



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:53 PM UTC

PDB ID : 5GON / pdb_00005gon
Title : Structures of a beta-lactam bridged analogue in complex with tubulin
Authors : Zhou, L.; Liu, Y.; Cheng, L.; Wang, Y.
Deposited on : 2016-07-28
Resolution : 2.48 Å(reported)

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

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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

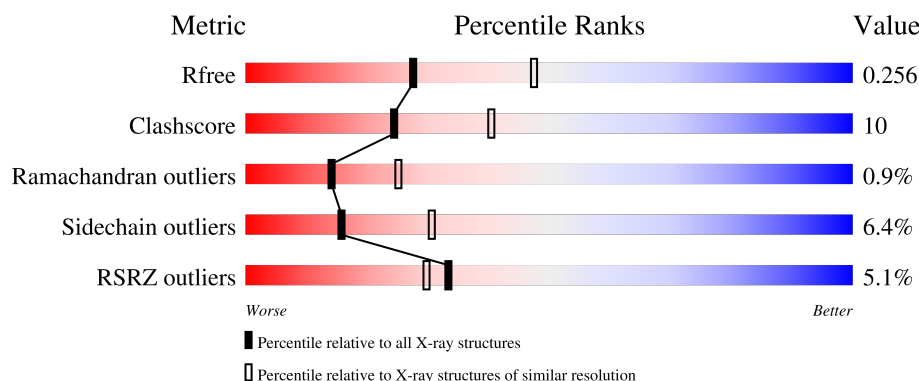
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	440	81% 17% .
1	C	440	85% 14% .
2	B	431	3% 75% 21% ..
2	D	431	4% 67% 28% ..
3	E	136	4% 69% 18% .. 11%

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Mol	Chain	Length	Quality of chain
4	F	378	

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
7	GOL	B	505	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 17847 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	13	0
			3488	2217	585	661	25			
1	C	440	Total	C	N	O	S	0	11	0
			3489	2209	588	668	24			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	1	11	0
			3374	2126	568	653	27			
2	D	421	Total	C	N	O	S	0	4	0
			3326	2094	562	642	28			

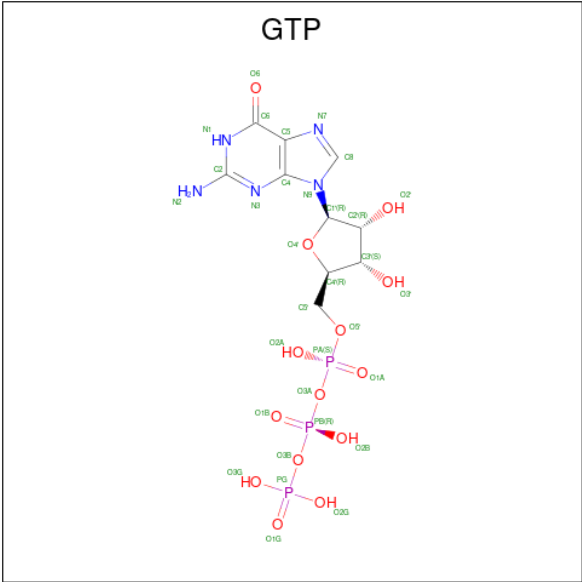
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	3	0
			1016	628	183	199	6			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	319	Total	C	N	O	S	0	5	0
			2633	1706	436	477	14			

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



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		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

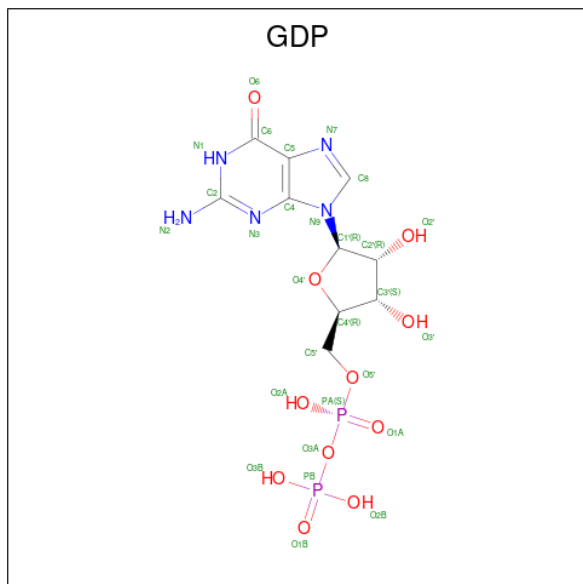


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

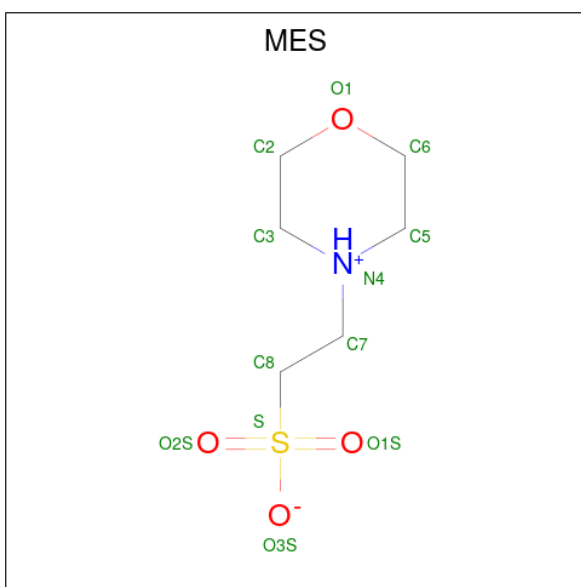
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

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



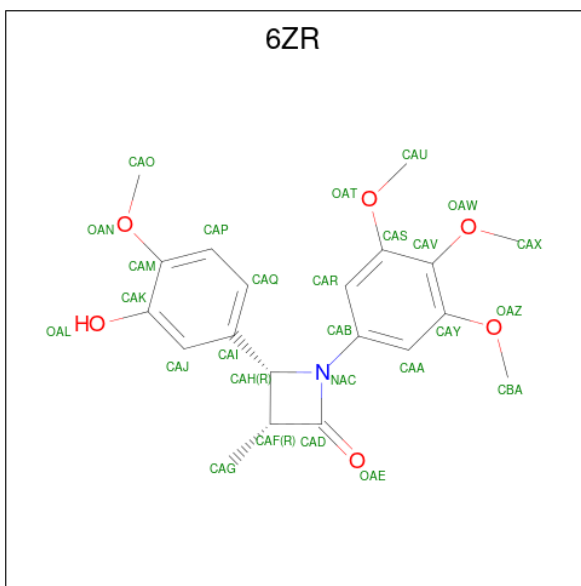
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



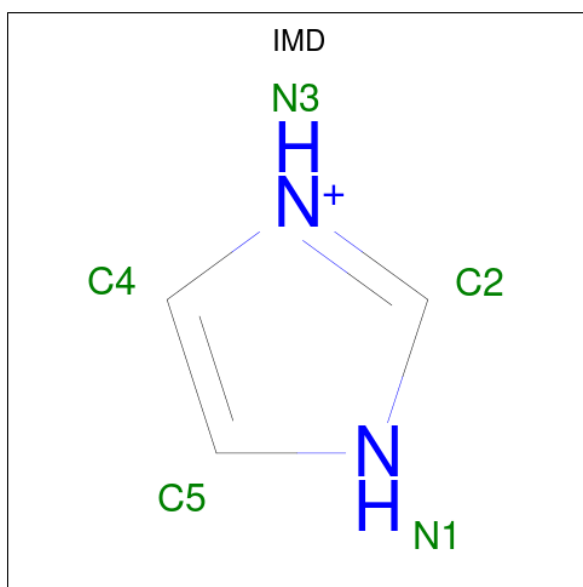
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3R,4R)-4-(4-methoxy-3-oxidanyl-phenyl)-3-methyl-1-(3,4,5-trimethoxyphenyl)azetidin-2-one (CCD ID: 6ZR) (formula: $C_{20}H_{23}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	20	1	6		

- Molecule 12 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	N	0	0
			5	3	2		
12	C	1	Total	C	N	0	0
			5	3	2		
12	C	1	Total	C	N	0	0
			5	3	2		

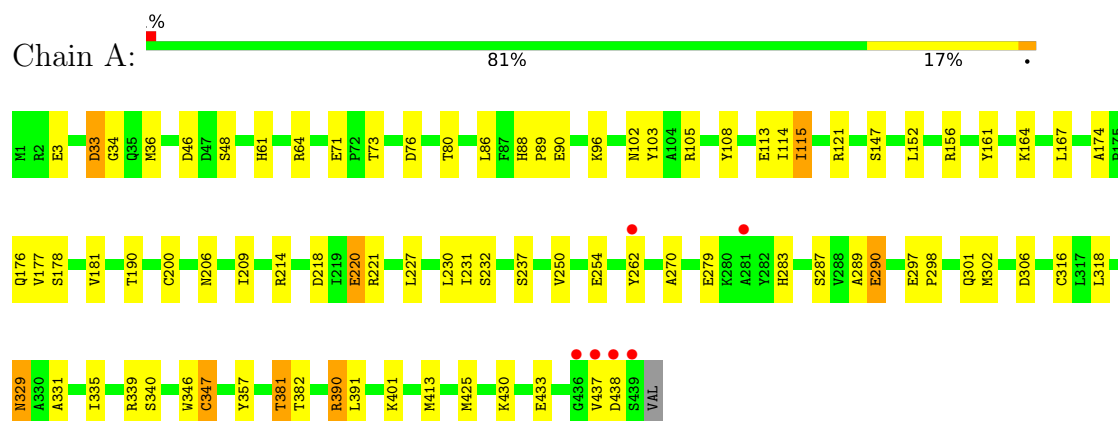
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	44	Total	O	0	0
			44	44		
13	B	52	Total	O	0	0
			52	52		
13	C	110	Total	O	0	0
			110	110		
13	D	25	Total	O	0	0
			25	25		
13	E	16	Total	O	0	0
			16	16		
13	F	20	Total	O	0	0
			20	20		

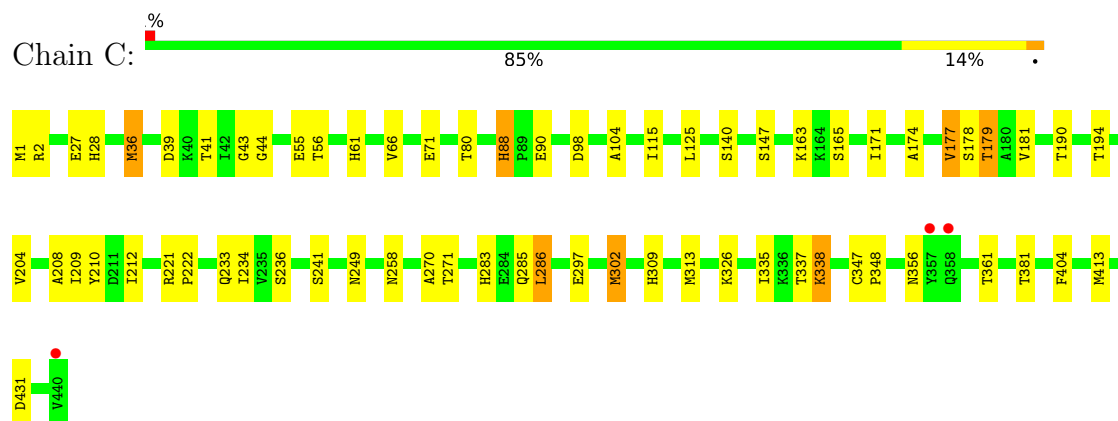
3 Residue-property plots

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.

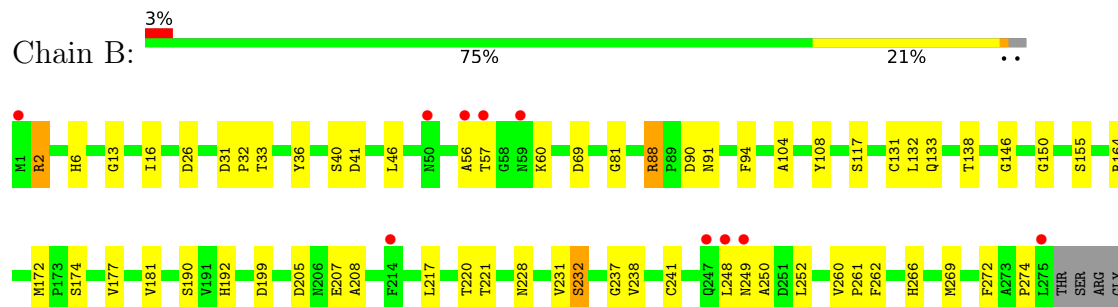
• Molecule 1: Tubulin alpha-1B chain

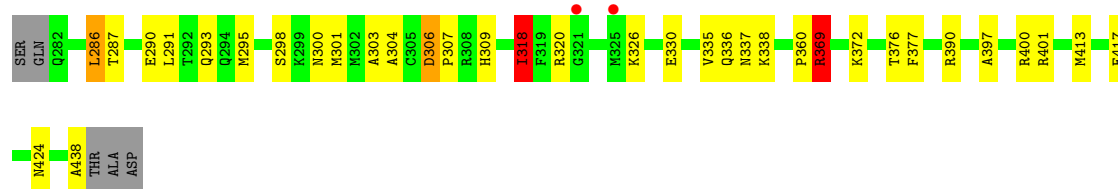


• Molecule 1: Tubulin alpha-1B chain

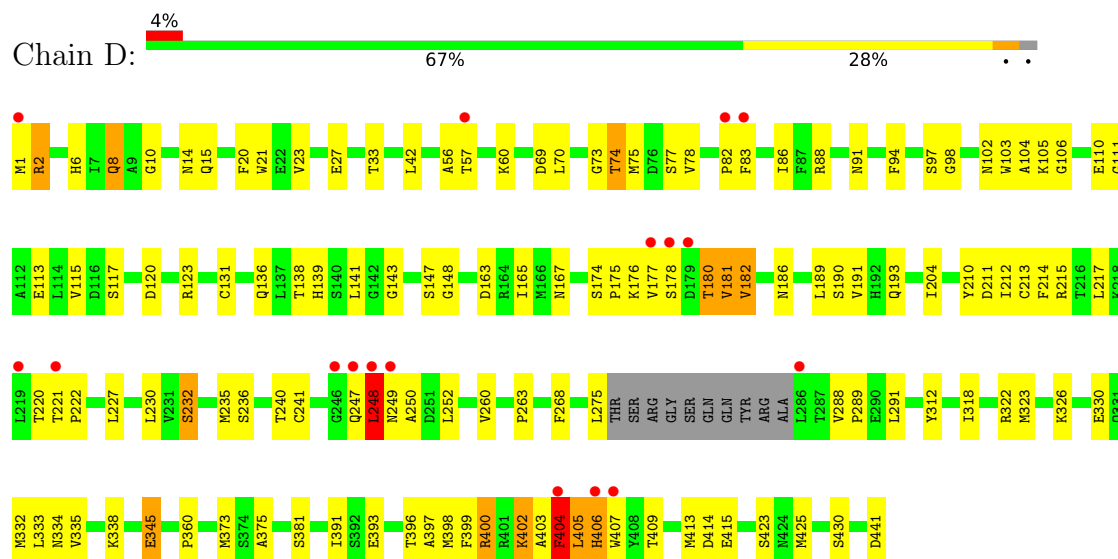


• Molecule 2: Tubulin beta-2B chain

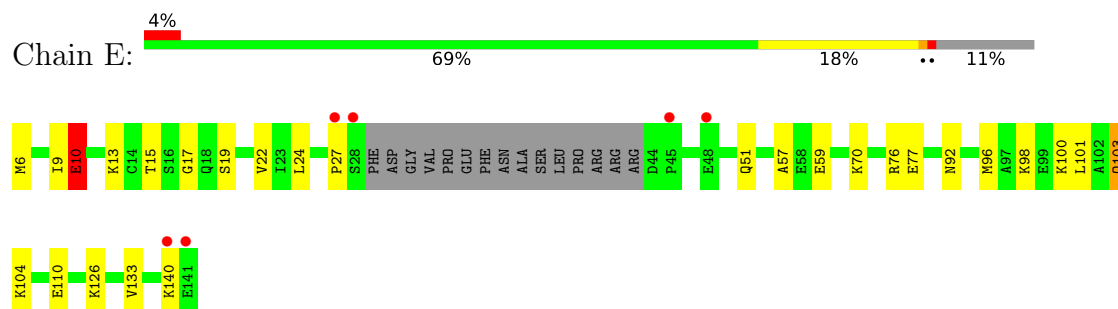




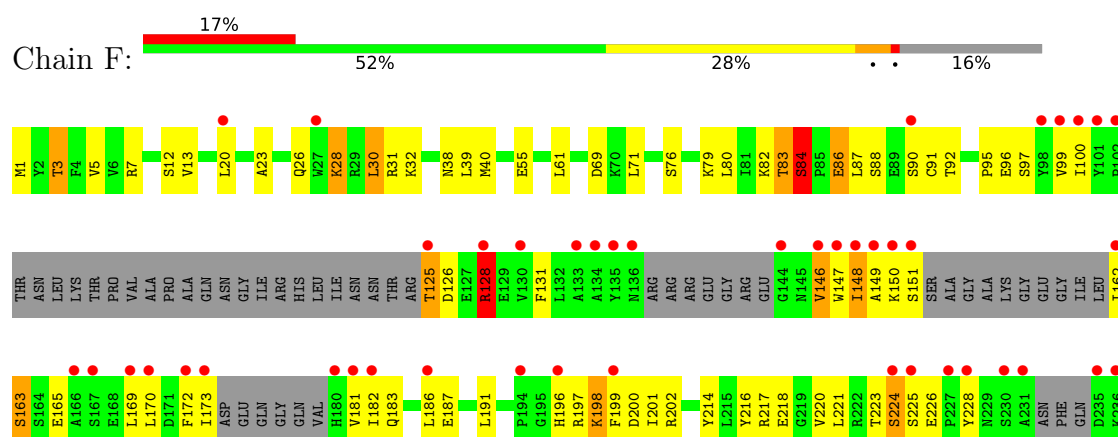
• Molecule 2: Tubulin beta-2B chain

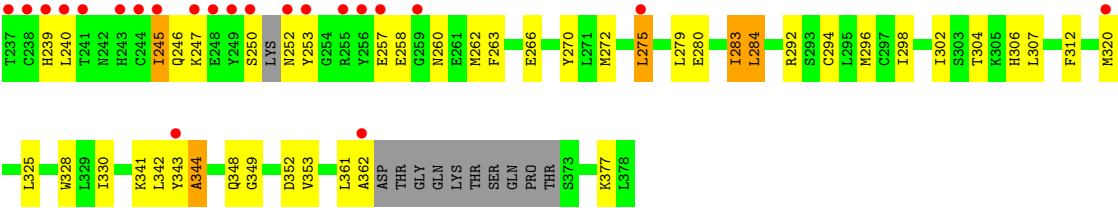


• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.51Å 156.46Å 181.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.60 – 2.48 118.60 – 2.48	Depositor EDS
% Data completeness (in resolution range)	92.9 (118.60-2.48) 93.2 (118.60-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.257 0.205 , 0.256	Depositor DCC
R_{free} test set	4920 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17847	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: MES, GOL, CA, MG, IMD, 6ZR, GTP, 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	1.01	2/3605 (0.1%)	1.05	10/4895 (0.2%)
1	C	1.17	3/3597 (0.1%)	1.08	11/4885 (0.2%)
2	B	1.09	2/3478 (0.1%)	1.04	7/4710 (0.1%)
2	D	1.02	3/3411 (0.1%)	1.07	10/4622 (0.2%)
3	E	1.05	0/1033	1.03	2/1370 (0.1%)
4	F	0.99	4/2704 (0.1%)	1.01	5/3650 (0.1%)
All	All	1.06	14/17828 (0.1%)	1.05	45/24132 (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	D	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	360	PRO	C-N	15.73	1.54	1.33
2	D	42	LEU	C-N	15.57	1.56	1.33
2	B	172	MET	SD-CE	-8.82	1.57	1.79
4	F	196	HIS	CE1-NE2	7.02	1.39	1.32
4	F	196	HIS	CG-CD2	6.94	1.43	1.35
1	A	88	HIS	CE1-NE2	6.82	1.39	1.32
1	C	309	HIS	CG-CD2	6.22	1.42	1.35
4	F	128	ARG	NE-CZ	6.12	1.39	1.33
1	C	283	HIS	CE1-NE2	5.81	1.38	1.32
1	A	88	HIS	CG-CD2	5.54	1.42	1.35
2	D	406	HIS	CG-CD2	5.52	1.42	1.35
2	B	6	HIS	CG-CD2	5.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	306	HIS	CG-CD2	5.15	1.41	1.35
1	C	28	HIS	CD2-NE2	-5.10	1.32	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	176	LYS	N-CA-C	-8.08	98.53	110.48
2	B	306	ASP	CA-C-N	8.04	127.76	119.56
2	B	306	ASP	C-N-CA	8.04	127.76	119.56
2	D	248	LEU	N-CA-C	-7.49	100.43	110.55
1	A	174	ALA	CA-C-N	6.93	127.22	119.32
1	A	174	ALA	C-N-CA	6.93	127.22	119.32
2	D	404	PHE	N-CA-C	6.76	120.85	112.47
4	F	283	ILE	N-CA-C	6.71	116.92	111.62
2	B	318	ILE	CB-CA-C	-6.56	100.39	110.95
3	E	133	VAL	N-CA-C	-6.42	106.54	112.96
2	D	260	VAL	N-CA-C	6.42	114.51	108.15
2	D	115	VAL	N-CA-C	6.38	117.90	110.62
3	E	57	ALA	N-CA-C	-6.36	106.11	114.31
2	B	260	VAL	N-CA-C	6.17	114.26	108.15
2	D	56	ALA	N-CA-C	6.05	116.58	108.23
1	A	283	HIS	N-CA-C	5.93	118.07	108.34
2	B	252	LEU	N-CA-C	5.87	117.67	111.28
1	C	233	GLN	N-CA-C	-5.78	105.06	111.36
1	C	313	MET	N-CA-C	-5.75	106.12	114.12
2	D	42	LEU	O-C-N	-5.74	115.66	122.20
1	C	88	HIS	CA-C-N	5.55	126.78	119.84
1	C	88	HIS	C-N-CA	5.55	126.78	119.84
4	F	55	GLU	CA-C-N	5.48	125.80	119.93
4	F	55	GLU	C-N-CA	5.48	125.80	119.93
2	D	268	PHE	N-CA-C	5.44	118.69	109.76
1	A	306	ASP	CA-C-N	5.39	125.01	119.56
1	A	306	ASP	C-N-CA	5.39	125.01	119.56
2	D	405	LEU	CB-CG-CD1	-5.34	94.67	110.70
1	C	174	ALA	CA-C-N	5.29	124.96	119.56
1	C	174	ALA	C-N-CA	5.29	124.96	119.56
2	B	81	GLY	CA-C-N	5.28	124.73	119.24
2	B	81	GLY	C-N-CA	5.28	124.73	119.24
1	A	390	ARG	N-CA-C	-5.28	105.44	111.14
4	F	84	SER	CA-C-N	5.24	125.30	119.32
4	F	84	SER	C-N-CA	5.24	125.30	119.32
1	C	347	CYS	CA-C-N	5.21	125.50	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	CYS	C-N-CA	5.21	125.50	119.92
2	D	2	ARG	NE-CZ-NH1	-5.20	116.31	121.50
1	A	329	ASN	N-CA-C	5.18	116.93	111.28
1	C	115	ILE	N-CA-C	5.09	115.81	110.62
1	A	290	GLU	N-CA-C	5.07	116.49	111.07
1	C	36	MET	CA-C-N	5.05	126.16	119.84
1	C	36	MET	C-N-CA	5.05	126.16	119.84
1	A	279	GLU	N-CA-C	-5.04	106.44	112.59
1	A	381	THR	CB-CA-C	-5.03	100.17	109.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	249	ASN	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	3488	0	3441	45	0
1	C	3489	0	3413	45	0
2	B	3374	0	3270	78	0
2	D	3326	0	3221	81	0
3	E	1016	0	1041	15	0
4	F	2633	0	2631	84	0
5	A	32	0	12	0	0
5	C	32	0	12	1	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
7	A	18	0	24	1	0
7	B	18	0	24	12	0
7	C	24	0	32	6	0
7	D	12	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	12	0	13	1	0
11	B	27	0	0	3	0
12	C	15	0	15	4	0
13	A	44	0	0	2	0
13	B	52	0	0	0	0
13	C	110	0	0	3	0
13	D	25	0	0	1	0
13	E	16	0	0	1	0
13	F	20	0	0	0	0
All	All	17847	0	17189	344	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (344) 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)
4:F:240:LEU:HD23	4:F:245:ILE:HD12	1.30	1.13
2:B:320:ARG:HH11	7:B:505:GOL:H11	1.05	1.10
4:F:1:MET:HG2	4:F:28:LYS:HD2	1.19	1.09
2:B:320:ARG:NH1	7:B:505:GOL:H11	1.68	1.06
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.34	1.05
4:F:240:LEU:CD2	4:F:245:ILE:HD12	1.99	0.93
4:F:163:SER:HB2	4:F:169:LEU:HG	1.47	0.93
4:F:240:LEU:HD23	4:F:245:ILE:CD1	1.99	0.93
1:A:214:ARG:NH1	1:A:220:GLU:O	2.01	0.93
4:F:149:ALA:HB2	4:F:182:ILE:HG12	1.55	0.89
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.54	0.89
1:C:221:ARG:NH1	7:C:505:GOL:O3	2.07	0.87
2:D:180:THR:HG22	2:D:181:VAL:N	1.88	0.86
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.56	0.86
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.49	0.86
4:F:320:MET:CG	4:F:330:ILE:HD11	2.07	0.84
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.12	0.84
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.11	0.82
4:F:1:MET:CG	4:F:28:LYS:HD2	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:O	4:F:91:CYS:HB3	1.78	0.82
2:D:180:THR:HG22	2:D:181:VAL:H	1.42	0.81
4:F:342:LEU:O	4:F:344:ALA:N	2.13	0.81
2:B:320:ARG:HH11	7:B:505:GOL:C1	1.91	0.80
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.44	0.80
4:F:170:LEU:O	4:F:173:ILE:CD1	2.29	0.80
1:C:210:TYR:OH	1:C:221:ARG:NH2	2.15	0.79
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.63	0.79
2:B:301:MET:HE1	2:B:377:PHE:CD2	2.18	0.78
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.18	0.78
4:F:31:ARG:HE	4:F:32:LYS:H	1.32	0.78
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.63	0.78
4:F:82:LYS:NZ	4:F:97:SER:O	2.13	0.78
4:F:1:MET:HG2	4:F:28:LYS:CD	2.09	0.78
4:F:240:LEU:CD2	4:F:245:ILE:CD1	2.59	0.76
1:C:286:LEU:H	1:C:286:LEU:HD12	1.50	0.76
2:B:306:ASP:HB3	2:B:309:HIS:HD2	1.52	0.75
7:C:506:GOL:O1	13:C:601:HOH:O	2.04	0.74
2:B:401:ARG:HE	7:B:503:GOL:H2	1.53	0.74
2:B:56:ALA:HB3	2:B:60:LYS:H	1.53	0.74
4:F:263:PHE:CE2	4:F:341:LYS:HE3	2.23	0.71
4:F:39:LEU:HD13	4:F:61:LEU:HD22	1.72	0.71
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.24	0.71
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD23	1.72	0.70
2:B:192:HIS:CD2	2:B:424[B]:ASN:HD22	2.10	0.70
1:C:39:ASP:OD2	1:C:55:GLU:OE2	2.10	0.70
1:C:1:MET:O	13:C:602:HOH:O	2.10	0.70
1:C:209:ILE:HD11	1:C:302:MET:HE2	1.72	0.70
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.73	0.69
4:F:170:LEU:O	4:F:173:ILE:HD13	1.92	0.69
4:F:125:THR:HG22	4:F:126:ASP:HA	1.75	0.68
2:B:2:ARG:HG3	2:B:2:ARG:HH11	1.59	0.68
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.29	0.67
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.74	0.67
2:B:301:MET:HE2	2:B:301:MET:HA	1.77	0.67
3:E:9:ILE:HG22	3:E:10:GLU:N	2.09	0.67
1:A:46:ASP:N	1:A:46:ASP:OD1	2.29	0.66
2:B:338:LYS:HG3	2:B:338:LYS:O	1.96	0.66
1:C:165:SER:OG	12:C:510:IMD:H2	1.96	0.65
4:F:61:LEU:HD21	4:F:312:PHE:CD1	2.31	0.65
2:B:360:PRO:HG3	7:B:505:GOL:H2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.15	0.64
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.30	0.64
1:A:220:GLU:CD	1:A:221:ARG:H	2.05	0.64
2:B:326:LYS:O	2:B:330:GLU:HG3	1.98	0.64
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.80	0.64
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.32	0.63
4:F:61:LEU:HD21	4:F:312:PHE:CE1	2.33	0.62
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.35	0.62
2:B:2:ARG:HG3	2:B:2:ARG:NH1	2.14	0.61
3:E:9:ILE:HG22	3:E:10:GLU:H	1.65	0.61
4:F:149:ALA:HA	4:F:181:VAL:O	2.00	0.61
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.36	0.60
4:F:100:ILE:HA	4:F:126:ASP:HB2	1.83	0.60
4:F:100:ILE:HA	4:F:126:ASP:CB	2.31	0.60
2:D:403:ALA:O	2:D:405:LEU:CD1	2.49	0.60
2:D:396:THR:O	2:D:400:ARG:HG2	2.02	0.60
1:A:329:ASN:O	3:E:6:MET:HE1	2.02	0.59
4:F:201:ILE:HG12	4:F:221:LEU:CD2	2.32	0.59
2:D:402:LYS:HB3	2:D:405:LEU:CD2	2.32	0.59
2:D:210:TYR:CE1	2:D:222:PRO:HG3	2.36	0.59
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.02	0.59
4:F:149:ALA:CB	4:F:182:ILE:HG12	2.30	0.59
1:A:262:TYR:CE1	1:A:346:TRP:CH2	2.91	0.58
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.85	0.58
11:B:508:6ZR:OAZ	11:B:508:6ZR:CAX	2.51	0.58
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.44	0.57
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.17	0.57
3:E:92:ASN:HD21	3:E:96:MET:HE1	1.68	0.57
4:F:169:LEU:O	4:F:172:PHE:HB2	2.05	0.57
1:A:390:ARG:NH2	13:A:602:HOH:O	2.37	0.56
2:D:104:ALA:HB2	2:D:413:MET:SD	2.45	0.56
2:D:393:GLU:O	2:D:396:THR:HG22	2.06	0.56
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.38	0.56
2:D:82:PRO:O	2:D:83:PHE:HB2	2.06	0.56
3:E:51:GLN:OE1	3:E:51:GLN:HA	2.07	0.55
4:F:96:GLU:OE2	4:F:147:TRP:HH2	1.89	0.55
2:D:414:ASP:OD1	2:D:415:GLU:N	2.40	0.55
2:D:334:ASN:OD1	2:D:338:LYS:HE2	2.07	0.55
4:F:320:MET:HG2	4:F:330:ILE:CD1	2.23	0.55
4:F:200:ASP:HB3	4:F:320:MET:SD	2.47	0.54
2:D:174:SER:O	2:D:178:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.90	0.54
2:D:180:THR:CG2	2:D:181:VAL:H	2.08	0.54
2:B:401:ARG:HE	7:B:503:GOL:C2	2.19	0.53
4:F:201:ILE:HG12	4:F:221:LEU:HD21	1.91	0.53
2:D:147:SER:OG	2:D:148:GLY:N	2.42	0.53
2:B:40:SER:OG	2:B:41:ASP:N	2.40	0.53
1:C:177:VAL:HG12	7:C:505:GOL:H32	1.89	0.53
4:F:99:VAL:HG22	4:F:181:VAL:HG12	1.91	0.53
2:D:402:LYS:CB	2:D:405:LEU:HD22	2.38	0.53
2:D:248:LEU:HD23	2:D:250:ALA:HB2	1.91	0.52
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.91	0.52
4:F:199:PHE:CD1	4:F:221:LEU:HD22	2.44	0.52
1:A:176:GLN:H	1:A:176:GLN:CD	2.18	0.52
2:D:291:LEU:HG	2:D:375:ALA:HB2	1.91	0.52
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.91	0.52
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.09	0.51
2:D:97:SER:HB2	2:D:110:GLU:OE1	2.09	0.51
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.93	0.51
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.40	0.51
1:A:287:SER:OG	1:A:290:GLU:HG3	2.11	0.51
2:D:403:ALA:O	2:D:405:LEU:HD13	2.10	0.51
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.92	0.51
12:C:509:IMD:C2	7:D:504:GOL:H2	2.41	0.51
4:F:170:LEU:O	4:F:173:ILE:HD11	2.11	0.51
1:A:237:SER:O	13:A:601:HOH:O	2.18	0.51
2:D:322:ARG:O	2:D:373:MET:HE1	2.11	0.51
12:C:509:IMD:H2	7:D:504:GOL:H2	1.93	0.50
2:B:104:ALA:HB2	2:B:413:MET:SD	2.51	0.50
1:C:1:MET:C	1:C:2:ARG:HG2	2.36	0.50
4:F:198:LYS:HZ3	4:F:228:TYR:HE1	1.59	0.50
1:A:250[B]:VAL:HG22	1:A:254:GLU:OE1	2.11	0.50
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.92	0.50
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.93	0.50
4:F:3:THR:O	4:F:38:ASN:HB2	2.11	0.50
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.93	0.50
2:B:272:PHE:HZ	7:B:505:GOL:HO2	1.54	0.49
4:F:148:ILE:HD13	4:F:162:ILE:HG13	1.94	0.49
2:B:174:SER:OG	2:B:207:GLU:OE1	2.31	0.49
1:C:39:ASP:OD2	1:C:55:GLU:CD	2.55	0.49
2:D:210:TYR:CE1	2:D:222:PRO:CG	2.96	0.49
4:F:262:MET:CG	4:F:266:GLU:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:O	1:A:121:ARG:HD2	2.13	0.49
3:E:103:GLN:HG3	3:E:104:LYS:N	2.27	0.49
2:B:269:MET:HG2	2:B:303:ALA:HB3	1.94	0.49
2:D:263:PRO:HD2	13:D:618:HOH:O	2.12	0.49
2:B:272:PHE:CE1	7:B:505:GOL:O2	2.67	0.48
1:C:27:GLU:OE1	1:C:236:SER:OG	2.26	0.48
2:D:10:GLY:O	2:D:14:ASN:ND2	2.40	0.48
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.37	0.48
3:E:92:ASN:ND2	3:E:96:MET:HE1	2.28	0.48
2:B:261:PRO:HG2	2:B:262:PHE:CD2	2.49	0.48
2:B:31:ASP:C	2:B:33:THR:H	2.21	0.48
2:D:248:LEU:CD2	2:D:250:ALA:HB2	2.44	0.48
2:D:404:PHE:HE1	2:D:407:TRP:CE2	2.32	0.48
2:D:33:THR:O	2:D:60:LYS:HD2	2.14	0.48
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.49	0.48
1:A:430:LYS:O	1:A:433:GLU:HB3	2.14	0.48
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.41	0.48
2:B:146:GLY:O	2:B:150:GLY:HA3	2.13	0.48
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.96	0.48
2:D:175:PRO:HA	2:D:178:SER:HB2	1.96	0.48
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.29	0.48
1:A:347:CYS:N	3:E:27:PRO:HB3	2.29	0.47
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.95	0.47
2:D:180:THR:HG22	2:D:182:VAL:H	1.79	0.47
2:D:143:GLY:O	2:D:186:ASN:ND2	2.47	0.47
4:F:96:GLU:OE2	4:F:147:TRP:CH2	2.67	0.47
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.95	0.47
2:D:323:MET:HE2	2:D:373:MET:SD	2.55	0.47
4:F:26:GLN:HE22	4:F:362:ALA:H	1.62	0.47
4:F:240:LEU:CD2	4:F:245:ILE:HD13	2.42	0.47
1:A:297:GLU:OE2	1:A:339:ARG:NH1	2.48	0.47
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.46	0.47
1:A:289:ALA:HA	1:A:331:ALA:HB2	1.96	0.47
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.14	0.47
3:E:13:LYS:NZ	13:E:201:HOH:O	2.32	0.47
2:B:2:ARG:HH11	2:B:2:ARG:CG	2.24	0.46
2:B:181:VAL:HG22	1:C:258:ASN:OD1	2.15	0.46
2:D:110:GLU:HA	2:D:113:GLU:HG2	1.97	0.46
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.97	0.46
2:D:322:ARG:O	2:D:373:MET:CE	2.63	0.46
2:D:345:GLU:CD	2:D:345:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:PHE:O	2:B:300:ASN:HB3	2.15	0.46
4:F:95:PRO:HB2	4:F:183:GLN:HG2	1.97	0.46
2:B:397:ALA:O	2:B:400:ARG:NH2	2.45	0.46
2:D:102:ASN:HB3	2:D:105:LYS:HD2	1.97	0.46
2:D:103:TRP:HD1	2:D:147:SER:OG	1.97	0.46
2:B:241:CYS:O	2:B:250:ALA:HB3	2.15	0.46
1:C:204:VAL:HG22	1:C:302:MET:SD	2.55	0.46
3:E:9:ILE:CG2	3:E:10:GLU:N	2.77	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.46
2:D:391:ILE:HG22	2:D:425:MET:HE1	1.97	0.46
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.51	0.46
11:B:508:6ZR:CAO	11:B:508:6ZR:OAL	2.63	0.46
2:D:106:GLY:O	2:D:111:GLY:HA3	2.15	0.46
4:F:292:ARG:O	4:F:296:MET:HB2	2.16	0.46
1:A:102:ASN:HB3	1:A:105:ARG:HB3	1.97	0.46
2:B:360:PRO:HG3	7:B:505:GOL:C2	2.45	0.45
2:B:306:ASP:HA	2:B:307:PRO:HD3	1.76	0.45
1:C:181:VAL:HG21	1:C:404:PHE:CZ	2.51	0.45
4:F:150:LYS:O	4:F:151:SER:HB3	2.15	0.45
2:B:56:ALA:CB	2:B:60:LYS:HB2	2.46	0.45
2:D:27:GLU:OE1	2:D:236:SER:OG	2.29	0.45
4:F:61:LEU:HD21	4:F:312:PHE:HD1	1.80	0.45
2:B:192:HIS:HD2	2:B:424[B]:ASN:HD22	1.57	0.45
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.97	0.45
2:D:332:MET:O	2:D:335:VAL:HG12	2.16	0.45
2:D:139:HIS:CE1	2:D:141:LEU:CD2	3.00	0.45
2:B:318:ILE:CD1	2:B:376:THR:HB	2.47	0.45
2:D:405:LEU:CD1	2:D:405:LEU:N	2.80	0.45
4:F:246:GLN:HA	4:F:250:SER:HB2	1.99	0.45
2:B:287:THR:O	2:B:290:GLU:N	2.46	0.45
3:E:9:ILE:CG2	3:E:10:GLU:H	2.29	0.45
4:F:1:MET:HG3	4:F:26:GLN:C	2.42	0.45
4:F:275[B]:LEU:HD23	4:F:275[B]:LEU:HA	1.64	0.45
1:C:39:ASP:OD1	1:C:41:THR:OG1	2.31	0.44
7:C:505:GOL:O1	2:D:247:GLN:OE1	2.30	0.44
4:F:128:ARG:O	4:F:131:PHE:HB3	2.16	0.44
2:B:56:ALA:HB3	2:B:60:LYS:N	2.26	0.44
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.86	0.44
1:A:115:ILE:HD13	1:A:152:LEU:HG	2.00	0.44
2:B:192:HIS:CE1	2:B:424[A]:ASN:OD1	2.70	0.44
2:D:139:HIS:CE1	2:D:141:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.98	0.44
4:F:262:MET:HG3	4:F:266:GLU:HG2	1.98	0.44
4:F:325:LEU:HA	4:F:325:LEU:HD23	1.77	0.44
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.32	0.44
2:B:274:PRO:HB3	2:B:286:LEU:HD22	2.00	0.44
2:D:180:THR:CG2	2:D:181:VAL:N	2.58	0.44
2:D:227:LEU:O	2:D:230:LEU:HB2	2.17	0.44
4:F:131:PHE:CD1	4:F:131:PHE:C	2.95	0.44
4:F:224:SER:C	4:F:226:GLU:H	2.25	0.44
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	2.00	0.44
2:B:164:ARG:HA	2:B:164:ARG:HD3	1.76	0.44
4:F:247:LYS:HA	4:F:253:TYR:HE2	1.83	0.44
1:C:44:GLY:HA2	1:C:55:GLU:HB2	1.99	0.44
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.44
4:F:149:ALA:O	4:F:150:LYS:HD2	2.17	0.44
4:F:270:TYR:C	4:F:270:TYR:CD2	2.95	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.44
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.99	0.44
2:B:272:PHE:CE1	7:B:505:GOL:H32	2.53	0.44
1:C:140:SER:HA	1:C:171:ILE:HB	1.99	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.43
2:B:56:ALA:N	2:B:60:LYS:O	2.49	0.43
2:B:318:ILE:HD11	2:B:376:THR:HB	2.00	0.43
2:B:318:ILE:HG12	11:B:508:6ZR:CAX	2.48	0.43
2:D:163:ASP:C	7:D:504:GOL:H32	2.43	0.43
4:F:146:VAL:HG13	4:F:187:GLU:OE2	2.18	0.43
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.33	0.43
1:C:209:ILE:HD11	1:C:302:MET:CE	2.43	0.43
1:C:234:ILE:HD13	1:C:302:MET:CE	2.48	0.43
4:F:26:GLN:HE22	4:F:362:ALA:HB3	1.83	0.43
1:C:163:LYS:HG2	7:C:507:GOL:O2	2.18	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.54	0.43
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.99	0.43
2:D:326:LYS:O	2:D:330:GLU:HG3	2.18	0.43
2:D:75:MET:O	2:D:78:VAL:HB	2.18	0.43
2:D:312:TYR:CD1	2:D:381:SER:HB2	2.54	0.43
1:A:115:ILE:HD11	1:A:156:ARG:HG3	2.01	0.43
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.54	0.43
4:F:198:LYS:NZ	4:F:239:HIS:HA	2.33	0.43
1:A:270:ALA:HB3	1:A:302[A]:MET:HG3	2.01	0.43
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.43
2:D:210:TYR:CD1	2:D:222:PRO:HG3	2.53	0.43
4:F:342:LEU:C	4:F:344:ALA:N	2.77	0.43
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.34	0.43
2:D:333:LEU:HD23	2:D:333:LEU:HA	1.84	0.43
2:B:199:ASP:O	2:B:266:HIS:HB2	2.19	0.42
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.59	0.42
1:C:147:SER:HB2	1:C:190:THR:HB	1.99	0.42
2:B:2:ARG:HA	2:B:131:CYS:O	2.20	0.42
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.18	0.42
2:B:181:VAL:HG12	1:C:348:PRO:CG	2.50	0.42
2:D:69:ASP:O	2:D:94:PHE:HA	2.18	0.42
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.42
1:A:425:MET:HE3	1:A:425:MET:HB3	1.90	0.42
1:C:208:ALA:O	1:C:212:ILE:HG13	2.20	0.42
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.01	0.42
4:F:284[A]:LEU:HD12	4:F:284[A]:LEU:HA	1.87	0.42
4:F:201:ILE:HG12	4:F:221:LEU:HD23	2.00	0.42
4:F:214:TYR:CE2	4:F:353[B]:VAL:HG11	2.54	0.42
2:B:413:MET:HE2	2:B:413:MET:HB3	1.86	0.42
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.44	0.42
2:D:103:TRP:NE1	2:D:148:GLY:HA2	2.35	0.42
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.42
4:F:280:GLU:HA	4:F:284[A]:LEU:HB2	2.01	0.42
1:A:33:ASP:OD1	1:A:33:ASP:N	2.52	0.42
2:B:286:LEU:HD23	2:B:291:LEU:HD23	2.02	0.42
2:D:406:HIS:CE1	2:D:407:TRP:HD1	2.37	0.42
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.54	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.42
1:C:43:GLY:HA2	1:C:56:THR:C	2.45	0.42
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.02	0.42
2:B:221:THR:HG21	1:C:326:LYS:HB2	2.01	0.42
2:B:301:MET:HE1	2:B:377:PHE:HD2	1.80	0.42
4:F:79:LYS:O	4:F:83:THR:HB	2.20	0.42
4:F:186:LEU:HD21	4:F:328:TRP:CE2	2.55	0.42
1:A:289:ALA:HA	1:A:331:ALA:CB	2.50	0.41
2:B:272:PHE:CZ	7:B:505:GOL:O2	2.67	0.41
1:C:43:GLY:HA2	1:C:56:THR:O	2.20	0.41
2:D:405:LEU:HA	2:D:405:LEU:HD12	1.89	0.41
2:B:2:ARG:H	2:B:2:ARG:HD2	1.86	0.41
2:B:237:GLY:HA2	7:B:505:GOL:H12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:80:LEU:O	4:F:84:SER:HB2	2.20	0.41
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.53	0.41
1:C:1:MET:HE2	1:C:1:MET:HB2	1.93	0.41
1:C:431:ASP:HB3	12:C:508:IMD:H2	2.01	0.41
2:B:88:ARG:O	2:B:91:ASN:HB2	2.21	0.41
2:B:228:ASN:O	2:B:232:SER:HB2	2.20	0.41
2:B:360:PRO:O	2:B:369:ARG:C	2.61	0.41
2:D:240:THR:HB	2:D:318:ILE:HD13	2.02	0.41
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.39	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.45	0.41
1:A:401:LYS:HE3	2:B:438:ALA:HB1	2.02	0.41
2:B:336:GLN:C	2:B:338:LYS:H	2.28	0.41
1:C:337:THR:OG1	1:C:338:LYS:HD2	2.20	0.41
4:F:223:THR:O	4:F:260:ASN:HB3	2.20	0.41
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.41
1:C:356[A]:ASN:OD1	13:C:603:HOH:O	2.21	0.41
2:D:330:GLU:O	2:D:334:ASN:HB2	2.20	0.41
2:D:402:LYS:O	2:D:405:LEU:HD13	2.19	0.41
3:E:101:LEU:HD12	3:E:101:LEU:HA	1.90	0.41
1:A:34:GLY:O	1:A:61:HIS:N	2.47	0.41
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.21	0.41
2:B:88:ARG:HH12	2:B:90:ASP:HB2	1.86	0.41
2:D:212:ILE:HG23	2:D:275:LEU:HD13	2.02	0.41
1:A:347:CYS:C	3:E:27:PRO:HB3	2.45	0.40
2:B:164:ARG:O	10:B:507:MES:H71	2.22	0.40
2:D:180:THR:HG22	2:D:181:VAL:HG12	2.03	0.40
2:D:211:ASP:OD1	2:D:211:ASP:N	2.53	0.40
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.51	0.40
4:F:198:LYS:HE2	4:F:198:LYS:HB2	1.75	0.40
1:A:103:TYR:CD1	1:A:103:TYR:C	2.99	0.40
1:C:179:THR:HG23	5:C:503:GTP:H3'	2.02	0.40
1:A:382:THR:O	7:A:504:GOL:H2	2.22	0.40
2:D:70:LEU:O	2:D:98:GLY:HA2	2.21	0.40
2:D:74:THR:O	2:D:78:VAL:HG23	2.22	0.40
4:F:86:GLU:O	4:F:87:LEU:HD23	2.21	0.40
4:F:221:LEU:HD23	4:F:221:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

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	450/440 (102%)	431 (96%)	19 (4%)	0	100	100
1	C	449/440 (102%)	437 (97%)	12 (3%)	0	100	100
2	B	429/431 (100%)	409 (95%)	18 (4%)	2 (0%)	24	40
2	D	421/431 (98%)	395 (94%)	18 (4%)	8 (2%)	6	10
3	E	120/136 (88%)	111 (92%)	8 (7%)	1 (1%)	16	28
4	F	307/378 (81%)	264 (86%)	34 (11%)	9 (3%)	3	5
All	All	2176/2256 (96%)	2047 (94%)	109 (5%)	20 (1%)	14	25

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	177	VAL
2	D	399	PHE
4	F	343	TYR
2	B	337	ASN
2	D	181	VAL
2	D	214	PHE
2	D	398	MET
2	D	402	LYS
4	F	128	ARG
2	B	369	ARG
2	D	73	GLY
2	D	180	THR
4	F	90	SER
4	F	225	SER
3	E	10	GLU
4	F	23	ALA
4	F	88	SER
4	F	92	THR
4	F	272	MET
4	F	344	ALA

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	383/371 (103%)	365 (95%)	18 (5%)	23	44
1	C	382/371 (103%)	369 (97%)	13 (3%)	32	57
2	B	375/372 (101%)	351 (94%)	24 (6%)	16	31
2	D	368/372 (99%)	344 (94%)	24 (6%)	15	30
3	E	112/122 (92%)	98 (88%)	14 (12%)	4	8
4	F	293/336 (87%)	261 (89%)	32 (11%)	6	11
All	All	1913/1944 (98%)	1788 (94%)	125 (6%)	16	30

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	48	SER
1	A	86	LEU
1	A	89	PRO
1	A	96	LYS
1	A	113	GLU
1	A	114	ILE
1	A	115	ILE
1	A	178	SER
1	A	181	VAL
1	A	218	ASP
1	A	220	GLU
1	A	232	SER
1	A	340	SER
1	A	347	CYS
1	A	381	THR
1	A	437	VAL
1	A	438	ASP
2	B	2	ARG
2	B	26	ASP
2	B	57	THR
2	B	88	ARG

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Mol	Chain	Res	Type
2	B	117	SER
2	B	132	LEU
2	B	155[A]	SER
2	B	155[B]	SER
2	B	177	VAL
2	B	190	SER
2	B	217	LEU
2	B	220	THR
2	B	232	SER
2	B	238	VAL
2	B	248	LEU
2	B	249	ASN
2	B	286	LEU
2	B	293	GLN
2	B	295	MET
2	B	298	SER
2	B	318	ILE
2	B	335	VAL
2	B	369	ARG
2	B	372	LYS
1	C	80	THR
1	C	177	VAL
1	C	178	SER
1	C	179	THR
1	C	241	SER
1	C	285	GLN
1	C	286	LEU
1	C	297	GLU
1	C	302	MET
1	C	335	ILE
1	C	338	LYS
1	C	361	THR
1	C	381	THR
2	D	1	MET
2	D	8	GLN
2	D	15	GLN
2	D	57	THR
2	D	74	THR
2	D	77	SER
2	D	117	SER
2	D	138	THR
2	D	182	VAL

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Mol	Chain	Res	Type
2	D	190	SER
2	D	204	ILE
2	D	215	ARG
2	D	220	THR
2	D	221[A]	THR
2	D	221[B]	THR
2	D	232	SER
2	D	248	LEU
2	D	345	GLU
2	D	400	ARG
2	D	404	PHE
2	D	409	THR
2	D	423	SER
2	D	430	SER
2	D	441	ASP
3	E	10	GLU
3	E	15	THR
3	E	19	SER
3	E	22	VAL
3	E	24	LEU
3	E	59	GLU
3	E	70	LYS
3	E	76	ARG
3	E	77	GLU
3	E	98	LYS
3	E	100	LYS
3	E	103	GLN
3	E	110	GLU
3	E	140	LYS
4	F	3	THR
4	F	12	SER
4	F	13	VAL
4	F	20	LEU
4	F	28	LYS
4	F	30	LEU
4	F	69	ASP
4	F	76[A]	SER
4	F	76[B]	SER
4	F	83	THR
4	F	84	SER
4	F	86	GLU
4	F	125	THR

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Mol	Chain	Res	Type
4	F	146	VAL
4	F	148	ILE
4	F	163	SER
4	F	165	GLU
4	F	191	LEU
4	F	198	LYS
4	F	202	ARG
4	F	217	ARG
4	F	220	VAL
4	F	224	SER
4	F	245	ILE
4	F	252	ASN
4	F	258	GLU
4	F	275[A]	LEU
4	F	275[B]	LEU
4	F	284[A]	LEU
4	F	284[B]	LEU
4	F	361	LEU
4	F	377	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	102	ASN
1	A	216	ASN
1	A	300	ASN
1	A	301	GLN
1	A	309	HIS
2	B	15	GLN
2	B	37	HIS
2	B	192	HIS
2	B	193	GLN
2	B	331	GLN
2	D	8	GLN
2	D	15	GLN
2	D	101	ASN
2	D	167	ASN
2	D	349	ASN
2	D	385	GLN
2	D	406	HIS
3	E	12	ASN

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Mol	Chain	Res	Type
3	E	92	ASN
3	E	136	ASN
4	F	26	GLN
4	F	145	ASN
4	F	196	HIS
4	F	243	HIS
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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	$\# Z > 2$
7	GOL	B	504	-	5,5,5	0.62	0	5,5,5	0.29	0
7	GOL	D	503	-	5,5,5	0.55	0	5,5,5	0.33	0
7	GOL	A	504	-	5,5,5	0.89	0	5,5,5	0.70	0
7	GOL	D	504	-	5,5,5	0.30	0	5,5,5	0.53	0
7	GOL	A	503	-	5,5,5	0.53	0	5,5,5	0.42	0
10	MES	B	507	-	12,12,12	2.24	1 (8%)	15,16,16	2.56	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	503	6	33,34,34	1.42	5 (15%)	50,54,54	1.90	11 (22%)
11	6ZR	B	508	-	28,29,29	2.28	7 (25%)	38,42,42	2.52	14 (36%)
7	GOL	C	506	-	5,5,5	0.57	0	5,5,5	0.60	0
12	IMD	C	509	-	5,5,5	0.75	0	5,5,5	0.87	0
7	GOL	C	507	-	5,5,5	0.94	0	5,5,5	0.81	0
9	GDP	B	501	6	29,30,30	1.71	5 (17%)	45,47,47	1.88	9 (20%)
5	GTP	A	501	6	33,34,34	1.32	4 (12%)	50,54,54	1.79	11 (22%)
7	GOL	C	505	-	5,5,5	0.62	0	5,5,5	0.63	0
9	GDP	D	501	6	29,30,30	1.38	4 (13%)	45,47,47	1.89	10 (22%)
7	GOL	C	502	-	5,5,5	0.96	0	5,5,5	0.65	0
7	GOL	A	506	-	5,5,5	0.58	0	5,5,5	0.85	0
12	IMD	C	510	-	5,5,5	0.74	0	5,5,5	0.75	0
12	IMD	C	508	-	5,5,5	0.68	0	5,5,5	0.78	0
7	GOL	B	503	-	5,5,5	0.47	0	5,5,5	1.19	0
7	GOL	B	505	-	5,5,5	0.66	0	5,5,5	0.42	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
7	GOL	B	504	-	-	0/4/4/4	-
7	GOL	D	503	-	-	0/4/4/4	-
7	GOL	A	504	-	-	0/4/4/4	-
7	GOL	D	504	-	-	2/4/4/4	-
7	GOL	A	503	-	-	3/4/4/4	-
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
5	GTP	C	503	6	-	8/22/38/38	0/3/3/3
11	6ZR	B	508	-	-	4/16/32/32	0/3/3/3
7	GOL	C	506	-	-	4/4/4/4	-
12	IMD	C	509	-	-	-	0/1/1/1
7	GOL	C	507	-	-	4/4/4/4	-
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
7	GOL	C	505	-	-	2/4/4/4	-
9	GDP	D	501	6	-	6/16/32/32	0/3/3/3
7	GOL	C	502	-	-	0/4/4/4	-
7	GOL	A	506	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	IMD	C	510	-	-	-	0/1/1/1
12	IMD	C	508	-	-	-	0/1/1/1
7	GOL	B	503	-	-	2/4/4/4	-
7	GOL	B	505	-	-	4/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	507	MES	C8-S	-7.37	1.67	1.77
11	B	508	6ZR	CAB-NAC	-6.18	1.32	1.43
11	B	508	6ZR	CAF-CAH	-5.46	1.50	1.57
9	B	501	GDP	PA-O3A	4.70	1.64	1.59
11	B	508	6ZR	CAI-CAH	-4.56	1.45	1.51
9	B	501	GDP	C6-N1	-4.25	1.30	1.38
11	B	508	6ZR	CAD-NAC	4.22	1.43	1.37
5	C	503	GTP	PB-O3B	4.03	1.63	1.59
9	D	501	GDP	PA-O3A	4.00	1.63	1.59
9	D	501	GDP	C5-C4	3.00	1.47	1.38
5	A	501	GTP	PA-O3A	2.89	1.62	1.59
5	A	501	GTP	C5-N7	-2.78	1.33	1.39
5	A	501	GTP	C6-N1	-2.75	1.33	1.38
5	C	503	GTP	C6-N1	-2.73	1.33	1.38
11	B	508	6ZR	CAH-NAC	-2.33	1.46	1.48
5	C	503	GTP	PB-O3A	2.31	1.62	1.59
9	B	501	GDP	C8-N9	-2.27	1.32	1.37
11	B	508	6ZR	CAG-CAF	2.22	1.57	1.53
9	D	501	GDP	C6-N1	-2.18	1.34	1.38
5	C	503	GTP	PB-O2B	-2.15	1.45	1.55
9	B	501	GDP	C5-C4	2.14	1.44	1.38
11	B	508	6ZR	CAK-CAM	2.08	1.43	1.40
5	A	501	GTP	PB-O3B	2.08	1.61	1.59
9	B	501	GDP	C2-N1	-2.08	1.32	1.37
9	D	501	GDP	C5-N7	-2.03	1.35	1.39
5	C	503	GTP	C5-N7	-2.02	1.35	1.39

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	507	MES	O1S-S-C8	6.74	116.91	106.73
11	B	508	6ZR	OAN-CAM-CAK	6.65	124.52	114.55
5	C	503	GTP	C5-C4-N3	-6.31	118.34	128.39
9	B	501	GDP	C5-C4-N3	-6.30	118.36	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	503	GTP	C2-N3-C4	6.08	122.78	112.30
11	B	508	6ZR	OAN-CAM-CAP	-6.06	114.08	124.30
9	D	501	GDP	C5-C4-N3	-6.05	118.77	128.39
5	A	501	GTP	C5-C4-N3	-5.70	119.31	128.39
11	B	508	6ZR	CAH-NAC-CAD	-5.09	90.84	95.30
9	B	501	GDP	C2-N3-C4	4.97	120.87	112.30
9	D	501	GDP	C2-N3-C4	4.83	120.62	112.30
9	D	501	GDP	N9-C4-N3	4.82	135.59	125.95
11	B	508	6ZR	CAI-CAH-NAC	4.73	121.13	115.79
5	A	501	GTP	N9-C4-N3	4.49	134.92	125.95
5	C	503	GTP	N9-C4-N3	4.30	134.56	125.95
9	B	501	GDP	N9-C4-N3	4.26	134.47	125.95
5	A	501	GTP	C2-N3-C4	4.09	119.35	112.30
11	B	508	6ZR	CAU-OAT-CAS	-3.88	111.83	117.51
9	D	501	GDP	C6-C5-N7	3.85	137.29	130.29
10	B	507	MES	C6-C5-N4	-3.71	104.48	110.12
11	B	508	6ZR	OAW-CAV-CAS	-3.60	114.97	120.12
10	B	507	MES	C5-N4-C3	3.46	116.29	108.84
9	B	501	GDP	C6-C5-N7	3.35	136.39	130.29
11	B	508	6ZR	CAB-NAC-CAH	3.31	135.19	130.33
5	C	503	GTP	C6-C5-N7	3.19	136.09	130.29
9	D	501	GDP	C4-C5-N7	-3.09	105.77	110.67
11	B	508	6ZR	OAZ-CAY-CAV	3.03	120.34	115.14
5	C	503	GTP	C2-N1-C6	-3.02	119.62	125.11
5	A	501	GTP	O3G-PG-O2G	2.88	118.59	107.80
5	C	503	GTP	C5-C6-N1	2.86	120.54	113.25
5	A	501	GTP	O6-C6-C5	-2.77	119.22	126.53
5	C	503	GTP	N9-C8-N7	-2.68	108.43	113.40
9	B	501	GDP	C4-C5-N7	-2.66	106.45	110.67
9	B	501	GDP	C5-C6-N1	2.66	120.03	113.25
9	D	501	GDP	C8-N7-C5	2.62	108.92	104.26
11	B	508	6ZR	OAW-CAV-CAY	2.61	123.87	120.12
10	B	507	MES	O2S-S-O1S	-2.57	105.47	113.82
11	B	508	6ZR	CBA-OAZ-CAY	-2.55	113.78	117.51
5	A	501	GTP	O2A-PA-O3A	2.53	114.11	107.27
9	B	501	GDP	C2-N1-C6	-2.51	120.57	125.11
11	B	508	6ZR	CAA-CAY-CAV	-2.50	117.44	120.22
9	B	501	GDP	O2B-PB-O3A	2.49	113.00	104.64
5	C	503	GTP	O6-C6-C5	-2.46	120.04	126.53
5	A	501	GTP	C6-C5-N7	2.45	134.75	130.29
10	B	507	MES	C2-C3-N4	-2.42	106.45	110.12
5	A	501	GTP	C2-N1-C6	-2.40	120.75	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	6ZR	CAQ-CAI-CAJ	2.37	121.49	118.74
5	C	503	GTP	C4-C5-N7	-2.32	107.00	110.67
5	A	501	GTP	C8-N7-C5	2.29	108.33	104.26
5	A	501	GTP	C4-C5-N7	-2.28	107.05	110.67
9	D	501	GDP	C5-C6-N1	2.27	119.02	113.25
5	A	501	GTP	N9-C8-N7	-2.25	109.23	113.40
5	C	503	GTP	C8-N7-C5	2.24	108.25	104.26
9	D	501	GDP	C8-N9-C4	2.23	110.21	106.03
11	B	508	6ZR	CAA-CAB-NAC	2.23	121.59	119.36
9	D	501	GDP	C2-N1-C6	-2.15	121.21	125.11
9	D	501	GDP	N9-C8-N7	-2.13	109.46	113.40
5	C	503	GTP	O2B-PB-O3A	2.11	112.99	107.27
9	B	501	GDP	O2A-PA-O3A	2.11	112.97	107.27
11	B	508	6ZR	OAE-CAD-NAC	2.06	134.58	131.85

There are no chirality outliers.

All (52) 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	C	503	GTP	C5'-O5'-PA-O3A
5	C	503	GTP	C5'-O5'-PA-O1A
5	C	503	GTP	C5'-O5'-PA-O2A
7	A	503	GOL	C1-C2-C3-O3
7	A	503	GOL	O2-C2-C3-O3
7	A	506	GOL	C1-C2-C3-O3
7	A	506	GOL	O2-C2-C3-O3
7	B	503	GOL	O1-C1-C2-C3
7	B	505	GOL	O1-C1-C2-C3
7	B	505	GOL	C1-C2-C3-O3
7	B	505	GOL	O2-C2-C3-O3
7	C	506	GOL	O1-C1-C2-C3
7	C	506	GOL	C1-C2-C3-O3
7	C	506	GOL	O2-C2-C3-O3
7	D	504	GOL	O1-C1-C2-O2
7	D	504	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
9	D	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
9	D	501	GDP	C5'-O5'-PA-O1A
11	B	508	6ZR	CAK-CAM-OAN-CAO
11	B	508	6ZR	CAP-CAM-OAN-CAO
11	B	508	6ZR	CAS-CAV-OAW-CAX
7	C	507	GOL	O1-C1-C2-C3
7	C	507	GOL	C1-C2-C3-O3
7	C	507	GOL	O1-C1-C2-O2
11	B	508	6ZR	CAY-CAV-OAW-CAX
7	B	503	GOL	O1-C1-C2-O2
7	B	505	GOL	O1-C1-C2-O2
7	C	506	GOL	O1-C1-C2-O2
7	C	507	GOL	O2-C2-C3-O3
5	C	503	GTP	PB-O3B-PG-O3G
9	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O2A
5	C	503	GTP	PB-O3B-PG-O1G
7	C	505	GOL	O1-C1-C2-C3
5	C	503	GTP	PB-O3A-PA-O2A
9	D	501	GDP	C3'-C4'-C5'-O5'
7	C	505	GOL	O1-C1-C2-O2
9	D	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	503	GTP	PB-O3B-PG-O2G
7	A	503	GOL	O1-C1-C2-O2
5	C	503	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

13 monomers are involved in 29 short contacts:

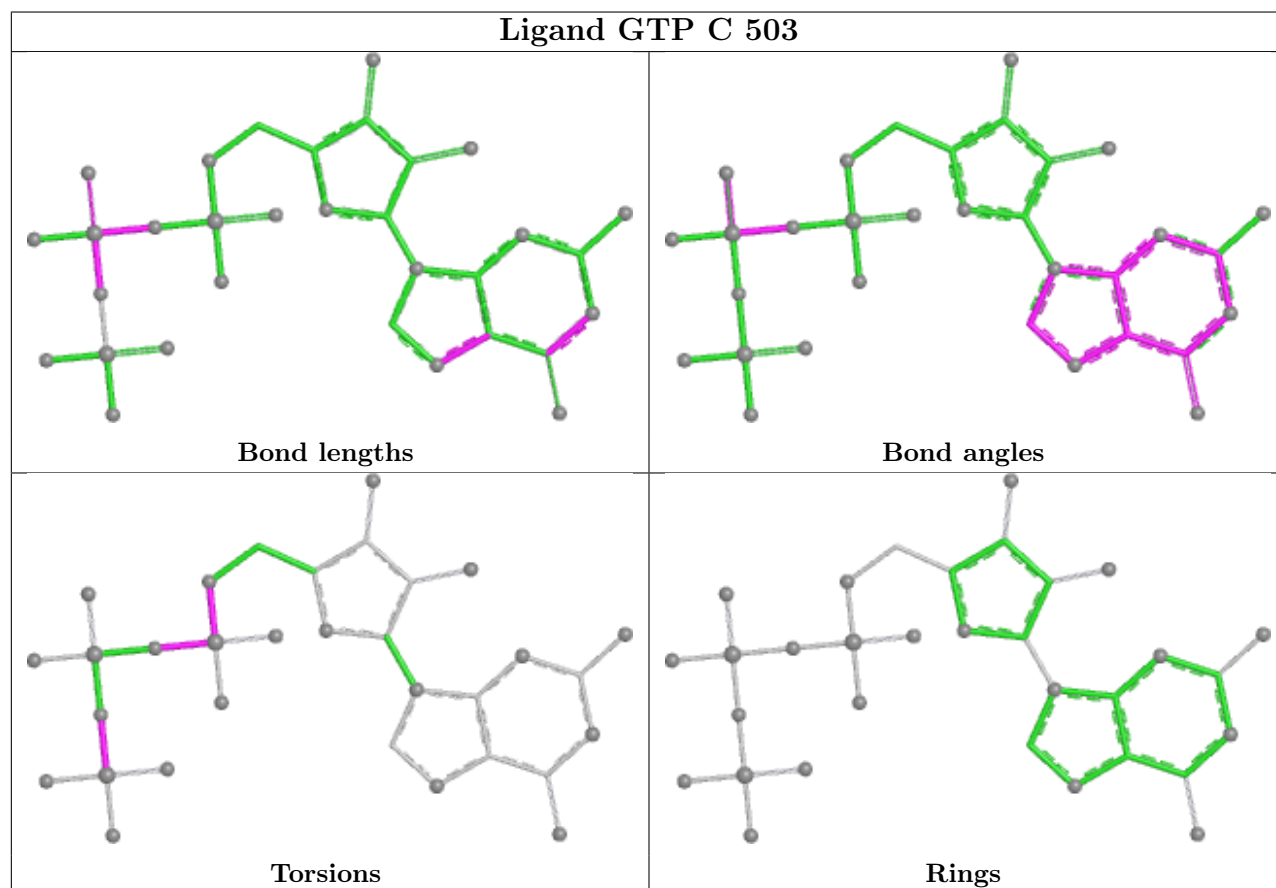
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	504	GOL	1	0
7	D	504	GOL	3	0
10	B	507	MES	1	0
5	C	503	GTP	1	0
11	B	508	6ZR	3	0
7	C	506	GOL	1	0
12	C	509	IMD	2	0
7	C	507	GOL	2	0

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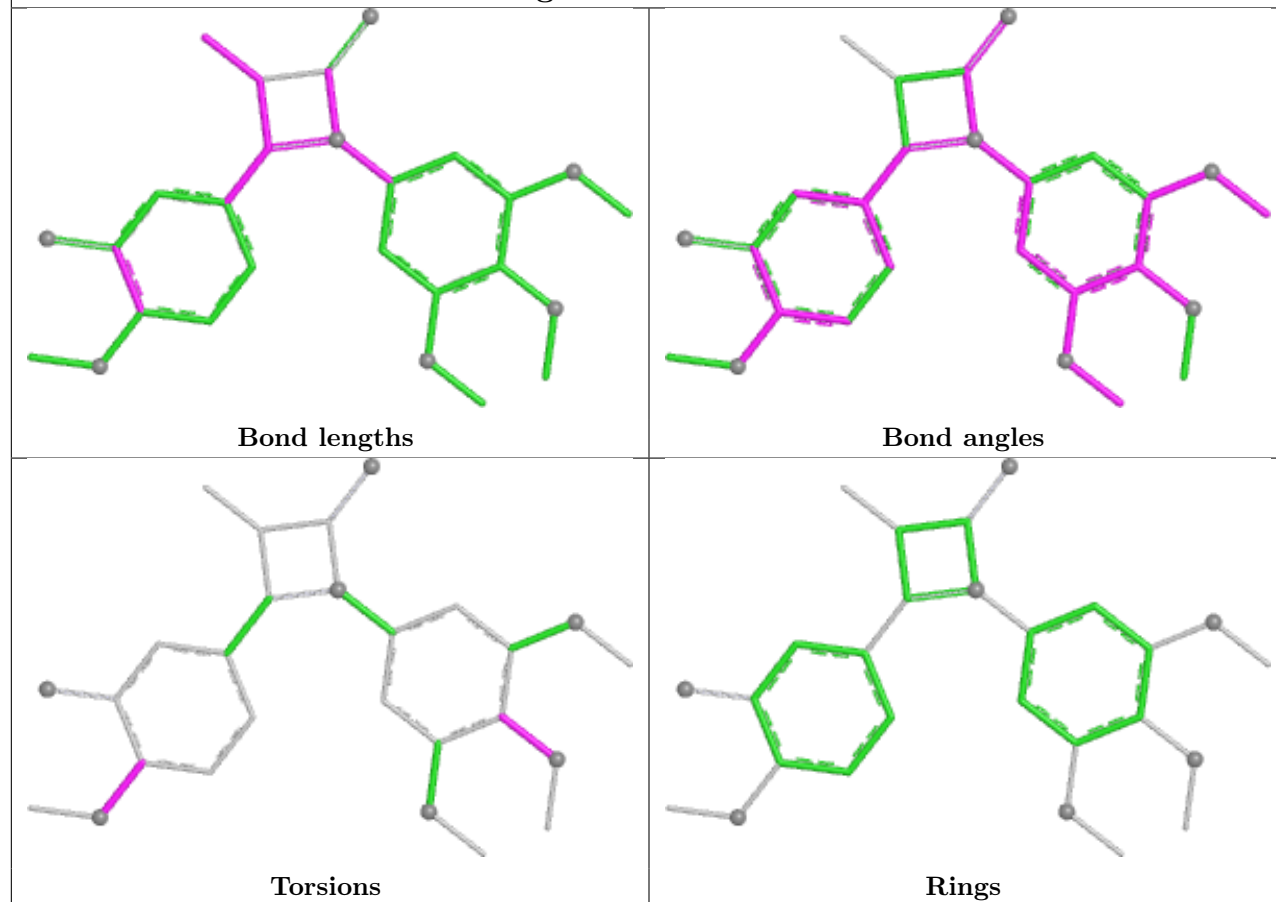
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	505	GOL	3	0
12	C	510	IMD	1	0
12	C	508	IMD	1	0
7	B	503	GOL	2	0
7	B	505	GOL	10	0

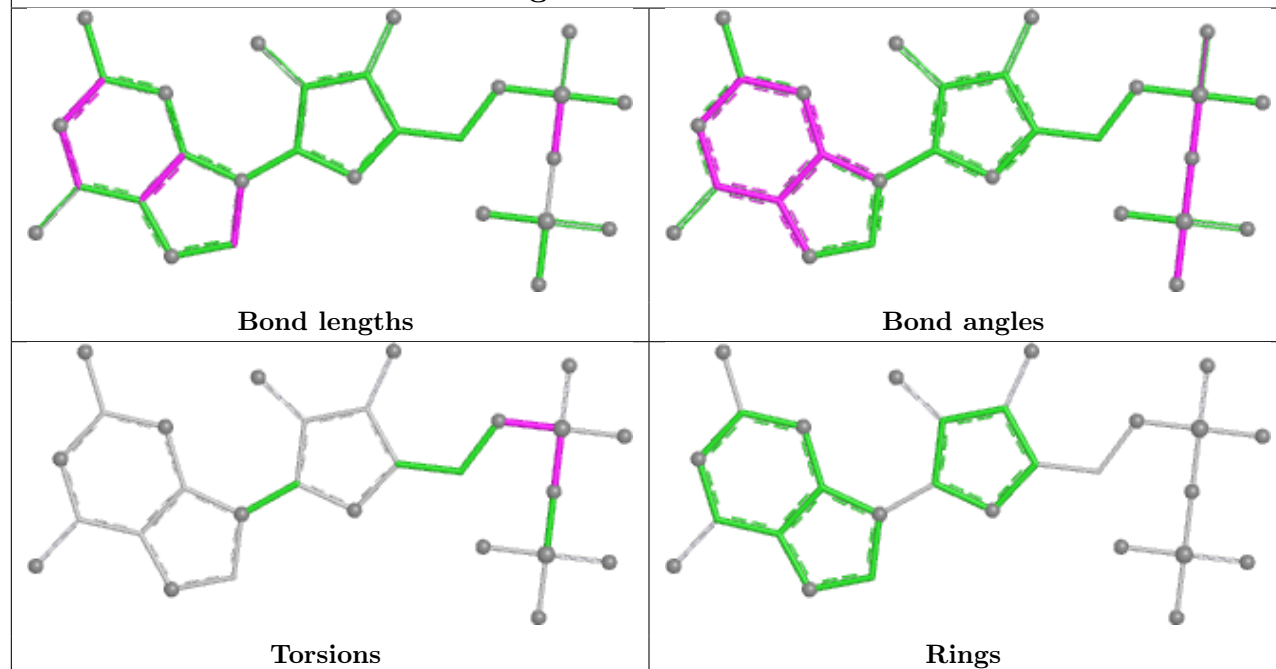
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

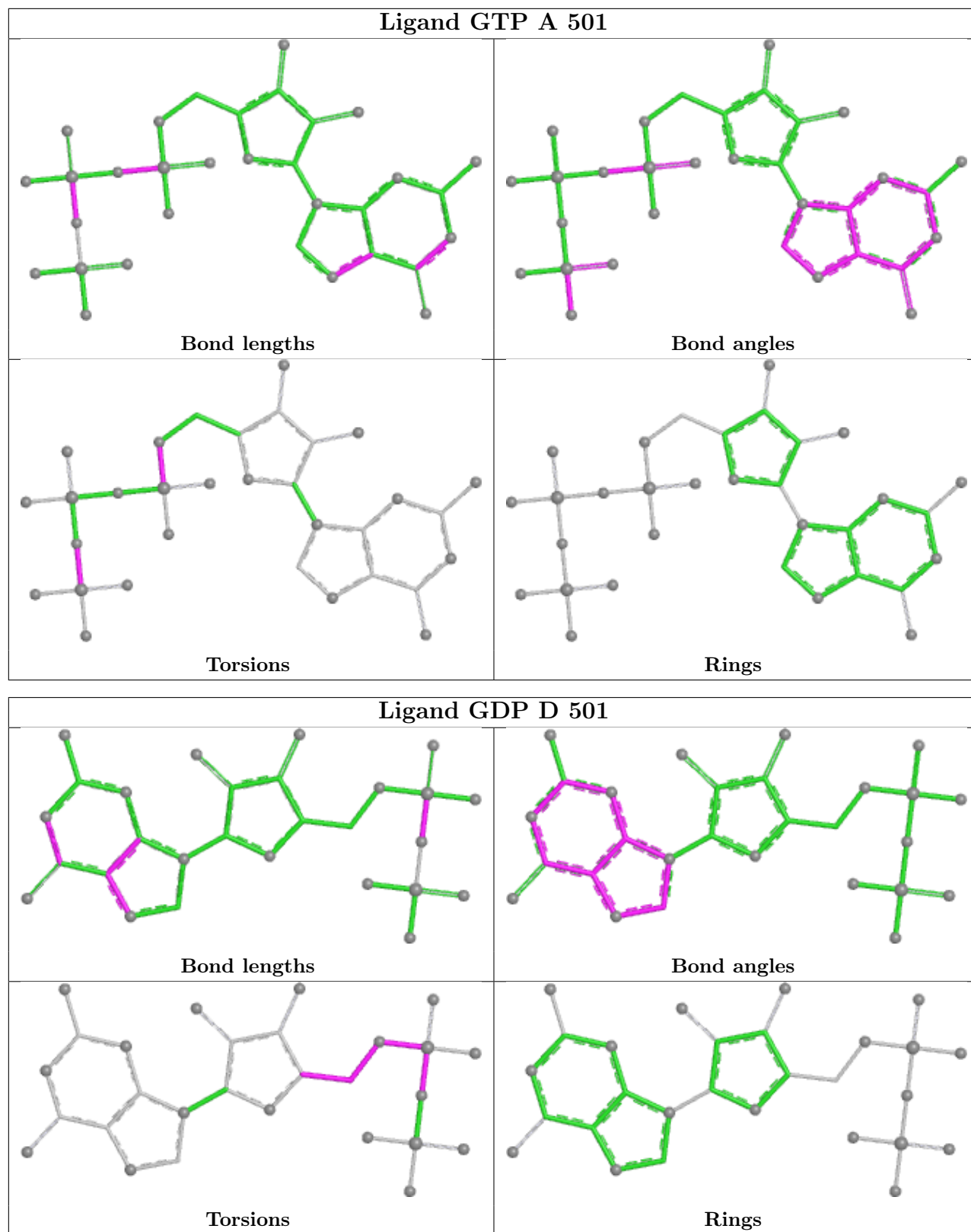


Ligand 6ZR B 508



Ligand GDP B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	439/440 (99%)	0.04	6 (1%) 73 71	17, 37, 62, 99	13 (2%)
1	C	440/440 (100%)	-0.50	3 (0%) 84 82	10, 22, 43, 59	11 (2%)
2	B	422/431 (97%)	-0.03	12 (2%) 55 51	10, 33, 65, 99	12 (2%)
2	D	421/431 (97%)	0.34	17 (4%) 42 38	21, 45, 73, 93	6 (1%)
3	E	121/136 (88%)	0.44	6 (4%) 34 30	12, 44, 76, 96	3 (2%)
4	F	319/378 (84%)	1.07	66 (20%) 2 2	24, 62, 143, 176	5 (1%)
All	All	2162/2256 (95%)	0.15	110 (5%) 33 30	10, 38, 79, 176	50 (2%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	6.9
4	F	173	ILE	5.9
4	F	102	PRO	5.7
4	F	245	ILE	5.6
4	F	231	ALA	5.4
4	F	170	LEU	5.3
2	B	249	ASN	4.4
4	F	256	TYR	4.3
4	F	259	GLY	4.3
4	F	253	TYR	4.0
4	F	249	TYR	3.8
2	D	179	ASP	3.8
4	F	151	SER	3.7
4	F	172	PHE	3.7
4	F	250	SER	3.7
4	F	244	CYS	3.7
4	F	180	HIS	3.6
4	F	135	TYR	3.6
2	D	249	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	247	GLN	3.5
2	B	248	LEU	3.5
2	B	247	GLN	3.4
4	F	237	THR	3.4
4	F	240	LEU	3.4
4	F	130	VAL	3.4
2	B	1	MET	3.3
2	D	1	MET	3.3
2	D	221[A]	THR	3.3
2	D	177	VAL	3.3
2	B	57	THR	3.3
2	D	82	PRO	3.2
4	F	90	SER	3.2
4	F	227	PRO	3.2
4	F	241	THR	3.2
4	F	100	ILE	3.2
4	F	236	LYS	3.2
4	F	162	ILE	3.2
4	F	169	LEU	3.1
4	F	133	ALA	3.1
4	F	186	LEU	3.1
4	F	166	ALA	3.1
2	D	219	LEU	3.1
4	F	181	VAL	3.1
4	F	182	ILE	3.1
1	A	437	VAL	3.0
3	E	28	SER	3.0
4	F	99	VAL	2.9
4	F	136	ASN	2.9
2	D	57	THR	2.9
4	F	125	THR	2.9
3	E	27	PRO	2.9
4	F	134	ALA	2.9
4	F	230	SER	2.8
4	F	148	ILE	2.8
4	F	239	HIS	2.8
4	F	150	LYS	2.8
4	F	228	TYR	2.8
2	D	406	HIS	2.8
1	A	439	SER	2.7
4	F	243	HIS	2.7
4	F	362	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	248	LEU	2.6
2	D	246	GLY	2.6
1	A	262	TYR	2.6
4	F	343	TYR	2.6
1	A	436	GLY	2.5
3	E	141	GLU	2.5
3	E	48	GLU	2.5
4	F	238	CYS	2.4
3	E	140	LYS	2.4
4	F	101	TYR	2.4
1	A	438	ASP	2.4
2	D	404	PHE	2.4
2	B	56	ALA	2.4
4	F	128	ARG	2.4
2	D	83	PHE	2.4
2	B	50[A]	ASN	2.4
2	D	178	SER	2.4
4	F	20	LEU	2.4
4	F	196	HIS	2.4
4	F	252	ASN	2.4
4	F	257	GLU	2.4
4	F	225	SER	2.3
1	C	440	VAL	2.3
4	F	199	PHE	2.3
2	B	275	LEU	2.3
4	F	247	LYS	2.3
4	F	255	ARG	2.3
4	F	27	TRP	2.3
4	F	146	VAL	2.3
2	B	325	MET	2.2
4	F	224	SER	2.2
3	E	45	PRO	2.2
2	B	59	ASN	2.2
4	F	98	TYR	2.2
4	F	144	GLY	2.2
1	A	281	ALA	2.2
2	D	407	TRP	2.2
1	C	357	TYR	2.1
2	B	214	PHE	2.1
4	F	147	TRP	2.1
2	B	321	GLY	2.1
4	F	248	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	2.1
4	F	320	MET	2.1
2	D	286	LEU	2.1
4	F	167	SER	2.1
4	F	275[A]	LEU	2.1
1	C	358[A]	GLN	2.0
4	F	235	ASP	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	GOL	D	503	6/6	0.67	0.18	74,81,86,87	0
7	GOL	A	506	6/6	0.75	0.16	52,63,69,73	0
6	MG	F	401	1/1	0.76	0.19	86,86,86,86	0
7	GOL	A	504	6/6	0.77	0.24	56,71,73,79	0
12	IMD	C	509	5/5	0.77	0.23	64,66,73,76	0
7	GOL	B	505	6/6	0.83	0.29	54,55,62,68	0
7	GOL	C	502	6/6	0.84	0.19	46,52,64,67	0
12	IMD	C	510	5/5	0.84	0.19	56,64,66,67	0
6	MG	A	502	1/1	0.86	0.16	37,37,37,37	0
7	GOL	B	503	6/6	0.86	0.20	42,49,52,72	0
7	GOL	B	504	6/6	0.86	0.19	53,62,69,71	0
6	MG	C	504	1/1	0.86	0.20	38,38,38,38	0
7	GOL	D	504	6/6	0.87	0.17	51,53,65,77	0
7	GOL	C	505	6/6	0.87	0.23	61,65,73,81	0
7	GOL	A	503	6/6	0.87	0.13	47,56,58,59	0
7	GOL	C	507	6/6	0.89	0.13	34,47,48,57	0

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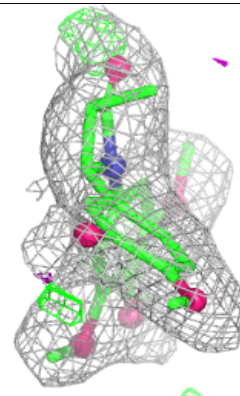
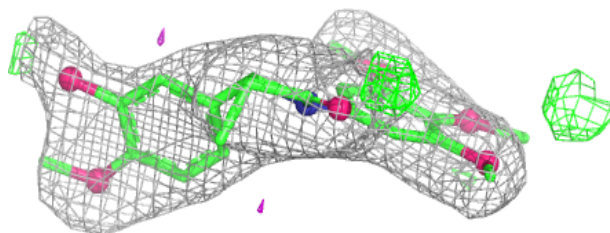
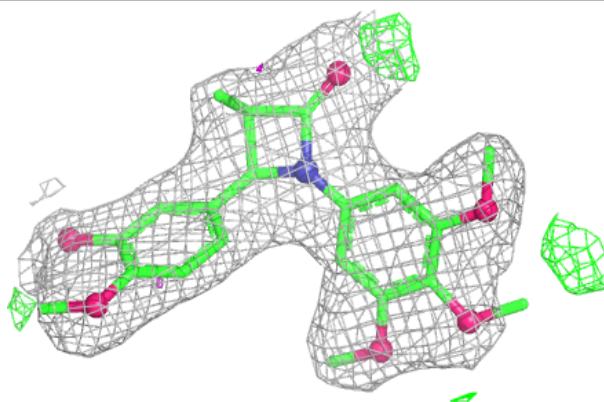
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	C	506	6/6	0.90	0.17	47,52,65,65	0
11	6ZR	B	508	27/27	0.90	0.12	35,47,53,58	0
6	MG	D	502	1/1	0.92	0.13	40,40,40,40	0
6	MG	B	502	1/1	0.93	0.13	16,16,16,16	0
8	CA	C	501	1/1	0.93	0.08	82,82,82,82	0
9	GDP	D	501	28/28	0.93	0.09	33,42,57,61	0
12	IMD	C	508	5/5	0.94	0.12	32,35,36,42	0
8	CA	B	506	1/1	0.95	0.08	81,81,81,81	0
10	MES	B	507	12/12	0.95	0.09	26,38,47,52	0
8	CA	A	505	1/1	0.97	0.04	59,59,59,59	0
5	GTP	A	501	32/32	0.98	0.05	18,23,30,33	0
5	GTP	C	503	32/32	0.98	0.05	12,16,20,22	0
9	GDP	B	501	28/28	0.99	0.05	13,18,21,24	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.

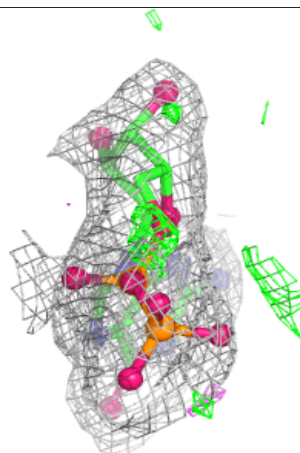
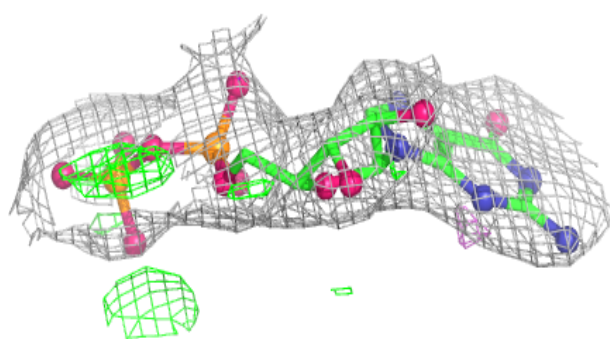
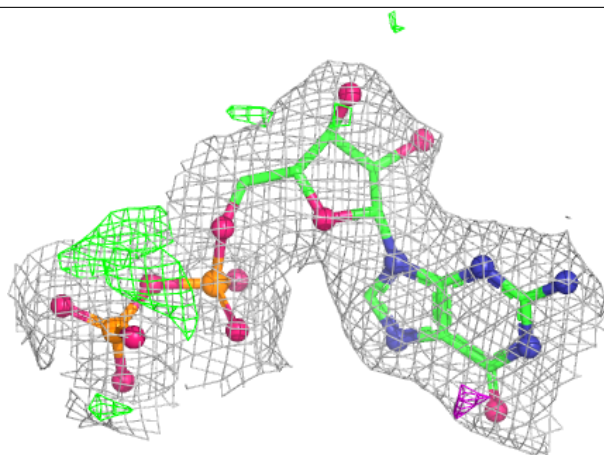
Electron density around 6ZR B 508:

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

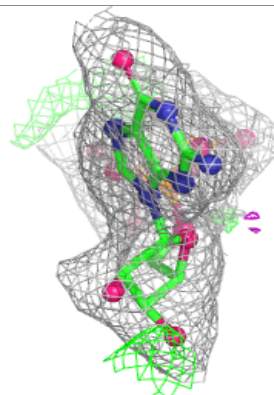
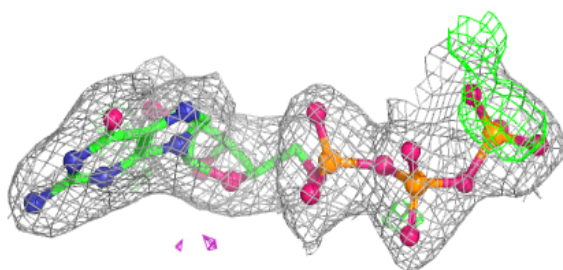
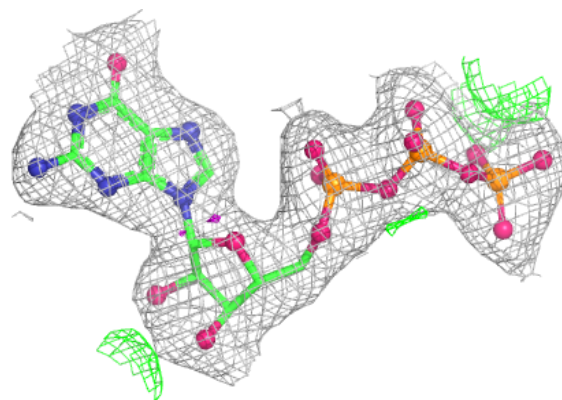


Electron density around GDP D 501:

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

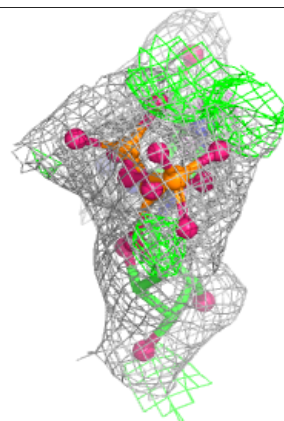
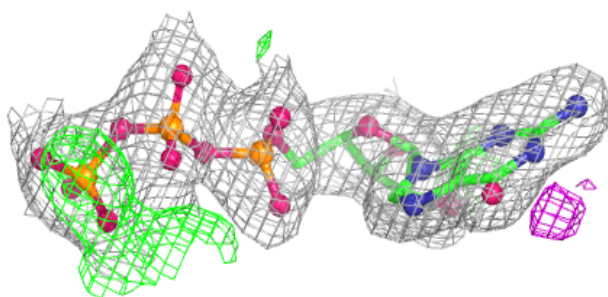
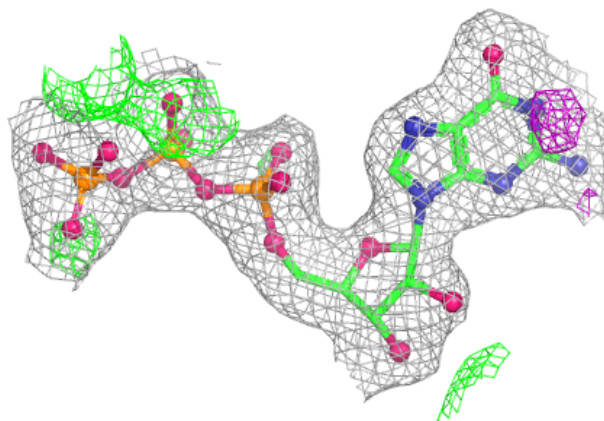
**Electron density around GTP A 501:**

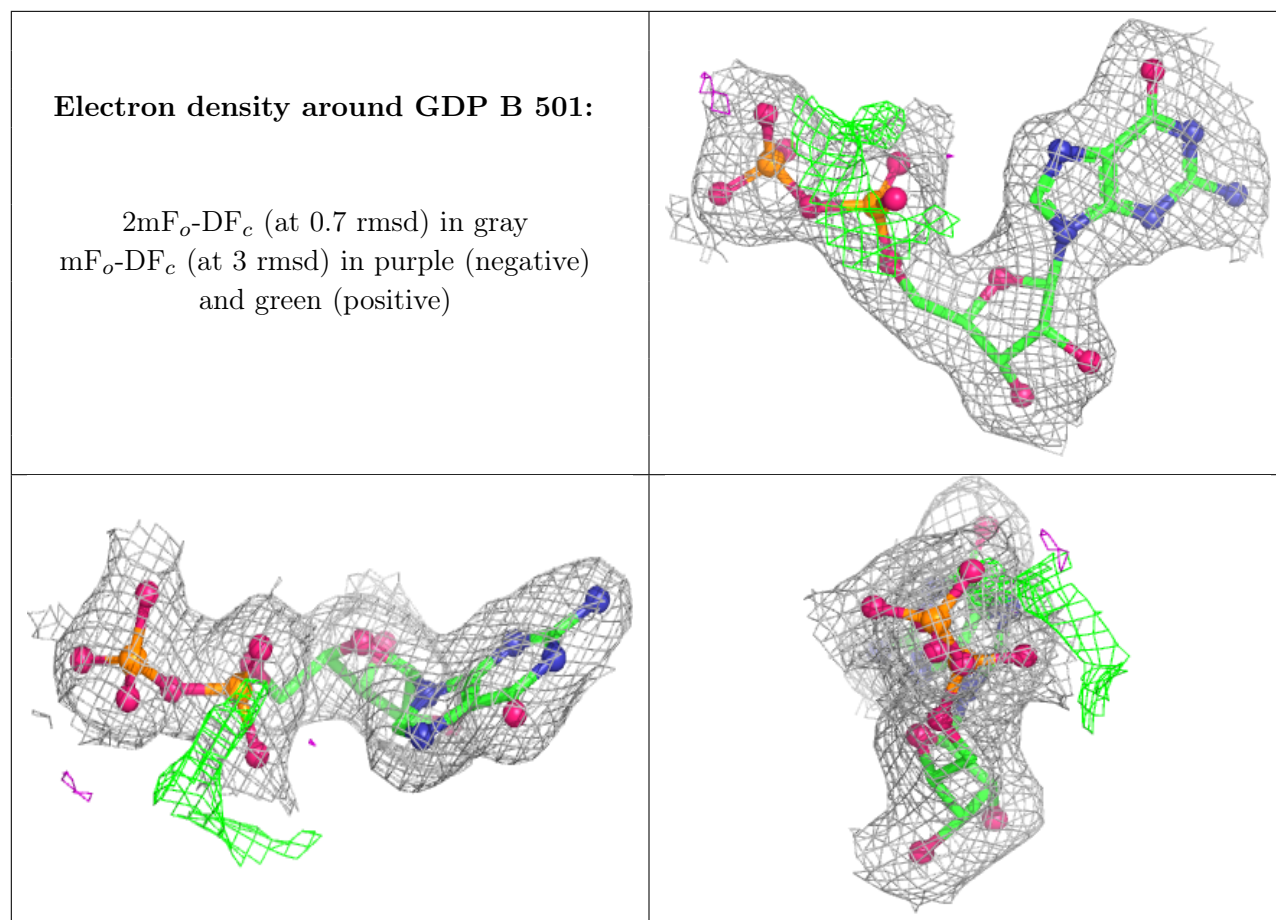
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP C 503:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.