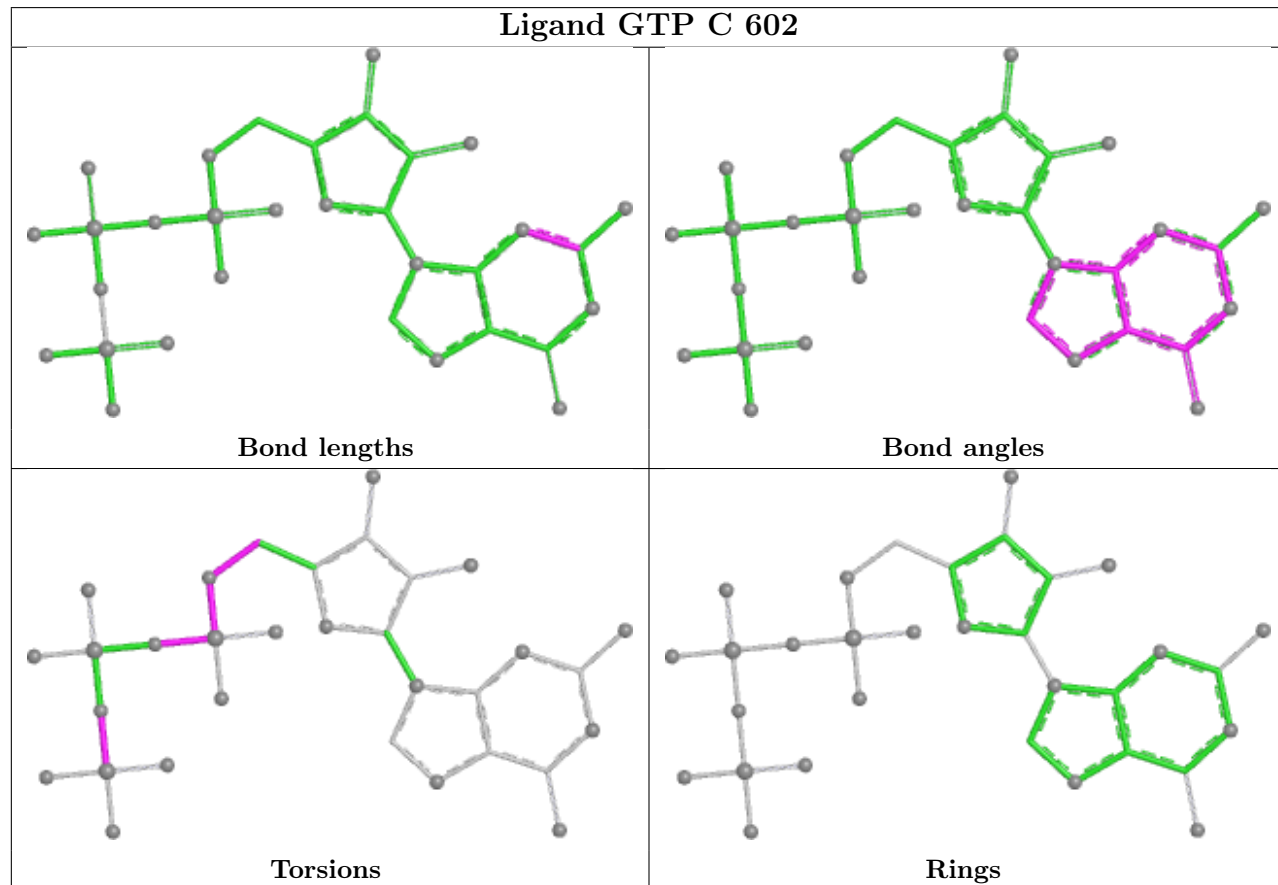
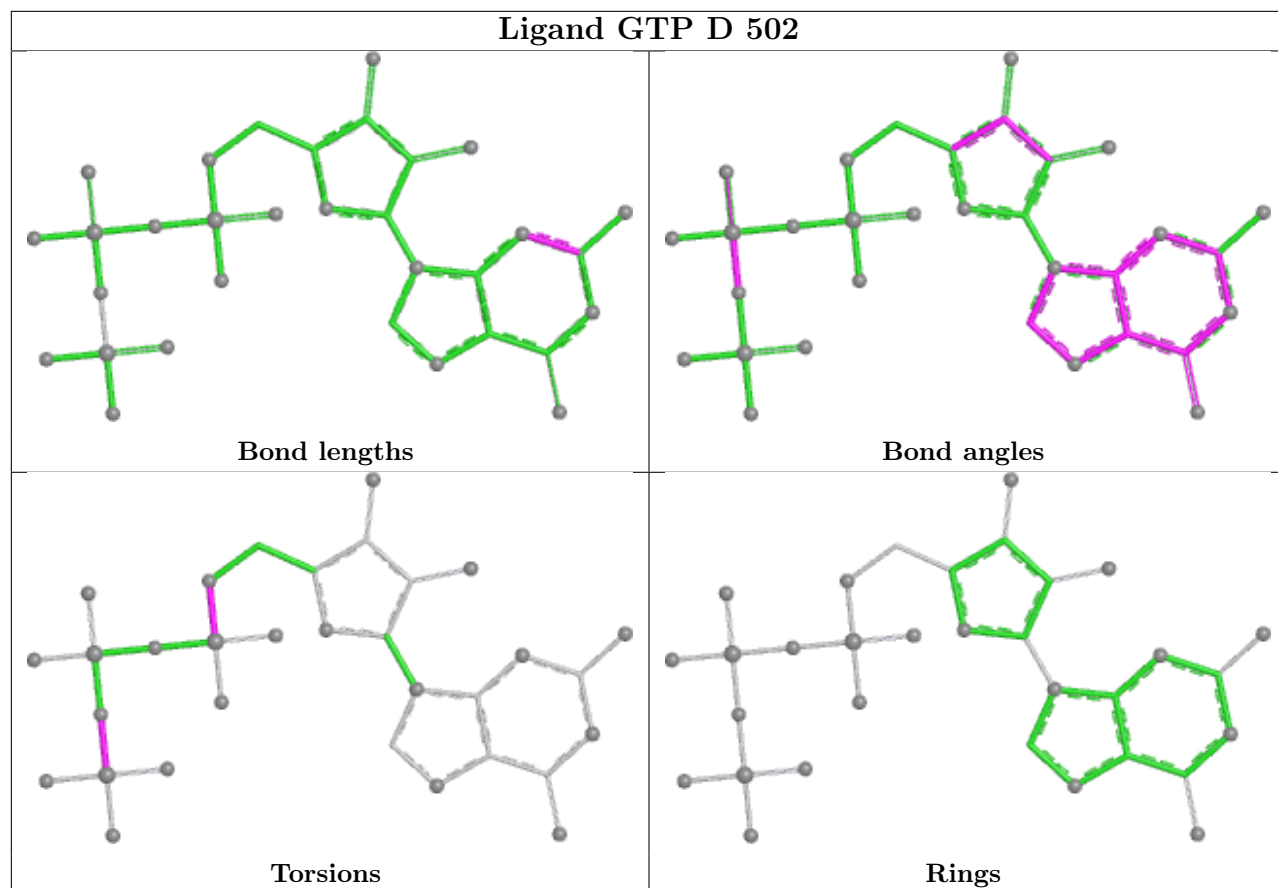
Mol	Chain	Res	Type	Atoms
5	C	602	GTP	PB-O3A-PA-O1A
11	C	601	G2X	C02-C01-N03-C04
11	C	605	G2X	C02-C01-N03-C04
5	A	501	GTP	PB-O3B-PG-O3G
5	C	602	GTP	PB-O3A-PA-O2A
12	D	503	6K9	C31-C32-C33-C34
5	C	602	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

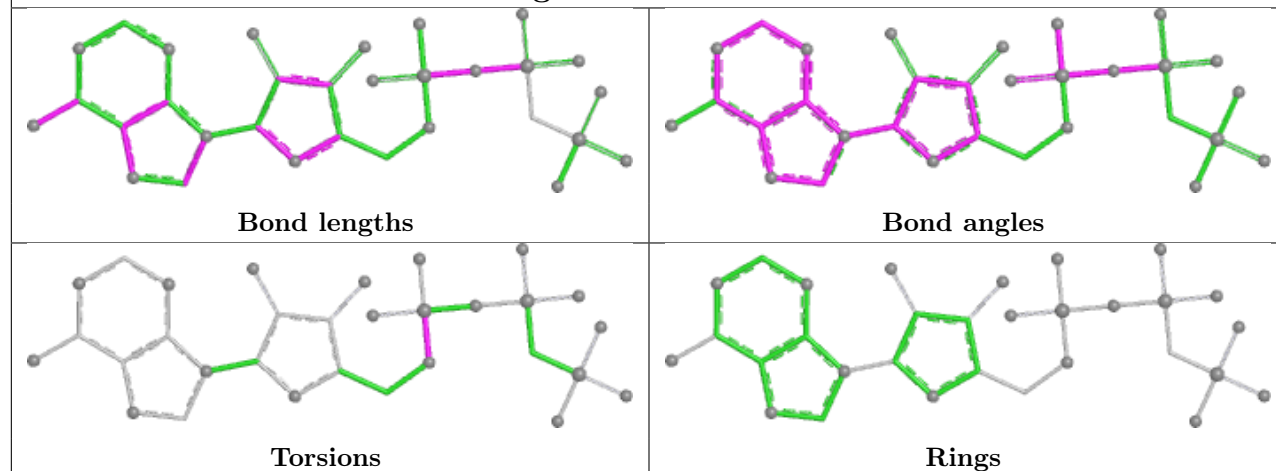
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	402	ACP	1	0
9	B	501	GDP	2	0
8	A	504	GOL	1	0
12	D	503	6K9	2	0

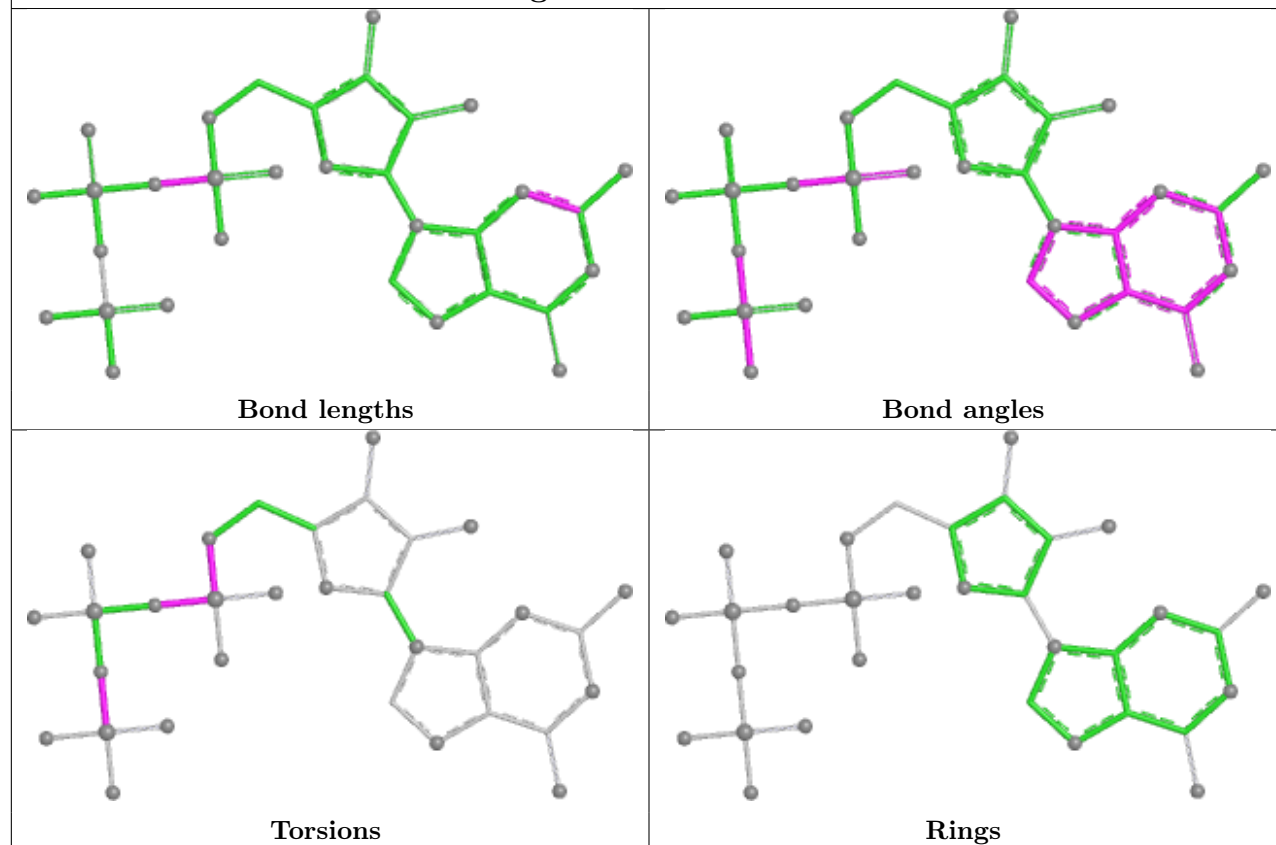
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

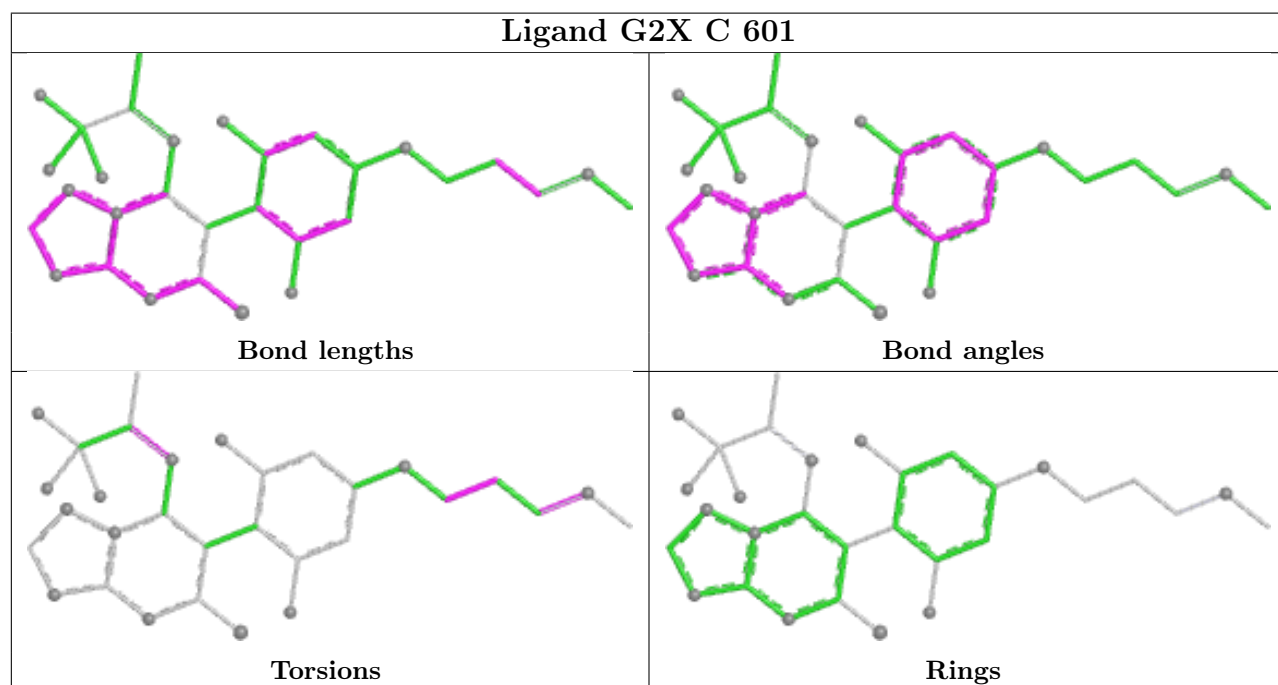
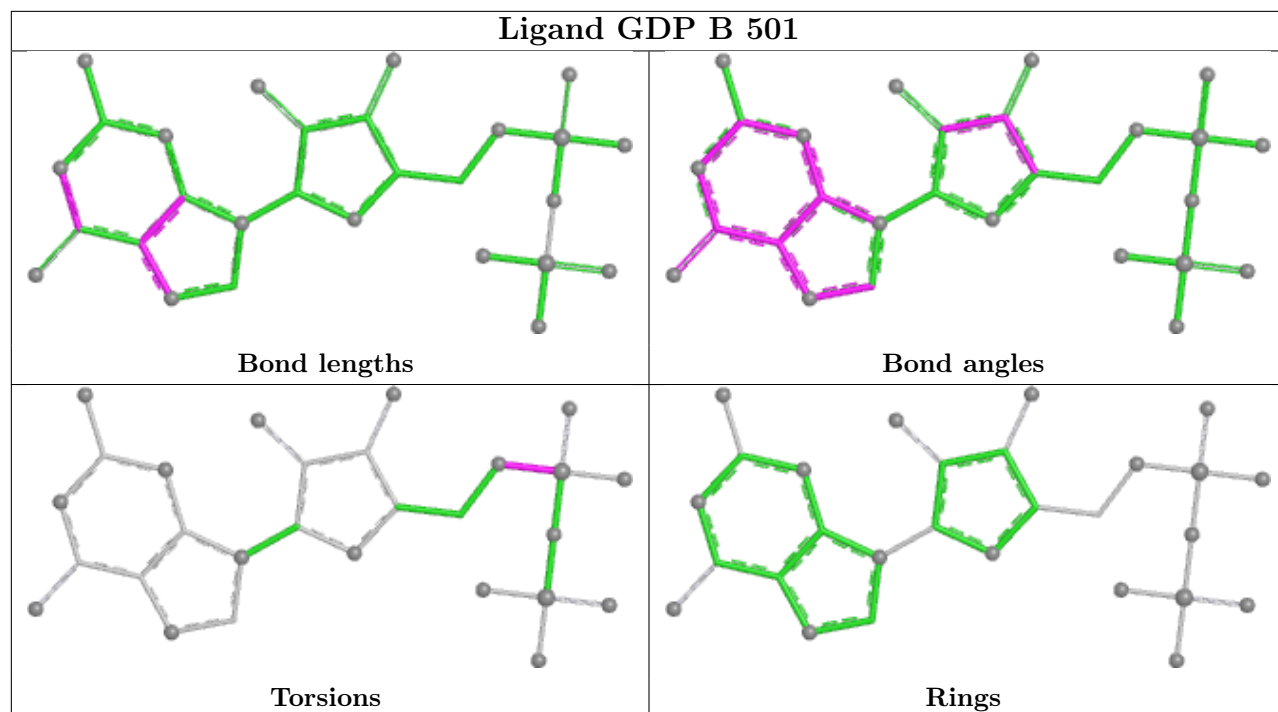


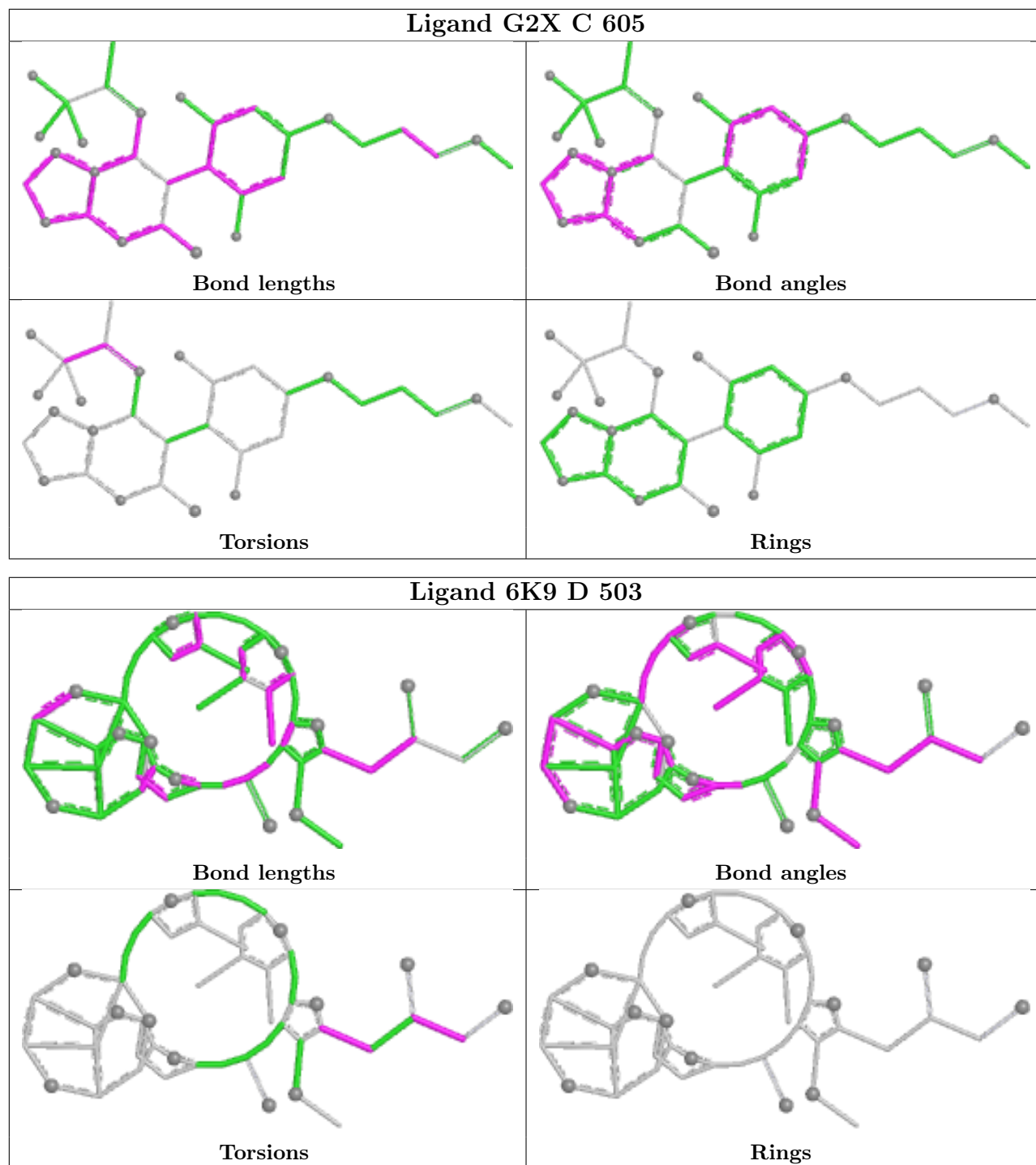
Ligand ACP F 402



Ligand GTP A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	438/450 (97%)	0.70	23 (5%)	32 29	31, 66, 86, 117	4 (0%)
1	C	440/450 (97%)	0.38	11 (2%)	58 59	26, 54, 71, 97	7 (1%)
2	B	418/445 (93%)	0.72	35 (8%)	17 14	32, 62, 84, 99	4 (0%)
2	D	426/445 (95%)	1.07	62 (14%)	6 4	39, 71, 90, 110	1 (0%)
3	E	123/143 (86%)	1.26	24 (19%)	3 2	30, 74, 99, 104	2 (1%)
4	F	351/384 (91%)	1.48	89 (25%)	1 1	34, 81, 120, 126	1 (0%)
All	All	2196/2317 (94%)	0.86	244 (11%)	10 8	26, 66, 99, 126	19 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	6.9
4	F	103	THR	6.5
1	A	283	HIS	5.6
1	A	346	TRP	5.5
1	C	151[A]	SER	5.3
4	F	155	ALA	5.1
4	F	233	PHE	4.9
4	F	380	HIS	4.9
4	F	172	PHE	4.8
2	B	1	MET	4.7
3	E	71[A]	HIS	4.7
3	E	143	ALA	4.6
2	D	1	MET	4.6
1	C	1	MET	4.4
4	F	249	TYR	4.4
1	A	262	TYR	4.4
4	F	166	ALA	4.3
1	C	340	SER	4.3
2	D	73	MET	4.2

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Mol	Chain	Res	Type	RSRZ
4	F	238	CYS	4.1
4	F	159	GLY	4.1
2	D	247	ASN	4.1
1	A	281	ALA	4.0
2	D	278	SER	4.0
2	D	402	PHE	4.0
3	E	6	MET	4.0
1	C	88[A]	HIS	3.9
1	A	282	TYR	3.9
2	B	438	ALA	3.9
4	F	149	ALA	3.9
4	F	239	HIS	3.9
2	D	284	LEU	3.9
4	F	100	ILE	3.8
1	C	440	VAL	3.7
3	E	12[A]	ASN	3.7
2	B	175	VAL	3.7
3	E	28	SER	3.7
2	D	92	PHE	3.6
3	E	115	HIS	3.6
4	F	125	THR	3.6
4	F	173	ILE	3.6
3	E	120	LEU	3.5
2	D	244	GLY	3.5
2	B	369	LEU	3.4
1	A	285	GLN	3.4
4	F	372	THR	3.4
2	B	414	MET	3.4
4	F	296[A]	MET	3.3
2	D	245	GLN	3.3
2	D	55	THR	3.3
4	F	146	VAL	3.3
1	C	283	HIS	3.3
3	E	45	PRO	3.3
3	E	123	LEU	3.3
4	F	363	ASP	3.2
4	F	245	ILE	3.2
4	F	148	ILE	3.2
4	F	227	PRO	3.1
2	D	331	LEU	3.1
2	B	246	LEU	3.1
2	D	2	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	119	MET	3.1
2	B	39	ASP	3.1
2	D	332	ASN	3.1
4	F	228	TYR	3.1
3	E	124	GLN	3.1
4	F	150	LYS	3.1
2	B	272	PRO	3.1
2	D	151	LEU	3.1
2	B	330	MET	3.0
4	F	132	LEU	3.0
2	D	439	ASP	3.0
4	F	163	SER	3.0
2	B	245	GLN	3.0
4	F	335	ALA	3.0
4	F	73	ARG	3.0
2	D	239	CYS	3.0
4	F	154	GLY	3.0
3	E	117	ALA	3.0
2	D	161	ASP	3.0
3	E	116	LEU	2.9
4	F	151	SER	2.9
4	F	334	GLY	2.9
4	F	70	LYS	2.9
3	E	53	LYS	2.9
2	B	290	THR	2.9
2	D	438	ALA	2.8
4	F	134	ALA	2.8
4	F	131	PHE	2.8
4	F	256	TYR	2.8
2	D	128	ASP	2.8
2	D	165	ASN	2.8
4	F	162	ILE	2.8
4	F	182	ILE	2.8
4	F	224	SER	2.8
2	B	55	THR	2.8
2	B	285	THR	2.8
2	B	411	MET	2.8
2	D	170	MET	2.8
4	F	178	GLN	2.8
2	D	371	MET	2.8
3	E	8	VAL	2.7
4	F	137	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	285	GLN	2.7
1	C	372	GLN	2.7
2	D	56	GLY	2.7
2	D	42	LEU	2.7
1	A	278	ALA	2.7
4	F	225	SER	2.7
2	B	323	MET	2.6
2	D	246	LEU	2.6
4	F	240	LEU	2.6
2	D	323	MET	2.6
1	C	284	GLU	2.6
4	F	153	ALA	2.6
2	B	216	LYS	2.6
2	D	276	ARG	2.6
3	E	139	LEU	2.6
4	F	156	LYS	2.6
2	D	71	GLY	2.6
2	D	289	LEU	2.6
2	B	73	MET	2.5
1	A	284	GLU	2.5
2	D	91	VAL	2.5
2	B	37	HIS	2.5
2	D	127	CYS	2.5
3	E	114	ALA	2.5
4	F	253	TYR	2.5
2	B	244	GLY	2.5
4	F	194	PRO	2.5
4	F	199	PHE	2.5
4	F	246	GLN	2.5
1	C	356	ASN	2.5
2	D	321	MET	2.5
2	D	277	GLY	2.5
4	F	254	GLY	2.5
4	F	127	GLU	2.5
2	D	250	LEU	2.5
4	F	186	LEU	2.5
2	D	370	LYS	2.5
4	F	161	LEU	2.5
4	F	236	LYS	2.5
2	B	92	PHE	2.5
2	D	405	TRP	2.5
2	D	401	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	115	ILE	2.4
2	B	203	ASP	2.4
4	F	160	ILE	2.4
2	D	194	GLU	2.4
4	F	200	ASP	2.4
4	F	285	LEU	2.4
4	F	343	TYR	2.4
4	F	333	ASN	2.4
4	F	147	TRP	2.4
4	F	231	ALA	2.4
2	D	274	THR	2.4
2	B	78	SER	2.4
2	D	330	MET	2.4
2	D	175	VAL	2.4
2	B	57	ASN	2.4
3	E	7	GLU	2.4
4	F	152	SER	2.3
2	D	222	TYR	2.3
2	D	57	ASN	2.3
2	D	419	ALA	2.3
4	F	282	SER	2.3
1	A	276	ILE	2.3
4	F	20	LEU	2.3
2	B	370	LYS	2.3
4	F	130	VAL	2.3
2	D	54	ALA	2.3
3	E	27	PRO	2.3
4	F	241	THR	2.3
3	E	51	GLN	2.3
4	F	101	TYR	2.3
2	D	358	PRO	2.3
4	F	252	ASN	2.3
4	F	177	GLY	2.3
2	B	293[A]	MET	2.3
3	E	44	ASP	2.3
4	F	181	VAL	2.3
2	D	173	PRO	2.2
4	F	176	GLN	2.2
4	F	277	THR	2.2
1	A	117	LEU	2.2
1	A	425	MET	2.2
4	F	171	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	165	GLU	2.2
1	A	182	VAL	2.2
4	F	229	ASN	2.2
2	D	37	HIS	2.2
4	F	32	LYS	2.2
4	F	98	TYR	2.2
2	D	319	GLY	2.2
2	D	70	PRO	2.2
2	D	80	PRO	2.2
4	F	263	PHE	2.2
2	D	238	THR	2.2
2	D	243	PRO	2.2
4	F	170	LEU	2.1
1	A	279	GLU	2.1
1	A	232	SER	2.1
1	A	88	HIS	2.1
1	A	18	ASN	2.1
4	F	30	LEU	2.1
2	B	316	ILE	2.1
1	C	282	TYR	2.1
2	B	251[A]	ARG	2.1
4	F	135	TYR	2.1
4	F	12	SER	2.1
2	B	170	MET	2.1
2	B	321	MET	2.1
2	B	76	VAL	2.1
2	B	117	LEU	2.1
2	D	217	LEU	2.1
4	F	221	LEU	2.1
1	A	94	THR	2.1
1	A	340	SER	2.1
1	A	438	ASP	2.1
2	B	435	ASP	2.1
4	F	164	SER	2.1
4	F	102	PRO	2.1
2	D	267	MET	2.1
2	D	333	VAL	2.1
3	E	118	ALA	2.1
2	B	218	THR	2.1
2	D	72	THR	2.1
2	B	124	SER	2.1
2	D	115	SER	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	234	GLN	2.0
1	A	96	LYS	2.0
2	D	107	THR	2.0
2	D	178	THR	2.0
2	D	59	TYR	2.0
2	D	399	ARG	2.0
4	F	255	ARG	2.0
1	A	338	LYS	2.0
3	E	128	LYS	2.0
4	F	157	GLY	2.0
1	A	337	THR	2.0
2	B	72	THR	2.0
3	E	96	MET	2.0
4	F	33	ASP	2.0
4	F	185	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	505	1/1	0.65	0.20	94,94,94,94	0
8	GOL	A	504	6/6	0.77	0.17	65,78,85,90	0
12	6K9	D	503	52/52	0.82	0.23	63,84,94,96	0
7	CA	B	504	1/1	0.85	0.13	101,101,101,101	0
6	MG	F	401	1/1	0.85	0.16	79,79,79,79	0
11	G2X	C	605	31/31	0.86	0.15	43,58,74,77	0
7	CA	A	506	1/1	0.87	0.17	96,96,96,96	0
6	MG	D	501	1/1	0.88	0.25	63,63,63,63	0

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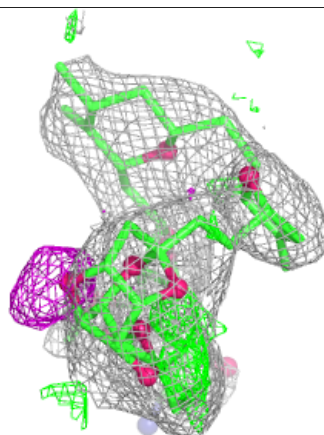
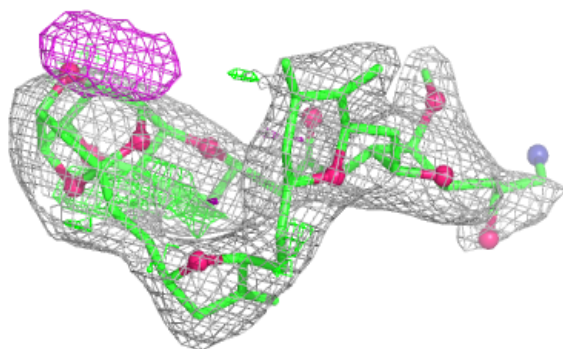
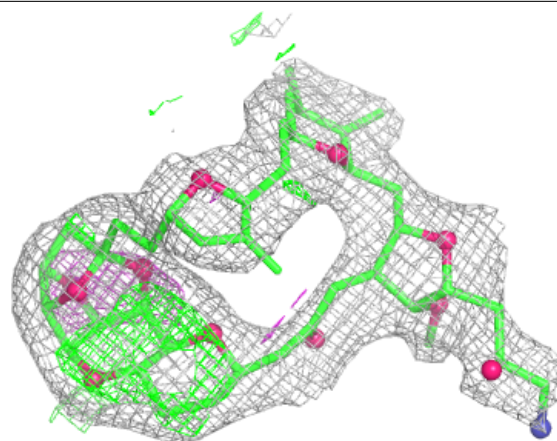
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	A	505	6/6	0.88	0.14	77,92,101,110	0
13	ACP	F	402	31/31	0.88	0.13	80,88,105,112	0
11	G2X	C	601	31/31	0.89	0.14	51,58,76,80	0
5	GTP	D	502	32/32	0.92	0.12	55,64,81,87	0
6	MG	B	502	1/1	0.94	0.12	65,65,65,65	0
7	CA	C	604	1/1	0.94	0.28	75,75,75,75	0
5	GTP	C	602	32/32	0.95	0.09	31,49,64,78	0
5	GTP	A	501	32/32	0.96	0.08	43,51,67,82	0
7	CA	A	503	1/1	0.96	0.07	82,82,82,82	0
9	GDP	B	501	28/28	0.96	0.10	31,55,77,92	0
10	MES	B	503	12/12	0.96	0.09	48,59,71,73	0
6	MG	C	603	1/1	0.98	0.05	40,40,40,40	0
6	MG	A	502	1/1	0.99	0.05	47,47,47,47	0
7	CA	C	606	1/1	0.99	0.03	47,47,47,47	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.

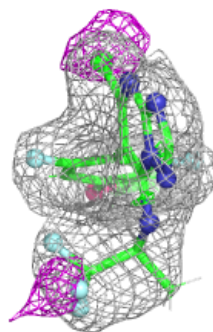
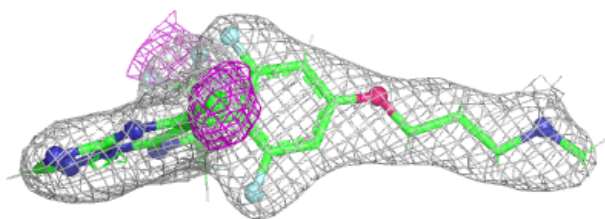
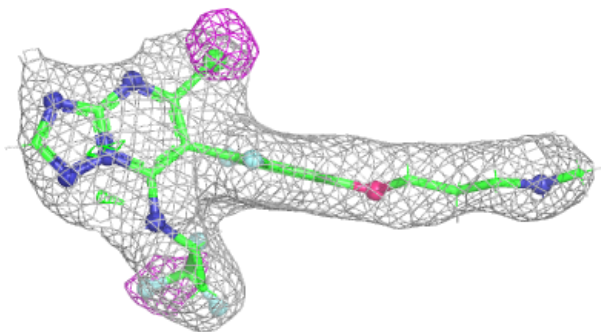
Electron density around 6K9 D 503:

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

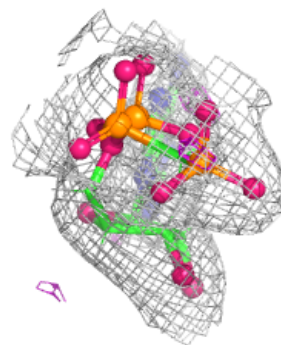
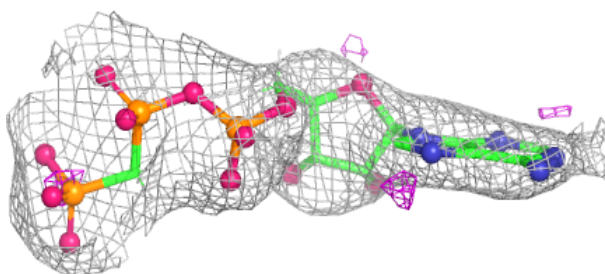
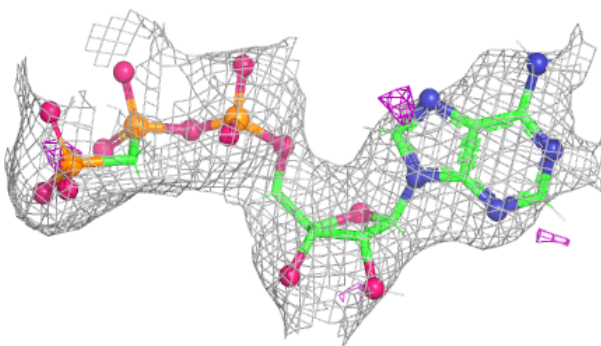


Electron density around G2X C 605:

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

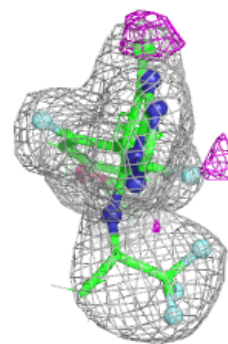
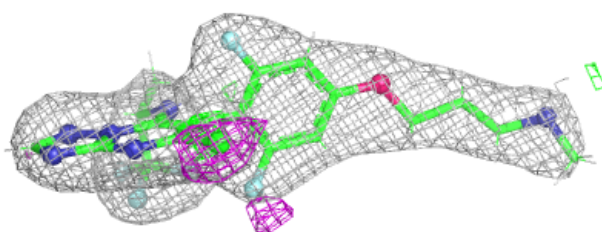
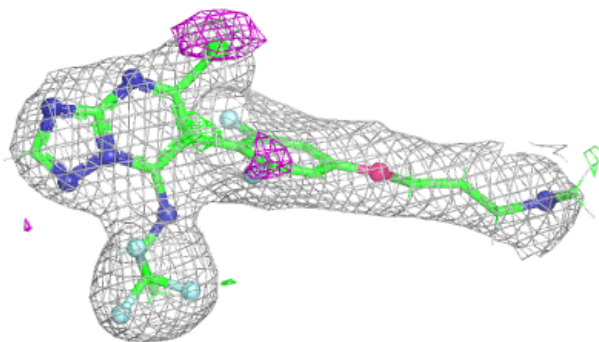
**Electron density around ACP F 402:**

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

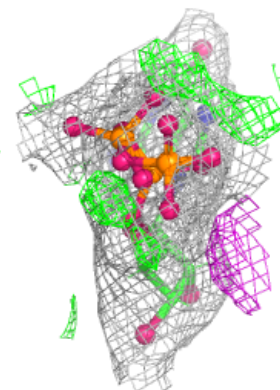
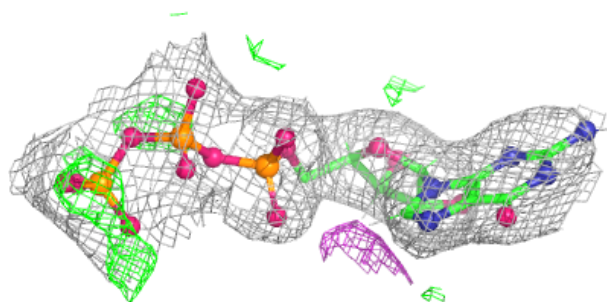
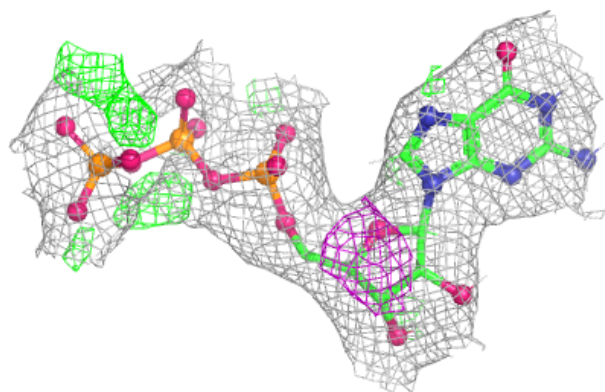


Electron density around G2X C 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

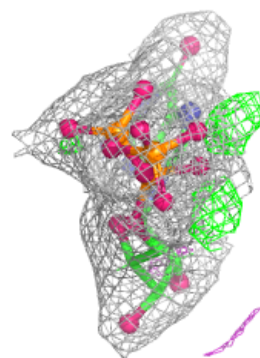
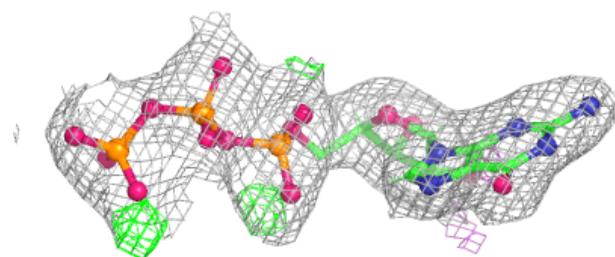
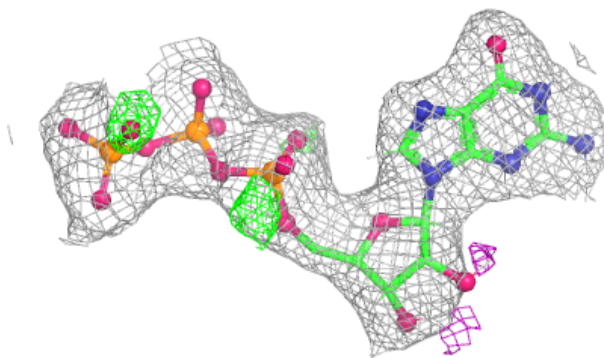
**Electron density around GTP D 502:**

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

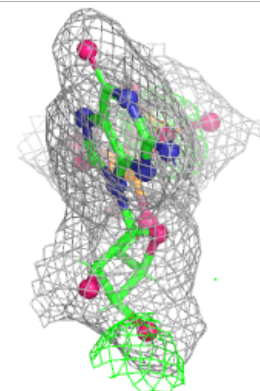
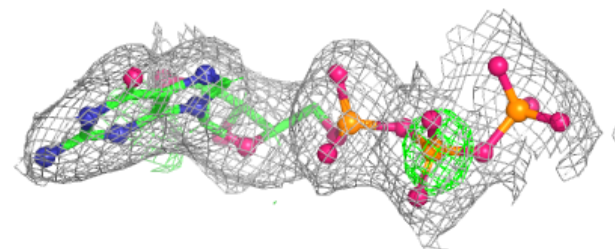
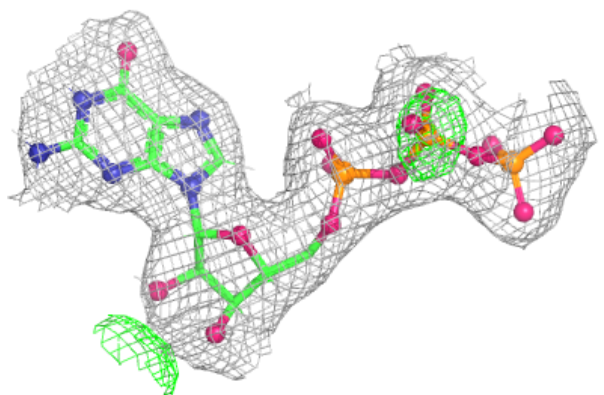


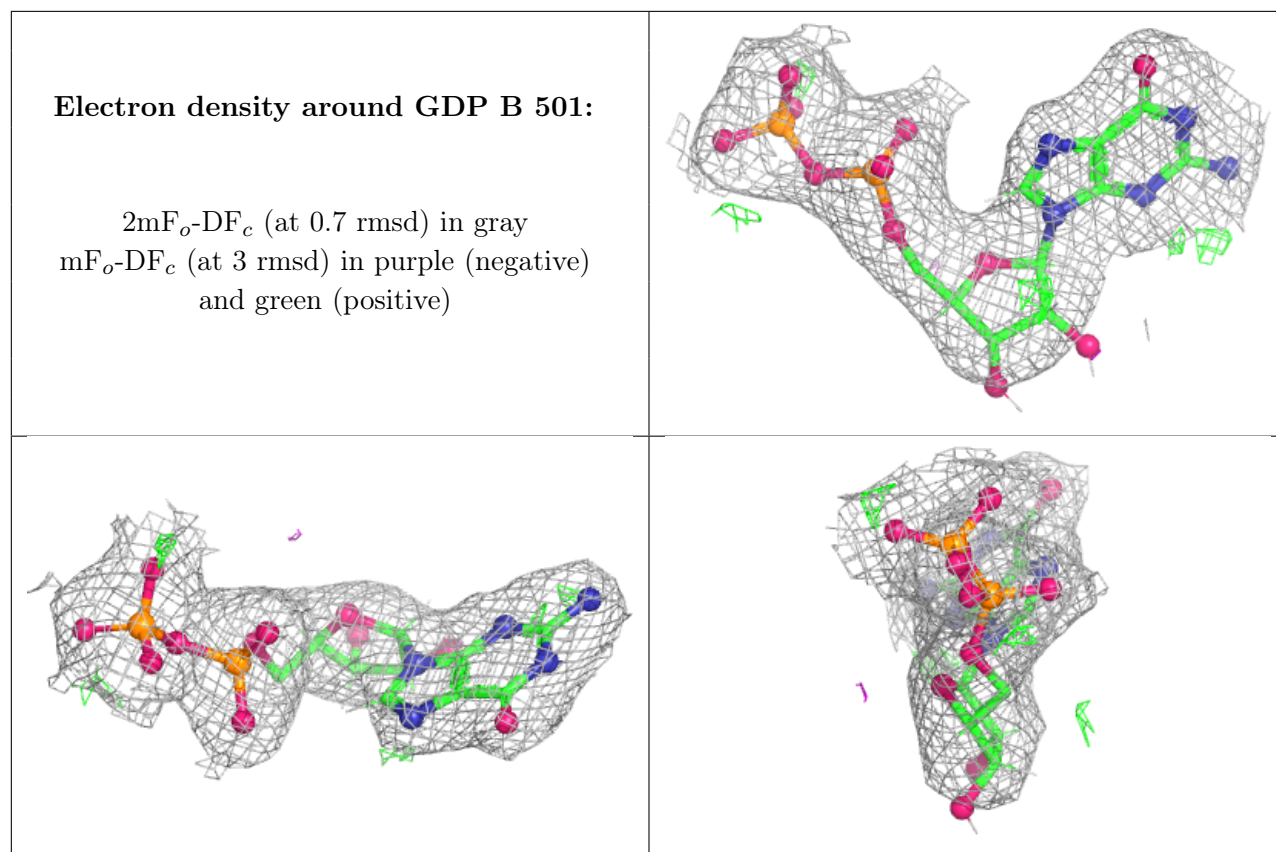
Electron density around GTP C 602:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.