



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:54 AM UTC

PDB ID : 5S5A / pdb_00005s5a
Title : Tubulin-Z1449748885-complex
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Deposited on : 2020-11-08
Resolution : 2.35 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

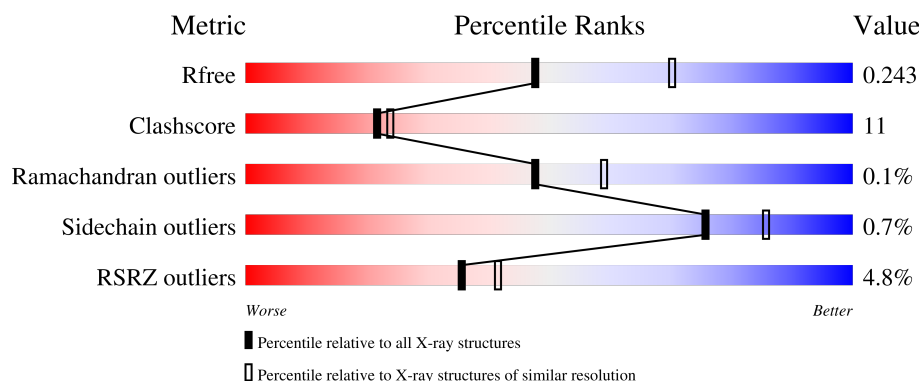
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	451	2% 72% 24% ..
1	C	451	3% 77% 20% .
2	B	445	4% 73% 23% .
2	D	445	6% 71% 25% ..
3	E	143	8% 69% 17% . 14%

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Mol	Chain	Length	Quality of chain
4	F	384	6% 70% 22% 8%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18104 atoms, of which 52 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	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	1	1	0
			3376	2119	580	650	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	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	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

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

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

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



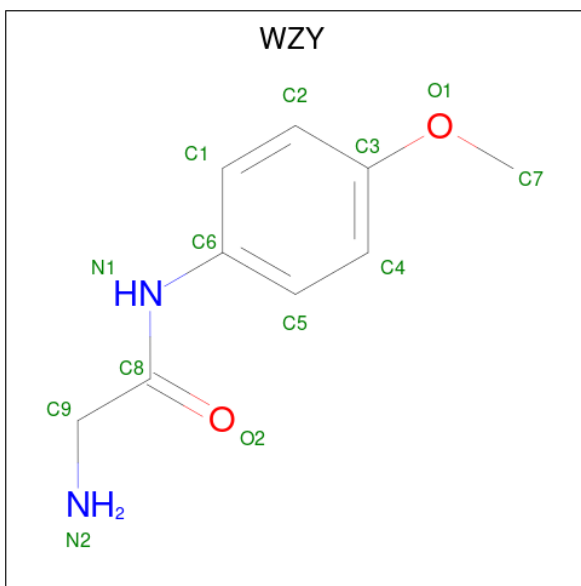
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is N-(4-methoxyphenyl)glycinamide (CCD ID: WZY) (formula: $C_9H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



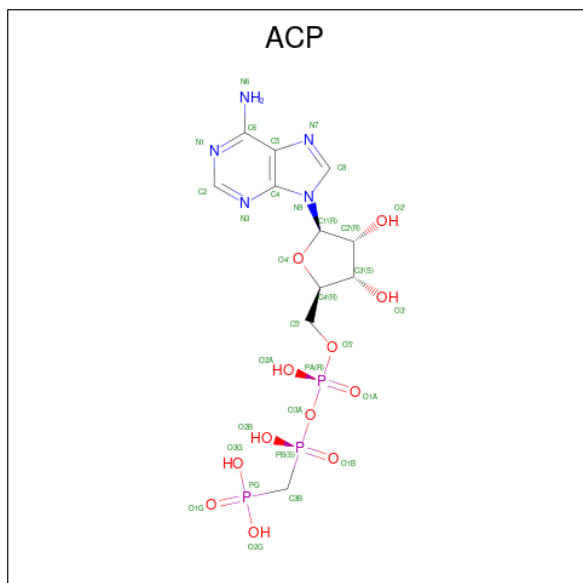
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			26	9	13	2	2		
10	C	1	Total	C	H	N	O	0	0
			26	9	13	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	H	N	O	0	0
			26	9	13	2	2		
10	E	1	Total	C	H	N	O	0	0
			26	9	13	2	2		

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



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

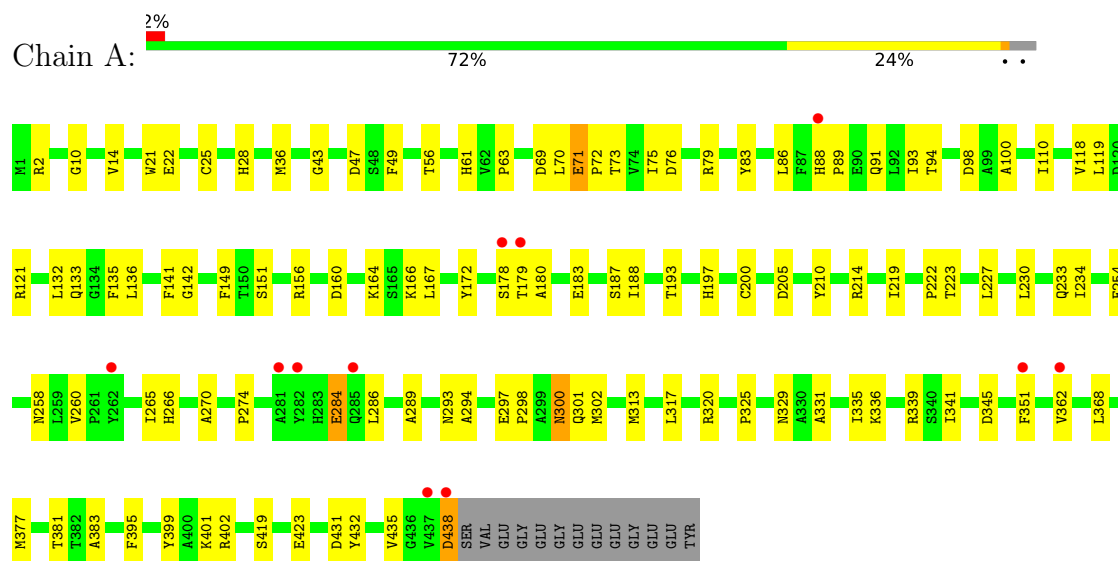
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	58	Total	O	0	0
			58	58		
12	B	62	Total	O	0	0
			62	62		
12	C	160	Total	O	0	0
			160	160		
12	D	30	Total	O	0	0
			30	30		
12	E	11	Total	O	0	0
			11	11		
12	F	5	Total	O	0	0
			5	5		

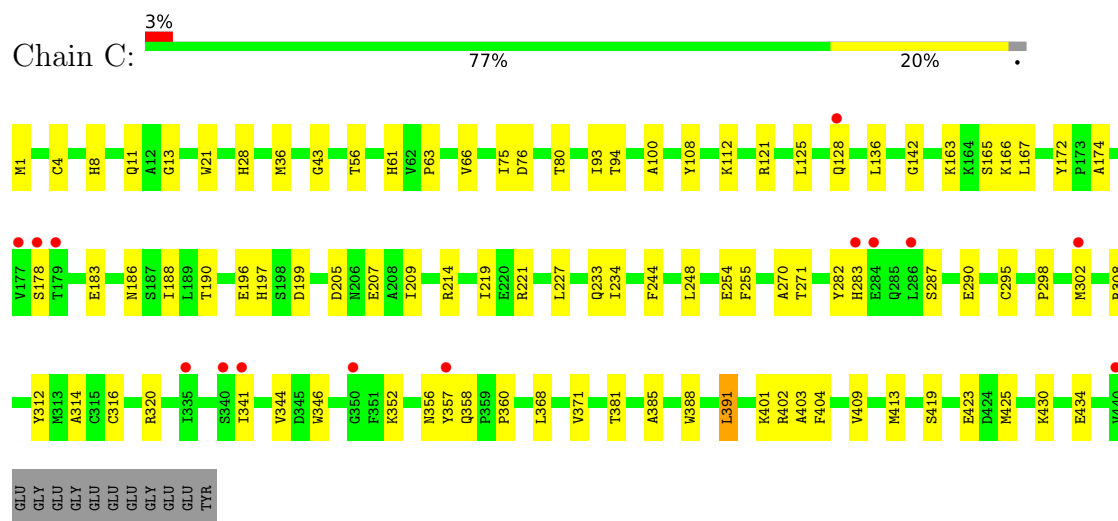
3 Residue-property plots

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

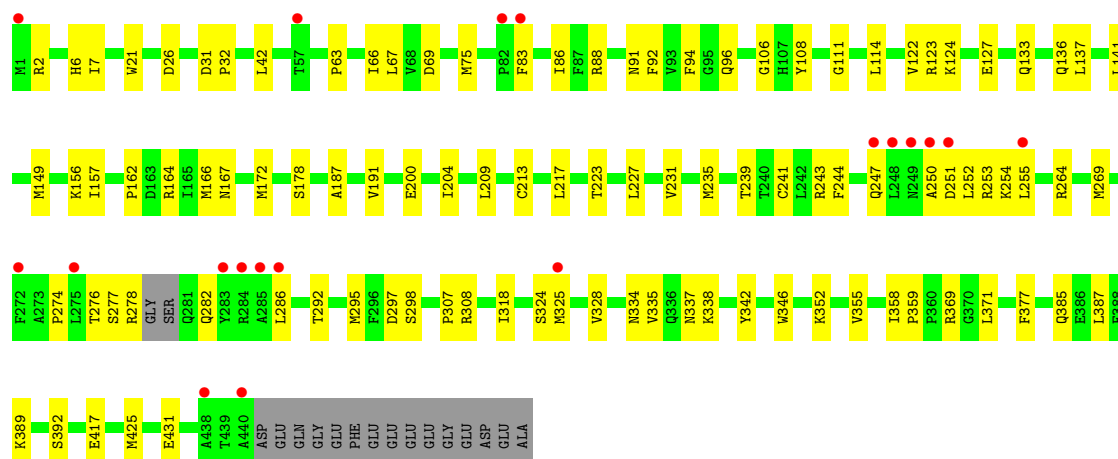


• Molecule 1: Tubulin alpha-1B chain

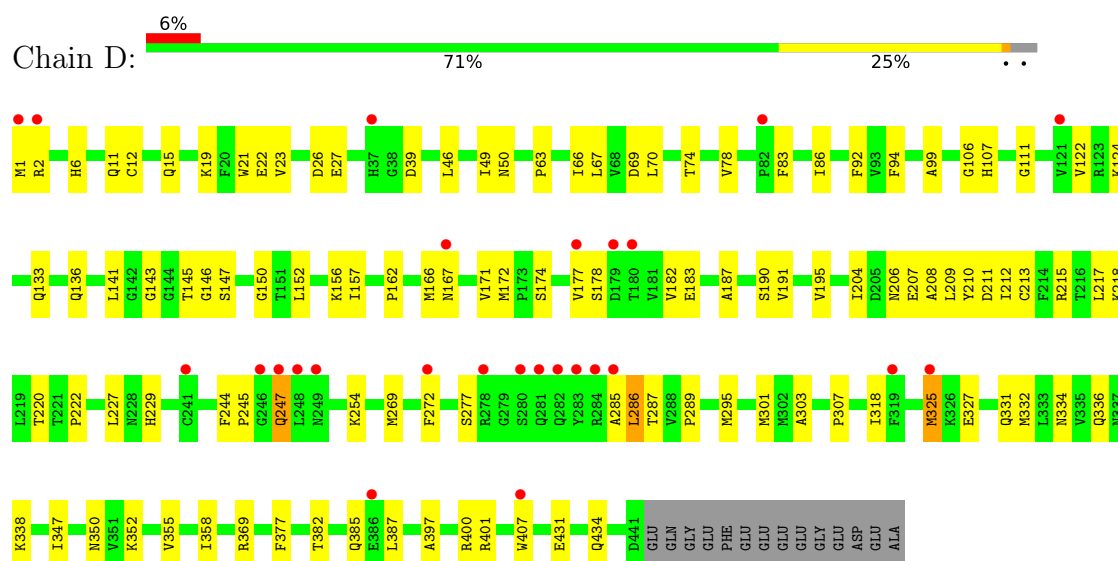


• Molecule 2: Tubulin beta-2B chain

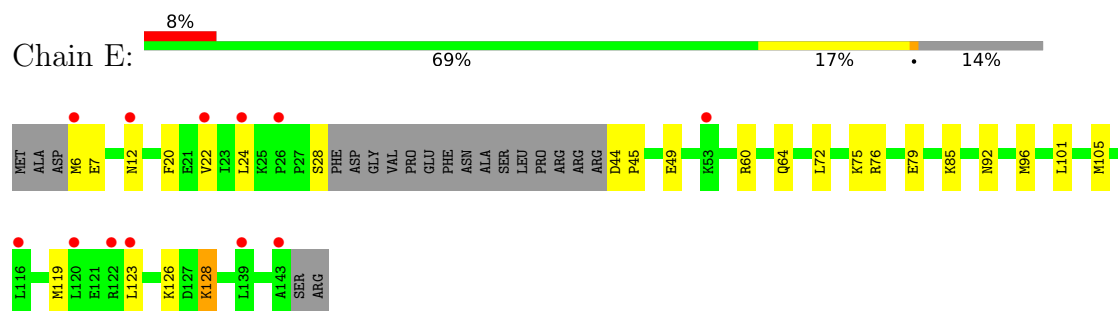




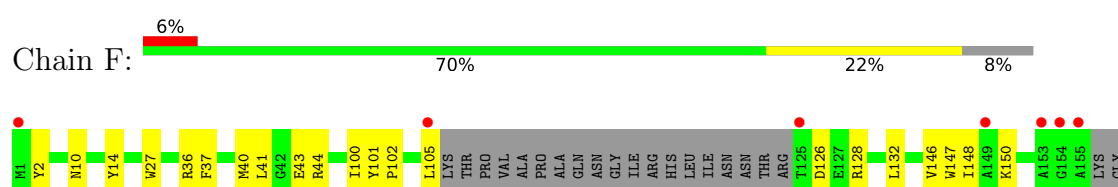
• Molecule 2: Tubulin beta-2B chain

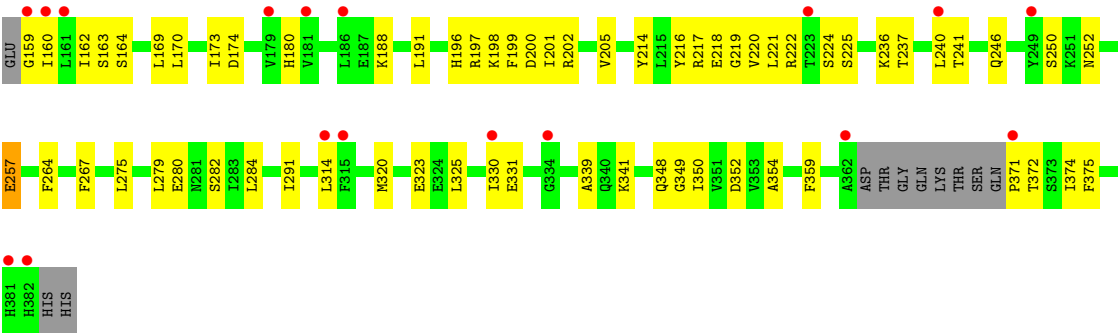


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.59Å 158.16Å 179.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.08 – 2.35 63.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.08-2.35) 99.8 (63.08-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.205 , 0.237 0.210 , 0.243	Depositor DCC
R_{free} test set	6345 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.3	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	0.96	EDS
Total number of atoms	18104	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, MG, MES, GDP, WZY, CA, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/3502	0.29	0/4754
1	C	0.13	0/3521	0.33	0/4780
2	B	0.12	0/3450	0.30	0/4671
2	D	0.10	0/3442	0.27	0/4664
3	E	0.11	0/1022	0.24	0/1356
4	F	0.09	0/2944	0.27	0/3978
All	All	0.11	0/17881	0.29	0/24203

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	84	0
1	C	3443	0	3352	69	0
2	B	3376	0	3252	79	0
2	D	3368	0	3236	86	0
3	E	1014	0	1029	20	0
4	F	2877	0	2839	62	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	3	0
9	B	12	0	12	3	0
10	B	13	13	0	1	0
10	C	13	13	0	0	0
10	D	13	13	0	0	0
10	E	13	13	0	1	0
11	F	31	0	14	3	0
12	A	58	0	0	3	0
12	B	62	0	0	3	0
12	C	160	0	0	4	0
12	D	30	0	0	4	0
12	E	11	0	0	2	0
12	F	5	0	0	0	0
All	All	18052	52	17116	377	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 11.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG22	1:A:383:ALA:H	1.20	1.07
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.37	1.06
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.40	0.99
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.47	0.93
1:C:209:ILE:HD11	1:C:302:MET:CE	2.04	0.88
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.58	0.84
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.61	0.83
1:A:297:GLU:HB2	1:A:300:ASN:HD21	1.43	0.82
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.97	0.82
2:B:167:ASN:OD1	2:B:200:GLU:HB2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.61	0.81
2:D:217:LEU:HA	2:D:277:SER:HB3	1.63	0.80
4:F:241:THR:OG1	11:F:401:ACP:O3'	1.98	0.80
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.62	0.79
1:A:294:ALA:O	1:A:300:ASN:ND2	2.18	0.76
1:A:300:ASN:OD1	12:A:601:HOH:O	2.02	0.76
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.51	0.76
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.51	0.76
1:C:76:ASP:O	1:C:80:THR:HG22	1.87	0.74
1:C:270:ALA:O	1:C:302:MET:HG2	1.89	0.73
2:D:162:PRO:CB	3:E:119:MET:HE1	2.19	0.72
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.71	0.72
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.71	0.72
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.71
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.24	0.71
2:D:83:PHE:O	2:D:86:ILE:HG22	1.93	0.69
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.75	0.69
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.27	0.69
2:D:431:GLU:OE1	12:D:601:HOH:O	2.10	0.68
1:C:234:ILE:HD13	1:C:302:MET:SD	2.33	0.68
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.23	0.68
2:B:83:PHE:O	2:B:86:ILE:HG22	1.94	0.68
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.12	0.68
1:A:179:THR:HA	2:B:352:LYS:HD2	1.75	0.67
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.77	0.66
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.31	0.66
2:D:11:GLN:O	2:D:15:GLN:HG2	1.96	0.66
4:F:371:PRO:HA	4:F:372:THR:HB	1.77	0.66
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.28	0.66
2:D:434:GLN:OE1	12:D:602:HOH:O	2.14	0.65
1:A:28:HIS:O	1:A:36:MET:HE3	1.97	0.65
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.27	0.65
2:D:162:PRO:HB2	3:E:119:MET:HE1	1.79	0.64
2:B:69:ASP:O	2:B:94:PHE:HA	1.98	0.64
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.33	0.64
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.97	0.64
1:C:282:TYR:O	1:C:283:HIS:HB2	1.98	0.64
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.81	0.63
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.64	0.63
1:C:234:ILE:HD13	1:C:302:MET:CE	2.28	0.63
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.81	0.62
4:F:371:PRO:HA	4:F:372:THR:O	1.99	0.62
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.82	0.62
2:B:96:GLN:CB	1:C:1:MET:HE2	2.30	0.62
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.80	0.62
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.14	0.61
4:F:188:LYS:HD3	4:F:323:GLU:OE2	2.00	0.61
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.80	0.61
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.82	0.61
2:D:215:ARG:O	2:D:218:LYS:HE3	2.00	0.61
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.60
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.66	0.60
1:C:221:ARG:CG	2:D:325:MET:HG2	2.24	0.60
2:D:325:MET:CE	2:D:355:VAL:HG21	2.32	0.60
2:D:285:ALA:O	2:D:286:LEU:HB2	2.02	0.59
4:F:246:GLN:O	4:F:250:SER:HB3	2.01	0.59
4:F:371:PRO:HA	4:F:372:THR:C	2.27	0.59
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.35	0.59
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.37	0.59
2:D:147:SER:HB2	2:D:190:SER:OG	2.02	0.59
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.02	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.85	0.58
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.85	0.58
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.39	0.58
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.18	0.58
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.33	0.58
2:B:324:SER:O	2:B:328:VAL:HG23	2.04	0.58
4:F:371:PRO:CA	4:F:372:THR:HB	2.33	0.57
4:F:159:GLY:C	4:F:160:ILE:HD12	2.30	0.57
2:B:136:GLN:HA	2:B:167:ASN:O	2.03	0.57
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.20	0.57
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.87	0.57
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.32	0.57
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.86	0.57
2:D:69:ASP:O	2:D:94:PHE:HA	2.04	0.57
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.36	0.56
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.85	0.56
1:A:431:ASP:O	1:A:435:VAL:HG23	2.05	0.56
2:B:325:MET:HE2	2:B:355:VAL:HG11	1.87	0.56
1:C:165:SER:HA	1:C:199:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.35	0.56
1:A:69:ASP:O	1:A:94:THR:HA	2.05	0.56
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.88	0.56
1:A:43:GLY:HA2	1:A:56:THR:O	2.06	0.56
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.39	0.56
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.36	0.56
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.89	0.55
1:A:223:THR:HB	2:B:247:GLN:HE22	1.72	0.55
1:C:214:ARG:HG2	1:C:219:ILE:O	2.07	0.55
2:D:152:LEU:O	2:D:156:LYS:HG2	2.07	0.55
2:B:278:ARG:HG2	2:B:282:GLN:NE2	2.21	0.55
1:C:28:HIS:O	1:C:36:MET:HE3	2.05	0.55
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.89	0.55
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.41	0.55
3:E:119:MET:HE2	10:E:201:WZY:C1	2.37	0.55
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.06	0.55
1:C:8:HIS:HB3	1:C:13:GLY:O	2.07	0.55
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.89	0.55
2:B:231:VAL:O	2:B:235:MET:HG3	2.08	0.54
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.32	0.54
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.87	0.54
2:B:164:ARG:O	9:B:504:MES:H31	2.07	0.54
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.88	0.54
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.43	0.54
1:C:271:THR:HG21	1:C:295:CYS:O	2.07	0.54
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.89	0.54
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.89	0.54
2:D:213:CYS:O	2:D:217:LEU:HB2	2.08	0.54
2:D:287:THR:HB	2:D:289:PRO:HD2	1.88	0.54
2:D:397:ALA:O	2:D:401:ARG:NH1	2.41	0.54
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.43	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.54
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.89	0.54
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.43	0.53
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.90	0.53
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.06	0.53
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.44	0.53
2:D:301:MET:HE3	2:D:307:PRO:HG3	1.91	0.53
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.24	0.53
2:B:141:LEU:HD12	2:B:172:MET:SD	2.49	0.53
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.44	0.53
4:F:350:ILE:O	4:F:354:ALA:HB3	2.09	0.53
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.91	0.52
1:C:360:PRO:HG2	1:C:371:VAL:HG23	1.90	0.52
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.89	0.52
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.90	0.52
2:D:124:LYS:C	2:D:124:LYS:HD3	2.34	0.52
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.24	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.08	0.52
2:D:146:GLY:O	2:D:150:GLY:HA3	2.10	0.52
2:B:295:MET:CG	2:B:377:PHE:HB2	2.39	0.52
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.44	0.52
3:E:12:ASN:HB3	12:E:307:HOH:O	2.09	0.52
3:E:128:LYS:O	3:E:128:LYS:HD3	2.09	0.52
1:A:419:SER:O	1:A:423:GLU:HG3	2.10	0.52
2:D:46:LEU:HA	2:D:49:ILE:HB	1.92	0.52
2:D:187:ALA:O	2:D:191:VAL:HG23	2.10	0.52
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.10	0.52
1:C:186:ASN:O	1:C:190:THR:HG22	2.10	0.51
2:D:69:ASP:HA	2:D:145:THR:HG21	1.91	0.51
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.10	0.51
2:D:332:MET:O	2:D:336:GLN:HG3	2.10	0.51
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.92	0.51
2:D:19:LYS:O	2:D:23:VAL:HG23	2.10	0.51
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.93	0.51
2:D:204:ILE:HG22	2:D:209:LEU:HD11	1.93	0.51
2:D:211:ASP:O	2:D:215:ARG:HB2	2.10	0.51
3:E:85:LYS:NZ	12:E:304:HOH:O	2.43	0.51
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.74	0.50
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.92	0.50
2:D:327:GLU:O	2:D:331:GLN:HG2	2.10	0.50
2:D:178:SER:HB3	2:D:183:GLU:OE2	2.11	0.50
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.11	0.50
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.50
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.41	0.50
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.94	0.50
4:F:197:ARG:HB2	4:F:224:SER:O	2.12	0.50
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.29	0.50
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.44	0.49
1:A:151:SER:HB2	1:A:193:THR:OG1	2.11	0.49
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.47	0.49
4:F:341:LYS:HG2	4:F:341:LYS:O	2.12	0.49
1:A:88:HIS:NE2	1:A:91:GLN:HG3	2.27	0.49
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.49
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.94	0.49
2:B:241:CYS:HB3	2:B:250:ALA:HB2	1.93	0.49
2:B:42:LEU:H	2:B:42:LEU:HD12	1.78	0.49
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.94	0.49
2:D:213:CYS:HA	2:D:217:LEU:HD12	1.94	0.49
1:A:320:ARG:HG3	12:A:646:HOH:O	2.11	0.49
2:B:178:SER:N	10:B:505:WZY:O2	2.27	0.49
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.48	0.49
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.94	0.49
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.95	0.49
4:F:198:LYS:HG2	4:F:199:PHE:H	1.76	0.49
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.13	0.49
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.42	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.49
2:D:191:VAL:O	2:D:195:VAL:HG23	2.13	0.49
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.48	0.49
1:A:119:LEU:HD12	1:A:156:ARG:NH2	2.27	0.48
2:B:164:ARG:HD2	12:B:655:HOH:O	2.14	0.48
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.43	0.48
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.29	0.48
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.95	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.48
1:A:214:ARG:HG2	1:A:219:ILE:O	2.13	0.48
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.48
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.44	0.48
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.94	0.48
1:C:221:ARG:HG3	2:D:325:MET:CG	2.26	0.48
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.96	0.48
4:F:162:ILE:HD11	4:F:240:LEU:HD11	1.95	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.47
2:D:208:ALA:O	2:D:212:ILE:HG13	2.13	0.47
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.96	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
1:C:287:SER:OG	1:C:290:GLU:HG3	2.14	0.47
1:A:284:GLU:CD	1:A:284:GLU:H	2.21	0.47
2:B:124:LYS:HD3	2:B:124:LYS:C	2.39	0.47
12:B:629:HOH:O	1:C:163:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:O	1:C:112:LYS:HG2	2.14	0.47
1:C:196:GLU:HG2	12:C:663:HOH:O	2.15	0.47
2:D:382:THR:O	2:D:385:GLN:HG2	2.14	0.47
2:B:297:ASP:OD1	2:B:298:SER:N	2.47	0.47
2:D:107:HIS:O	2:D:152:LEU:HD22	2.14	0.47
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.96	0.47
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.15	0.47
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.96	0.47
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.97	0.47
1:A:71:GLU:HG2	1:A:72:PRO:N	2.29	0.47
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.47	0.47
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.50	0.47
2:B:318:ILE:N	2:B:318:ILE:HD12	2.30	0.47
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.47
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.45	0.47
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.50	0.47
2:D:141:LEU:HA	2:D:147:SER:HB3	1.97	0.47
4:F:191:LEU:HD13	4:F:196:HIS:CD2	2.50	0.47
1:C:270:ALA:HB3	1:C:302:MET:CG	2.45	0.46
2:D:145:THR:HB	8:D:501:GDP:O2B	2.15	0.46
1:C:401:LYS:NZ	12:C:608:HOH:O	2.47	0.46
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.16	0.46
1:A:381:THR:HG22	1:A:383:ALA:N	2.05	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.46
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.98	0.46
2:B:392:SER:HB2	2:B:425:MET:HE3	1.96	0.46
1:C:419:SER:O	1:C:423:GLU:HG3	2.14	0.46
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.50	0.46
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.46
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.16	0.46
2:B:114:LEU:O	2:B:114:LEU:HG	2.15	0.46
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.45	0.46
2:D:162:PRO:HB3	3:E:119:MET:HE1	1.95	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.16	0.46
4:F:101:TYR:N	4:F:126:ASP:OD1	2.31	0.46
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.49	0.46
1:C:178:SER:OG	2:D:352:LYS:NZ	2.49	0.46
1:C:205:ASP:HB3	1:C:302:MET:O	2.15	0.46
1:A:289:ALA:HA	1:A:331:ALA:CB	2.46	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:HB2	1:A:300:ASN:ND2	2.22	0.45
1:A:141:PHE:HB3	1:A:187:SER:OG	2.16	0.45
1:A:438:ASP:OD1	1:A:438:ASP:N	2.49	0.45
1:A:10:GLY:O	1:A:14:VAL:HG23	2.15	0.45
2:D:141:LEU:HD12	2:D:172:MET:SD	2.56	0.45
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.45	0.45
2:B:334:ASN:ND2	2:B:338:LYS:HD2	2.32	0.45
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.45
2:D:74:THR:O	2:D:78:VAL:HG23	2.17	0.45
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.52	0.45
4:F:2:TYR:O	4:F:27:TRP:HA	2.16	0.45
1:A:362:VAL:HG22	12:A:602:HOH:O	2.16	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45
2:B:387:LEU:C	2:B:387:LEU:HD23	2.42	0.45
1:C:43:GLY:HA2	1:C:56:THR:O	2.17	0.45
3:E:101:LEU:O	3:E:105:MET:HG2	2.17	0.45
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.98	0.45
4:F:202:ARG:HB3	4:F:220:VAL:CG2	2.47	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
1:C:401:LYS:O	1:C:402:ARG:HB2	2.17	0.44
3:E:92:ASN:O	3:E:96:MET:HG2	2.16	0.44
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.97	0.44
1:A:132:LEU:O	1:A:164:LYS:NZ	2.51	0.44
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.98	0.44
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.45	0.44
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.40	0.44
2:B:276:THR:HG22	2:B:277:SER:O	2.18	0.44
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.83	0.44
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.53	0.44
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.82	0.43
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.53	0.43
1:A:135:PHE:C	1:A:136:LEU:HD23	2.44	0.43
1:A:234:ILE:HD12	1:A:234:ILE:N	2.33	0.43
2:B:96:GLN:HB2	1:C:1:MET:HE2	2.00	0.43
2:D:325:MET:HE2	2:D:355:VAL:HG21	1.99	0.43
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.53	0.43
1:A:118:VAL:HG21	1:A:149:PHE:HZ	1.83	0.43
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.53	0.43
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.59	0.43
2:D:66:ILE:HD12	2:D:122:VAL:HG22	2.01	0.43
2:D:220:THR:O	2:D:222:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.00	0.43
1:A:119:LEU:HD13	1:A:160:ASP:OD2	2.19	0.43
2:B:88:ARG:NH2	2:B:124:LYS:HE3	2.33	0.43
4:F:148:ILE:HD11	4:F:160:ILE:HG21	2.00	0.43
2:B:42:LEU:HD12	2:B:42:LEU:N	2.34	0.43
2:D:325:MET:HE1	2:D:355:VAL:HG21	2.00	0.43
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.00	0.43
1:A:70:LEU:HD13	1:A:110:ILE:HG21	2.00	0.43
2:B:278:ARG:HG2	2:B:282:GLN:HE22	1.83	0.43
2:B:359:PRO:HB2	2:B:371:LEU:O	2.18	0.42
1:C:75:ILE:HB	1:C:94:THR:CG2	2.48	0.42
1:C:174:ALA:HB2	1:C:207:GLU:N	2.35	0.42
2:D:177:VAL:HG11	2:D:206:ASN:ND2	2.34	0.42
2:B:223:THR:O	2:B:227:LEU:HD13	2.20	0.42
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.54	0.42
2:D:182:VAL:HG11	2:D:407:TRP:CE3	2.55	0.42
2:D:174:SER:OG	2:D:207:GLU:OE1	2.35	0.42
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.02	0.42
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.55	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.02	0.42
2:D:19:LYS:HE3	12:D:620:HOH:O	2.19	0.42
1:A:47:ASP:HB2	1:A:49:PHE:CE2	2.55	0.42
1:A:329:ASN:HB3	3:E:6:MET:CE	2.49	0.42
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.02	0.42
2:B:156:LYS:HE3	12:B:641:HOH:O	2.19	0.42
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.20	0.42
4:F:240:LEU:HD12	4:F:240:LEU:N	2.35	0.42
1:A:399:TYR:O	1:A:402:ARG:NH1	2.51	0.42
2:B:114:LEU:HD23	2:B:149:MET:HE1	2.01	0.42
2:B:251:ASP:HB3	2:B:254:LYS:HB2	2.01	0.41
2:B:269:MET:HE1	2:B:307:PRO:HG3	2.01	0.41
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.55	0.41
2:D:220:THR:C	2:D:222:PRO:HD3	2.45	0.41
3:E:7:GLU:O	3:E:22:VAL:HA	2.20	0.41
3:E:123:LEU:O	3:E:126:LYS:HB2	2.21	0.41
1:A:223:THR:HB	2:B:247:GLN:NE2	2.34	0.41
3:E:44:ASP:HB3	3:E:45:PRO:HD2	2.03	0.41
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.55	0.41
4:F:237:THR:O	4:F:246:GLN:NE2	2.46	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:HB2	2:B:123:ARG:CZ	2.51	0.41
1:C:409:VAL:HA	1:C:413:MET:O	2.21	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.03	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.54	0.41
4:F:236:LYS:O	4:F:240:LEU:HD13	2.21	0.41
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.01	0.41
2:B:187:ALA:O	2:B:191:VAL:HG23	2.21	0.41
1:C:128:GLN:NE2	12:C:615:HOH:O	2.54	0.41
2:B:162:PRO:O	9:B:504:MES:H72	2.21	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.03	0.41
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.56	0.41
1:A:75:ILE:HD12	1:A:94:THR:CG2	2.49	0.41
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.21	0.41
1:C:75:ILE:HB	1:C:94:THR:HG21	2.03	0.41
4:F:163:SER:HB3	4:F:169:LEU:CD2	2.50	0.41
4:F:320:MET:HG3	4:F:330:ILE:HD11	2.03	0.41
1:A:230:LEU:O	1:A:234:ILE:HD13	2.20	0.41
3:E:60:ARG:O	3:E:64:GLN:HG3	2.20	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.56	0.41
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.21	0.40
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.90	0.40
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.21	0.40
4:F:150:LYS:NZ	11:F:401:ACP:N7	2.62	0.40
2:B:63:PRO:HD2	2:B:86:ILE:O	2.21	0.40
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.54	0.40
1:C:403:ALA:O	1:C:404:PHE:HB2	2.21	0.40
2:D:213:CYS:SG	2:D:227:LEU:HD23	2.61	0.40
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.02	0.40
4:F:225:SER:O	4:F:252:ASN:HB2	2.21	0.40
1:A:223:THR:O	1:A:227:LEU:HG	2.22	0.40
2:B:88:ARG:CZ	2:B:124:LYS:HE3	2.52	0.40
2:B:239:THR:O	2:B:243:ARG:HG3	2.22	0.40
2:D:23:VAL:O	2:D:27:GLU:HG3	2.21	0.40
2:D:272:PHE:HE2	12:D:624:HOH:O	2.03	0.40
1:A:270:ALA:HB3	1:A:302:MET:CG	2.52	0.40
1:C:314:ALA:HB2	12:C:632:HOH:O	2.22	0.40
2:D:157:ILE:CG2	2:D:166:MET:HE1	2.52	0.40
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.40	0.40
4:F:275:LEU:N	4:F:275:LEU:HD22	2.37	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	436/451 (97%)	426 (98%)	10 (2%)	0	100	100
1	C	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
2	B	425/445 (96%)	410 (96%)	15 (4%)	0	100	100
2	D	429/445 (96%)	413 (96%)	14 (3%)	2 (0%)	24	27
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	344/384 (90%)	327 (95%)	17 (5%)	0	100	100
All	All	2192/2319 (94%)	2124 (97%)	66 (3%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	286	LEU
2	D	245	PRO

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	369/379 (97%)	364 (99%)	5 (1%)	59	73
1	C	372/379 (98%)	370 (100%)	2 (0%)	81	89
2	B	369/383 (96%)	369 (100%)	0	100	100
2	D	368/383 (96%)	364 (99%)	4 (1%)	65	79
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	315/342 (92%)	313 (99%)	2 (1%)	78	87
All	All	1903/1993 (96%)	1889 (99%)	14 (1%)	76	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	178	SER
1	A	284	GLU
1	A	300	ASN
1	A	438	ASP
1	C	381	THR
1	C	391	LEU
2	D	39	ASP
2	D	229	HIS
2	D	247	GLN
2	D	325	MET
3	E	128	LYS
4	F	43	GLU
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	249	ASN
1	A	258	ASN
1	A	300	ASN
1	A	301	GLN
1	A	309	HIS
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN
2	B	15	GLN
2	B	136	GLN
2	B	193	GLN
2	B	247	GLN
2	B	282	GLN
2	B	294	GLN
2	B	349	ASN
1	C	11	GLN

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Mol	Chain	Res	Type
1	C	356	ASN
1	C	406	HIS
2	D	96	GLN
2	D	133	GLN
2	D	294	GLN
2	D	349	ASN
3	E	12	ASN
3	E	103	GLN
3	E	136	ASN
4	F	180	HIS
4	F	196	HIS
4	F	269	GLN
4	F	306	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	$\# Z > 2$
8	GDP	D	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.74	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	501	6	33,34,34	1.03	4 (12%)	50,54,54	1.50	8 (16%)
9	MES	B	504	-	12,12,12	2.32	1 (8%)	15,16,16	2.05	5 (33%)
10	WZY	B	505	-	12,13,13	0.13	0	14,16,16	0.32	0
10	WZY	C	504	-	12,13,13	0.11	0	14,16,16	0.43	0
10	WZY	E	201	-	12,13,13	0.13	0	14,16,16	0.59	0
8	GDP	B	501	6	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
5	GTP	A	501	6	33,34,34	1.03	2 (6%)	50,54,54	1.50	8 (16%)
11	ACP	F	401	6	31,33,33	1.71	9 (29%)	47,52,52	1.87	10 (21%)
10	WZY	D	503	-	12,13,13	0.13	0	14,16,16	0.45	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
8	GDP	D	501	6	-	6/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	WZY	B	505	-	-	4/8/8/8	0/1/1/1
10	WZY	C	504	-	-	0/8/8/8	0/1/1/1
10	WZY	E	201	-	-	0/8/8/8	0/1/1/1
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
11	ACP	F	401	6	-	12/19/38/38	0/3/3/3
10	WZY	D	503	-	-	2/8/8/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.71	1.66	1.77
11	F	401	ACP	C5-C4	4.73	1.47	1.39
8	D	501	GDP	C5-C4	3.12	1.47	1.38
11	F	401	ACP	PG-O2G	3.06	1.61	1.55
11	F	401	ACP	PG-O3G	3.00	1.61	1.55
8	B	501	GDP	C5-C4	2.98	1.46	1.38
11	F	401	ACP	PB-O3A	2.98	1.61	1.58
11	F	401	ACP	C5-C6	2.76	1.48	1.41
5	A	501	GTP	PB-O3B	2.43	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C6-N1	-2.42	1.34	1.38
5	C	501	GTP	PA-O3A	2.36	1.62	1.59
8	D	501	GDP	C6-N1	-2.36	1.34	1.38
5	A	501	GTP	PA-O3A	2.36	1.62	1.59
5	C	501	GTP	PB-O3A	2.35	1.62	1.59
11	F	401	ACP	PA-O3A	2.33	1.62	1.59
11	F	401	ACP	C8-N7	2.30	1.36	1.31
11	F	401	ACP	PB-O2B	2.19	1.61	1.56
11	F	401	ACP	C5-N7	-2.19	1.35	1.39
5	C	501	GTP	PB-O3B	2.16	1.61	1.59
5	C	501	GTP	C2-N3	2.07	1.38	1.33
8	B	501	GDP	C5-N7	-2.04	1.35	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-6.07	118.73	128.39
8	B	501	GDP	C5-C4-N3	-5.83	119.11	128.39
11	F	401	ACP	C5-C4-N3	-5.72	118.83	126.72
8	D	501	GDP	C2-N3-C4	5.09	121.07	112.30
8	B	501	GDP	C2-N3-C4	5.00	120.91	112.30
5	C	501	GTP	C5-C4-N3	-4.68	120.94	128.39
5	A	501	GTP	C5-C4-N3	-4.61	121.05	128.39
11	F	401	ACP	N3-C4-N9	4.61	135.00	127.17
5	A	501	GTP	C2-N3-C4	4.51	120.07	112.30
8	D	501	GDP	N9-C4-N3	4.46	134.88	125.95
9	B	504	MES	C5-N4-C3	4.42	118.36	108.84
8	B	501	GDP	N9-C4-N3	4.33	134.60	125.95
5	C	501	GTP	C2-N3-C4	4.30	119.71	112.30
11	F	401	ACP	PB-O3A-PA	-3.83	119.89	132.37
11	F	401	ACP	C2-N3-C4	3.67	120.79	111.83
9	B	504	MES	C6-C5-N4	-3.48	104.83	110.12
8	B	501	GDP	C6-C5-N7	3.43	136.53	130.29
11	F	401	ACP	C4-C5-N7	-3.37	106.73	110.58
8	D	501	GDP	C6-C5-N7	3.34	136.38	130.29
11	F	401	ACP	N3-C2-N1	-3.27	123.63	128.58
5	C	501	GTP	N9-C4-N3	2.86	131.67	125.95
5	C	501	GTP	C2-N1-C6	-2.81	120.01	125.11
5	A	501	GTP	N9-C4-N3	2.79	131.53	125.95
5	A	501	GTP	C2-N1-C6	-2.71	120.20	125.11
5	C	501	GTP	N9-C8-N7	-2.68	108.43	113.40
11	F	401	ACP	C4-N9-C8	2.67	108.54	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N9-C8-N7	-2.67	108.46	113.40
8	D	501	GDP	C4-C5-N7	-2.63	106.50	110.67
11	F	401	ACP	C3'-C2'-C1'	2.63	106.43	101.46
8	B	501	GDP	C4-C5-N7	-2.56	106.61	110.67
5	C	501	GTP	C8-N7-C5	2.52	108.75	104.26
11	F	401	ACP	C5-N7-C8	2.50	107.37	103.45
5	A	501	GTP	C8-N7-C5	2.47	108.65	104.26
5	A	501	GTP	C5-C6-N1	2.39	119.33	113.25
5	A	501	GTP	O6-C6-C5	-2.36	120.29	126.53
5	C	501	GTP	O6-C6-C5	-2.30	120.46	126.53
5	C	501	GTP	C5-C6-N1	2.29	119.08	113.25
8	B	501	GDP	O6-C6-C5	-2.28	120.51	126.53
9	B	504	MES	C2-C3-N4	-2.22	106.74	110.12
9	B	504	MES	C7-N4-C5	2.21	117.14	111.24
8	D	501	GDP	O6-C6-C5	-2.11	120.95	126.53
9	B	504	MES	C7-N4-C3	2.08	116.79	111.24
11	F	401	ACP	C6-C5-N7	2.06	136.05	132.09

There are no chirality outliers.

All (45) 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	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
10	B	505	WZY	N1-C8-C9-N2
10	B	505	WZY	O2-C8-C9-N2
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
9	B	504	MES	C7-C8-S-O3S
10	D	503	WZY	O2-C8-C9-N2
10	D	503	WZY	N1-C8-C9-N2
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	PA-O3A-PB-O1B
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
10	B	505	WZY	C4-C3-O1-C7
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	505	WZY	C2-C3-O1-C7
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	PA-O3A-PB-O3B
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O1A

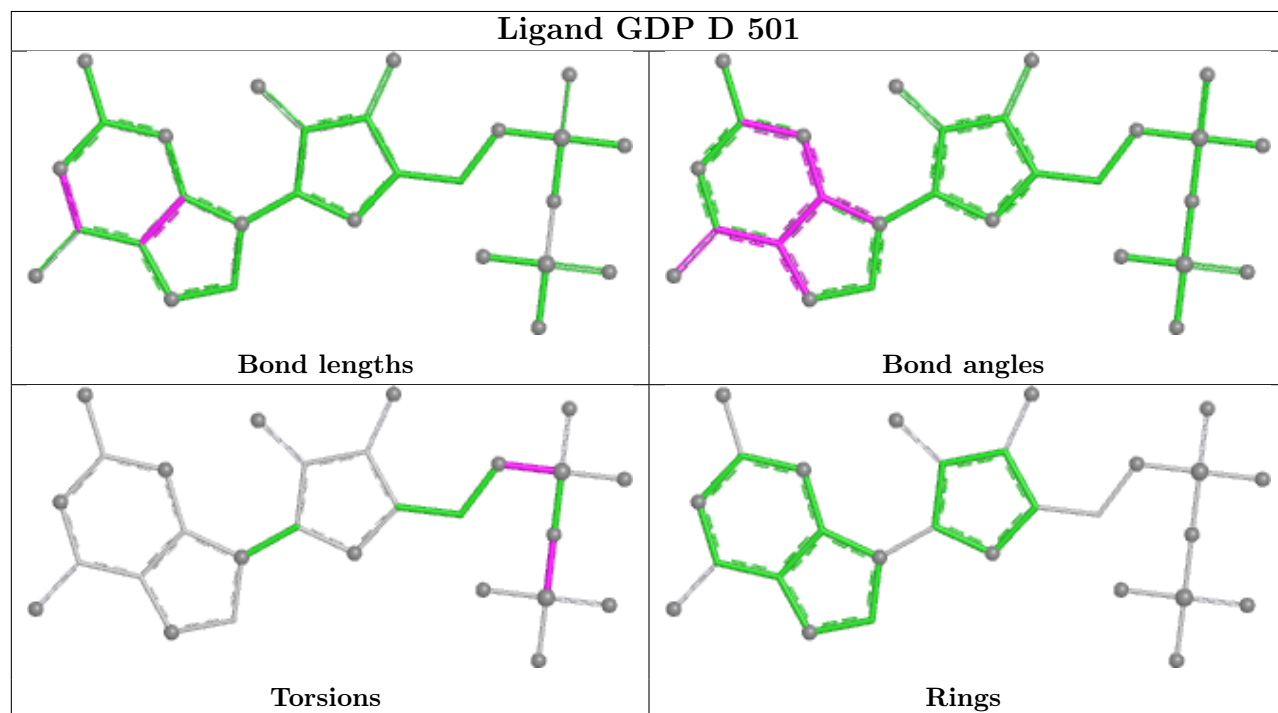
There are no ring outliers.

6 monomers are involved in 12 short contacts:

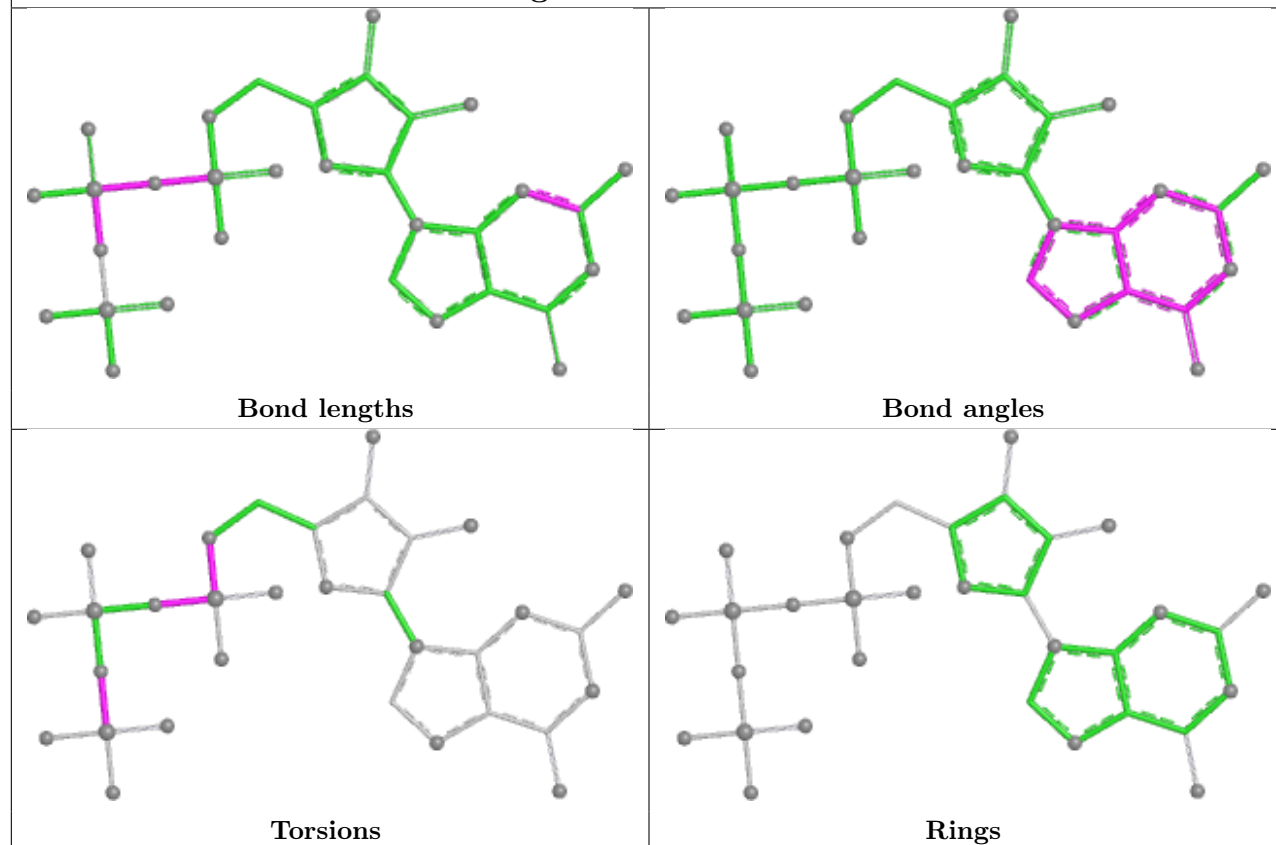
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	3	0
9	B	504	MES	3	0
10	B	505	WZY	1	0
10	E	201	WZY	1	0
5	A	501	GTP	1	0
11	F	401	ACP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

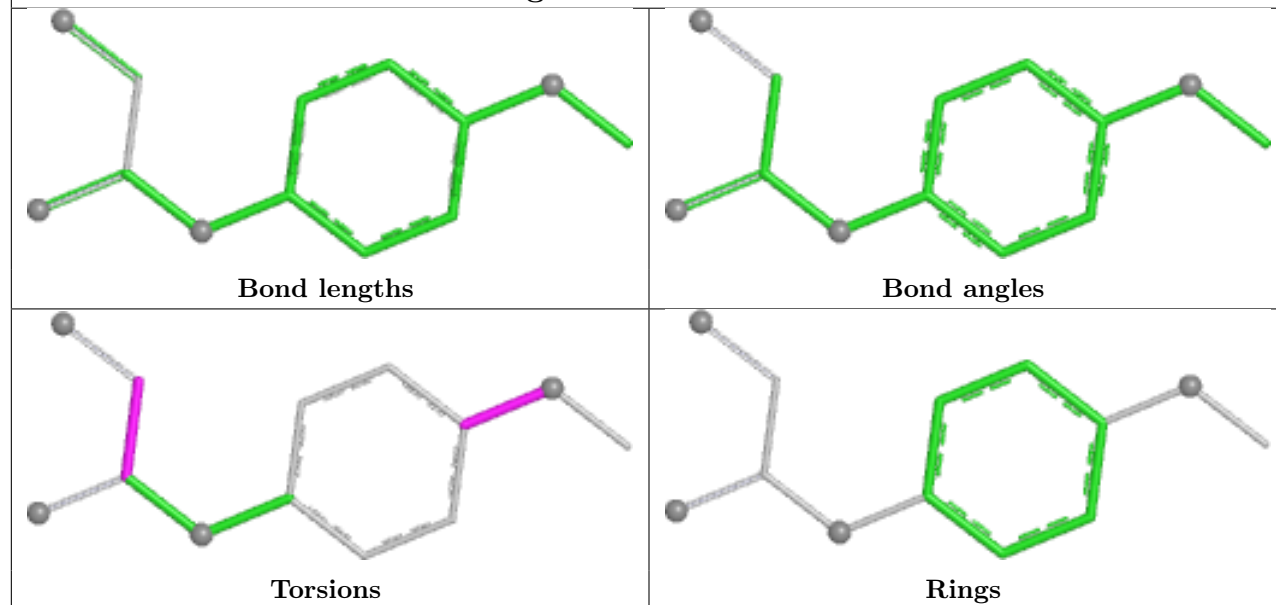
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

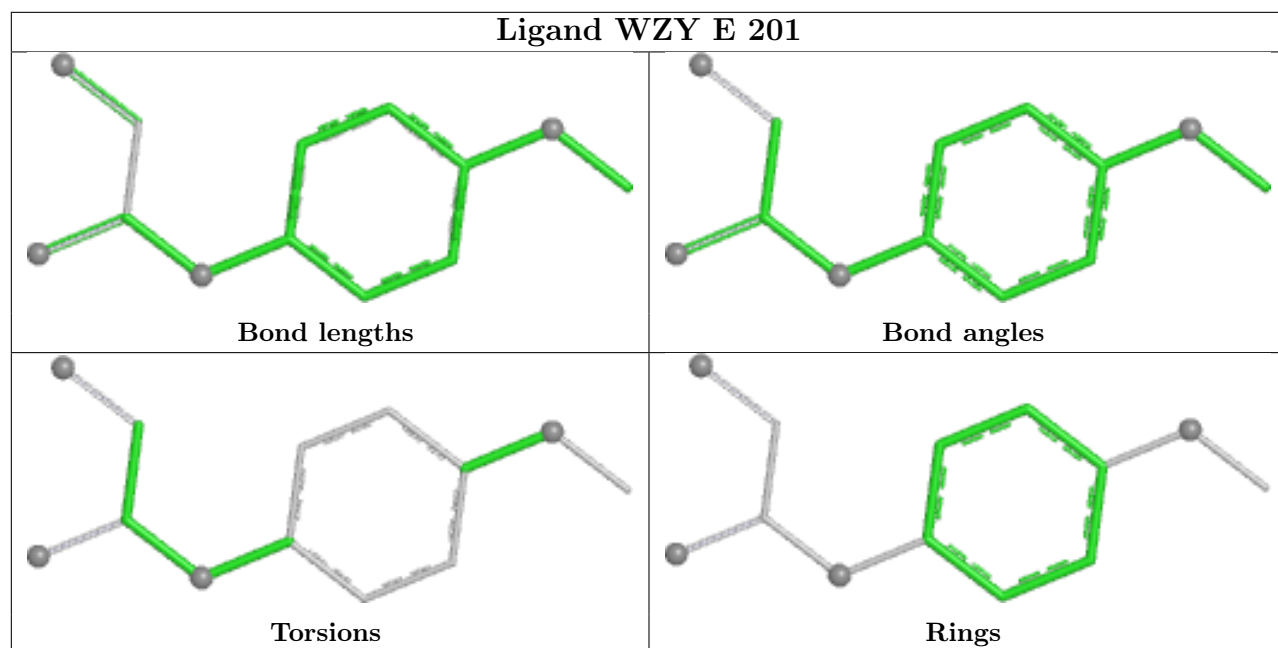
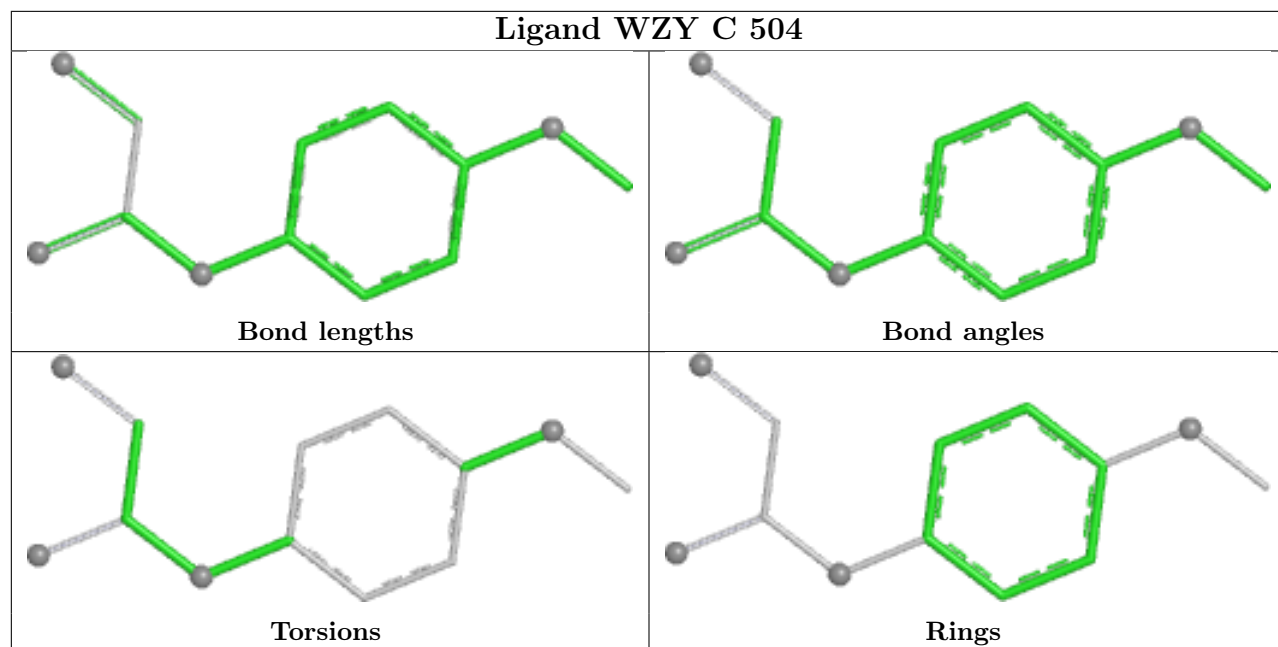


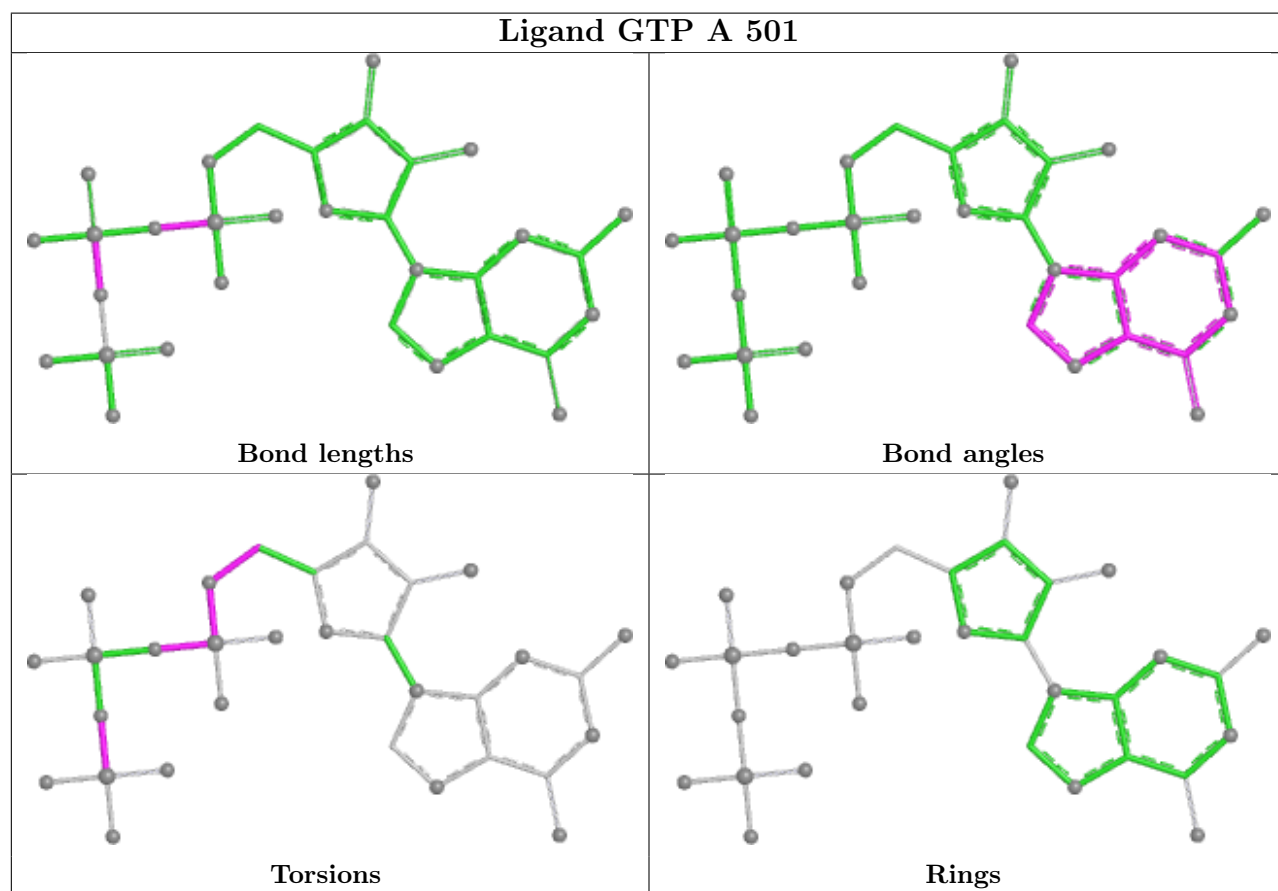
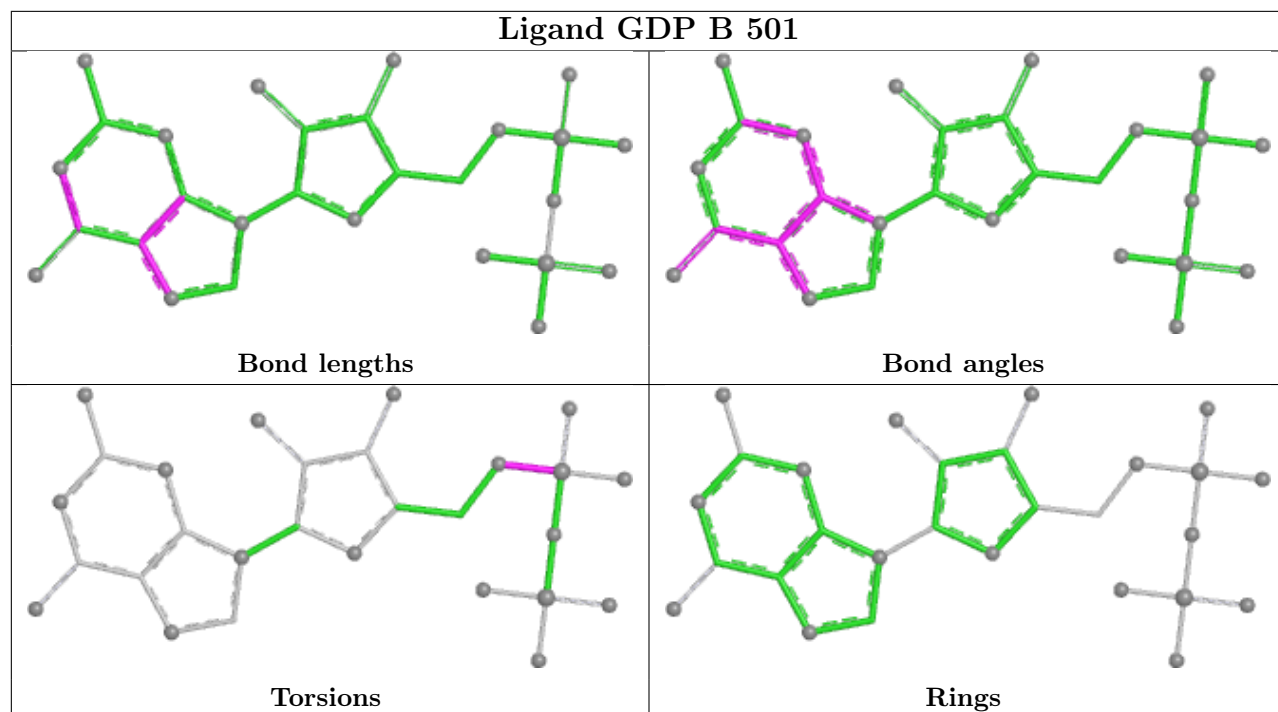
Ligand GTP C 501

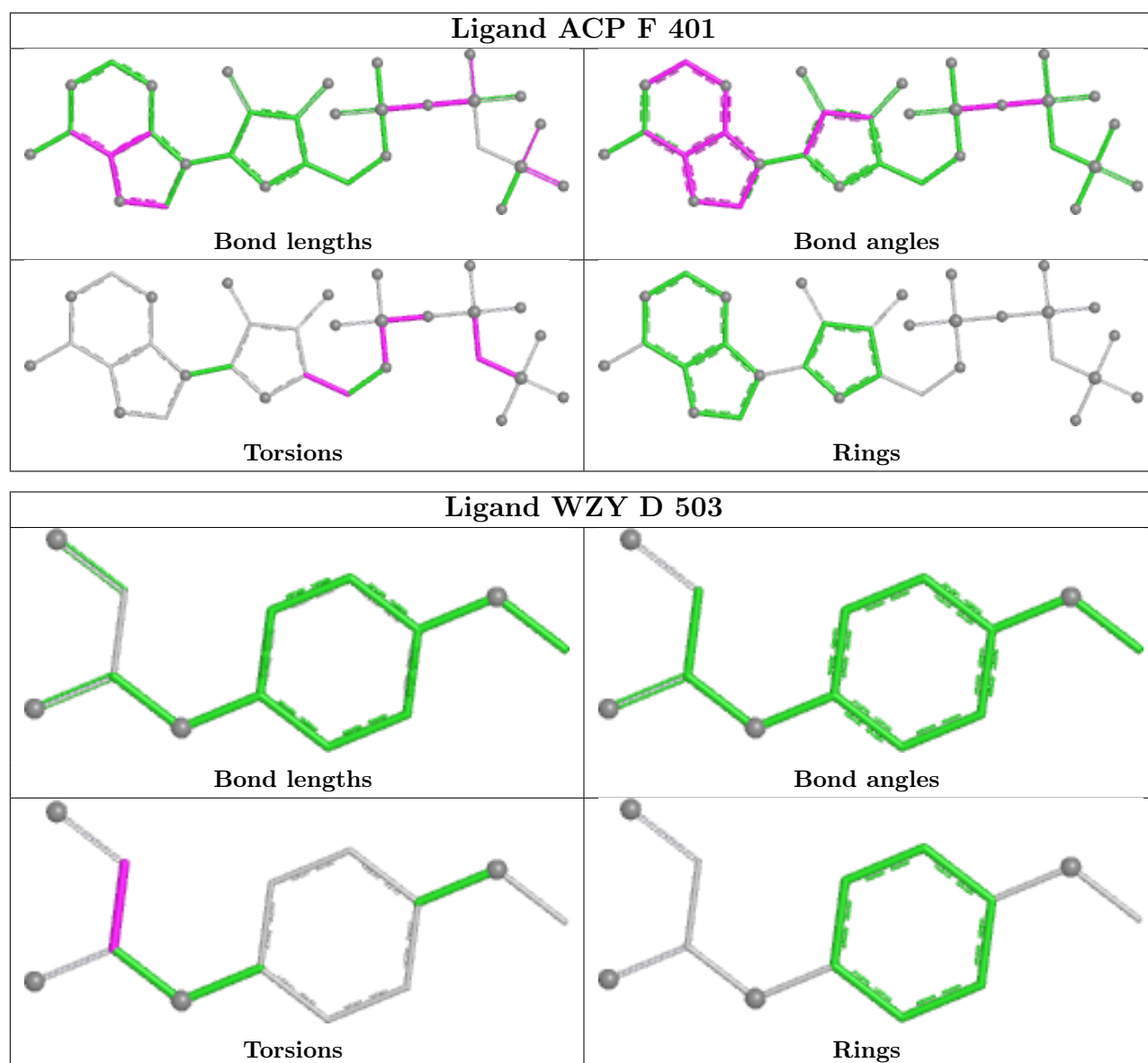


Ligand WZY B 505









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	438/451 (97%)	0.35	11 (2%)	58	64	51, 69, 109, 184	0
1	C	440/451 (97%)	0.13	14 (3%)	50	57	29, 58, 83, 131	1 (0%)
2	B	428/445 (96%)	0.39	19 (4%)	39	45	34, 66, 116, 164	2 (0%)
2	D	431/445 (96%)	0.53	26 (6%)	27	31	54, 78, 114, 192	4 (0%)
3	E	123/143 (86%)	0.71	12 (9%)	13	15	57, 79, 129, 163	0
4	F	352/384 (91%)	0.79	24 (6%)	23	26	67, 103, 169, 206	0
All	All	2212/2319 (95%)	0.44	106 (4%)	35	41	29, 72, 135, 206	7 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	249	ASN	7.5
4	F	155	ALA	6.8
2	B	248	LEU	6.2
4	F	159	GLY	5.1
2	D	283	TYR	5.1
1	C	440	VAL	4.9
1	A	179	THR	4.6
3	E	24	LEU	4.4
2	D	407	TRP	4.2
2	D	284	ARG	4.0
2	D	248	LEU	3.9
4	F	125	THR	3.8
2	D	282	GLN	3.7
1	A	351	PHE	3.7
4	F	371	PRO	3.7
4	F	186	LEU	3.5
1	C	357	TYR	3.5
4	F	240	LEU	3.5
2	B	285	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	179	VAL	3.5
2	B	1	MET	3.3
2	D	249	ASN	3.2
4	F	160	ILE	3.2
2	D	272	PHE	3.1
1	C	341	ILE	3.1
1	C	177	VAL	3.1
4	F	153	ALA	3.1
3	E	143	ALA	3.0
1	C	286	LEU	3.0
1	A	262	TYR	3.0
2	D	280	SER	3.0
2	B	275	LEU	3.0
4	F	249	TYR	3.0
2	B	283	TYR	2.9
2	D	281	GLN	2.9
2	D	121	VAL	2.9
2	B	57	THR	2.9
1	A	282	TYR	2.9
1	C	128	GLN	2.9
2	B	251	ASP	2.9
1	A	437	VAL	2.8
1	A	88	HIS	2.8
4	F	381	HIS	2.8
1	C	340	SER	2.8
2	D	241	CYS	2.8
4	F	382	HIS	2.7
4	F	149	ALA	2.6
2	B	250	ALA	2.6
2	B	272	PHE	2.6
2	D	177	VAL	2.6
2	B	255	LEU	2.6
2	B	284	ARG	2.5
1	C	302	MET	2.5
3	E	6	MET	2.5
1	A	281	ALA	2.5
1	C	179	THR	2.4
2	D	386	GLU	2.4
4	F	161	LEU	2.4
4	F	314	LEU	2.4
1	C	284	GLU	2.4
2	B	325	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	123	LEU	2.4
1	A	438	ASP	2.3
2	D	246	GLY	2.3
2	D	180	THR	2.3
1	C	283	HIS	2.3
2	B	82	PRO	2.3
2	D	82	PRO	2.3
4	F	181	VAL	2.3
1	A	178	SER	2.3
4	F	330	ILE	2.3
3	E	116	LEU	2.2
1	C	350	GLY	2.2
4	F	223	THR	2.2
2	D	37	HIS	2.2
2	D	247	GLN	2.2
2	D	285	ALA	2.2
3	E	22	VAL	2.2
4	F	1	MET	2.2
3	E	122	ARG	2.2
1	A	285	GLN	2.2
2	B	247	GLN	2.2
1	C	178	SER	2.2
4	F	334	GLY	2.1
2	D	1	MET	2.1
4	F	105	LEU	2.1
2	D	179	ASP	2.1
3	E	12	ASN	2.1
3	E	26	PRO	2.1
2	B	438	ALA	2.1
2	B	440	ALA	2.1
4	F	362	ALA	2.1
1	C	335	ILE	2.1
2	D	167	ASN	2.1
2	D	2	ARG	2.1
2	D	278	ARG	2.1
3	E	120	LEU	2.1
1	A	362	VAL	2.1
2	B	83	PHE	2.1
2	D	319	PHE	2.1
2	B	286	LEU	2.0
3	E	139	LEU	2.0
4	F	154	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	315	PHE	2.0
3	E	53	LYS	2.0
2	D	325	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

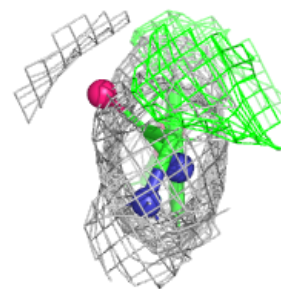
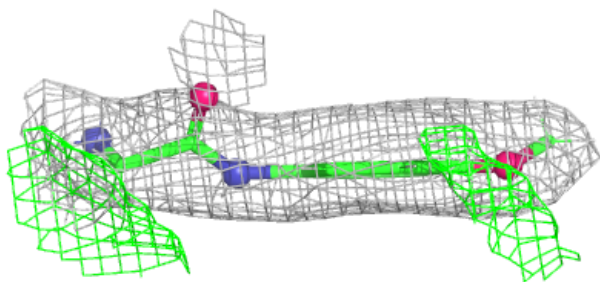
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MES	B	504	12/12	0.45	0.25	65,84,94,102	0
10	WZY	B	505	13/13	0.78	0.15	61,73,90,92	26
6	MG	D	502	1/1	0.79	0.12	79,79,79,79	0
10	WZY	C	504	13/13	0.82	0.14	71,79,93,95	26
11	ACP	F	401	31/31	0.86	0.10	98,109,119,124	0
7	CA	B	503	1/1	0.88	0.12	96,96,96,96	0
10	WZY	E	201	13/13	0.89	0.14	67,73,88,88	26
10	WZY	D	503	13/13	0.89	0.12	59,71,82,83	26
6	MG	F	402	1/1	0.92	0.08	99,99,99,99	0
8	GDP	D	501	28/28	0.93	0.10	67,72,81,85	0
7	CA	A	503	1/1	0.95	0.06	94,94,94,94	0
7	CA	A	504	1/1	0.95	0.06	96,96,96,96	0
6	MG	B	502	1/1	0.96	0.09	45,45,45,45	0
5	GTP	C	501	32/32	0.98	0.06	42,50,55,60	0
8	GDP	B	501	28/28	0.98	0.06	43,52,55,60	0
5	GTP	A	501	32/32	0.98	0.06	46,54,60,62	0
7	CA	C	503	1/1	0.99	0.02	70,70,70,70	0
6	MG	A	502	1/1	1.00	0.06	53,53,53,53	0
6	MG	C	502	1/1	1.00	0.04	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.

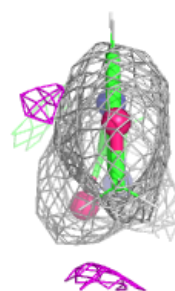
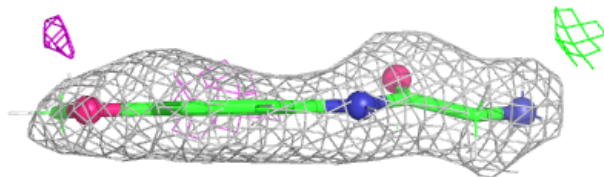
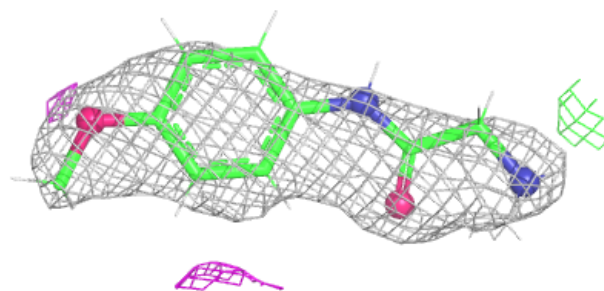
Electron density around WZY B 505:

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

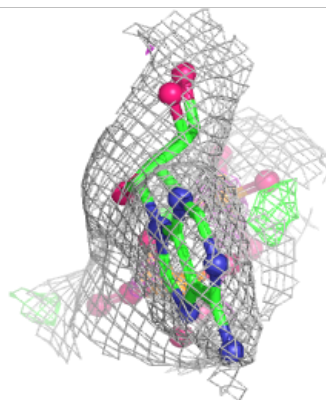
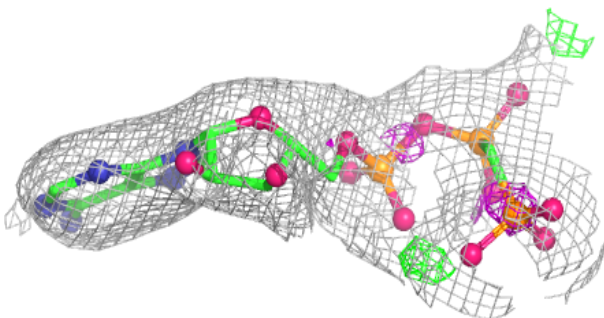
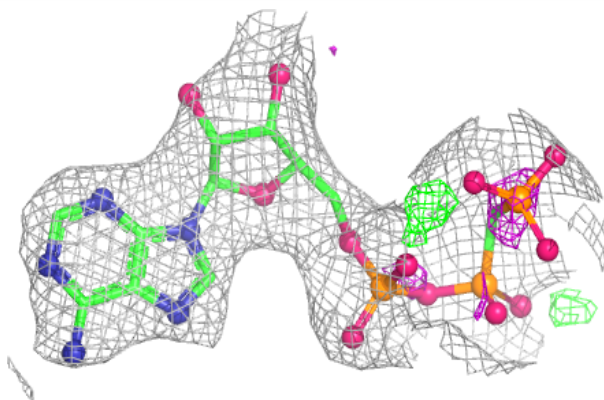


Electron density around WZY C 504:

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

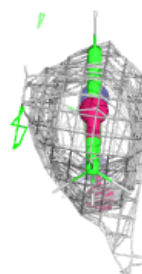
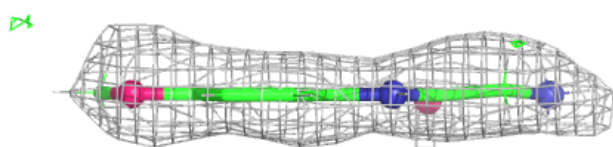
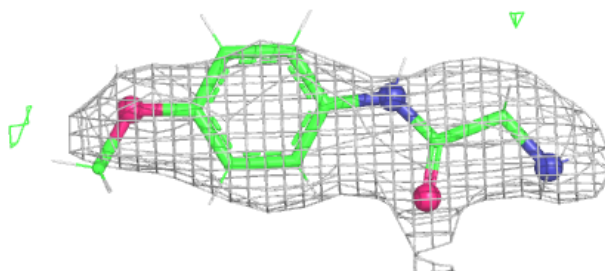
**Electron density around ACP F 401:**

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

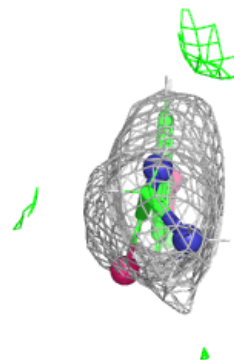
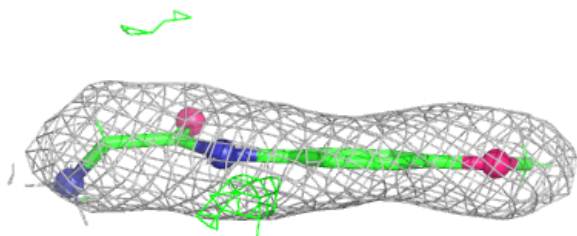
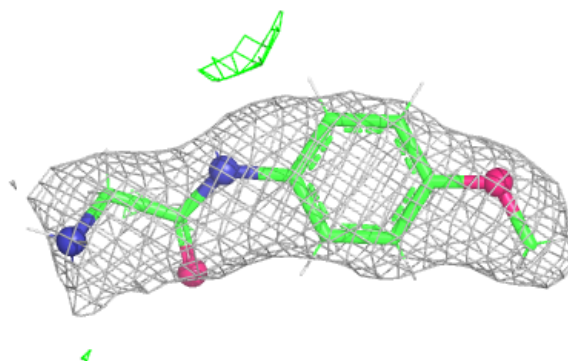


Electron density around WZY E 201:

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

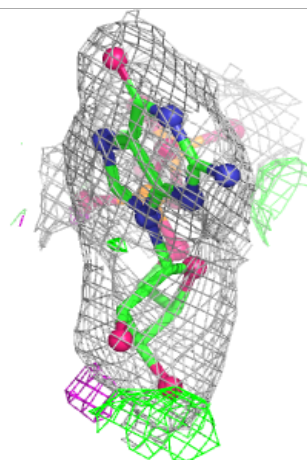
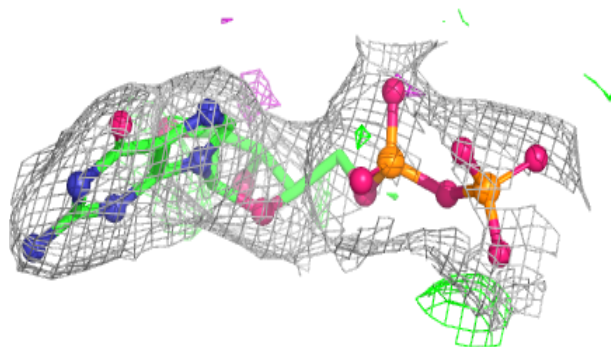
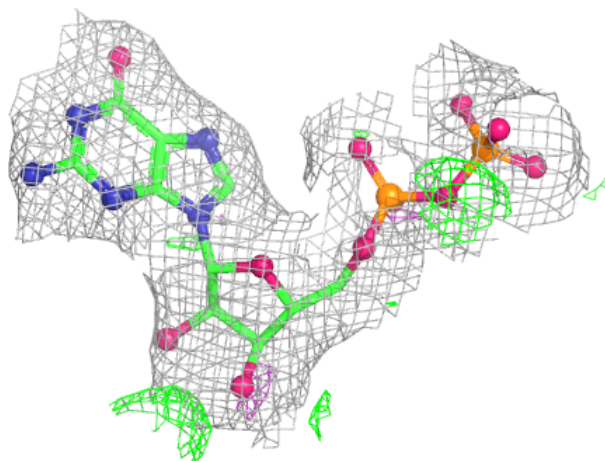
**Electron density around WZY D 503:**

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



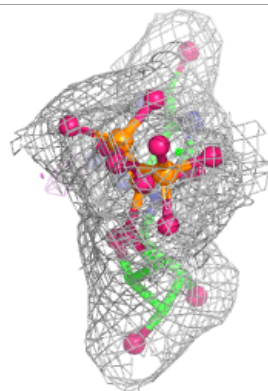
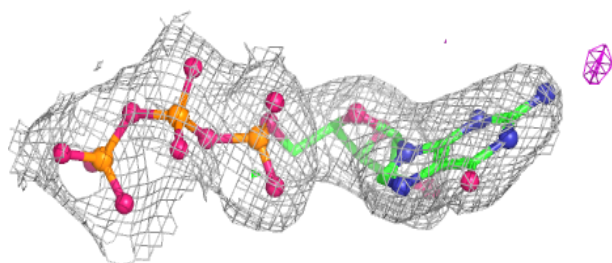
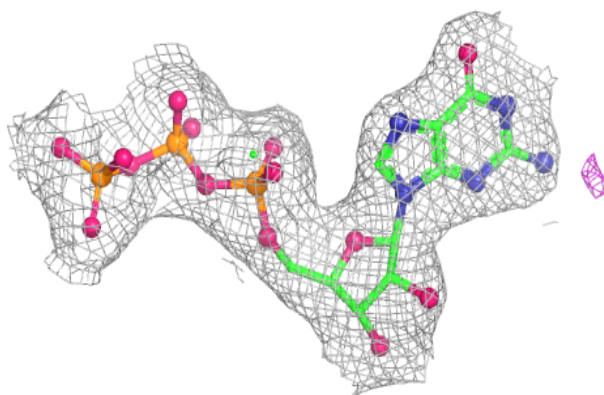
Electron density around GDP D 501:

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

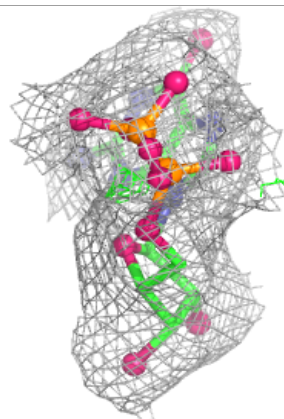
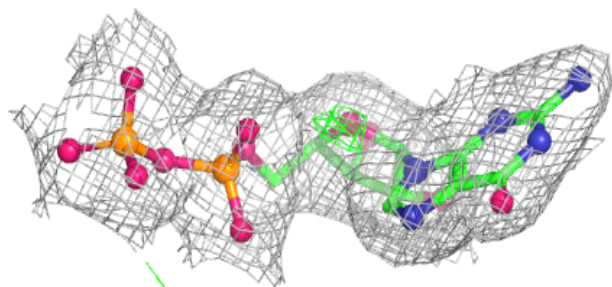
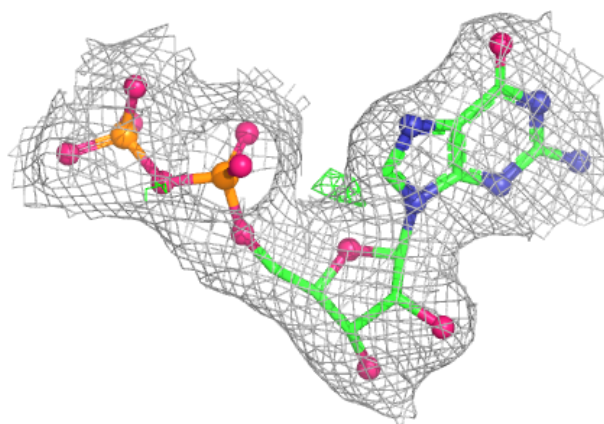


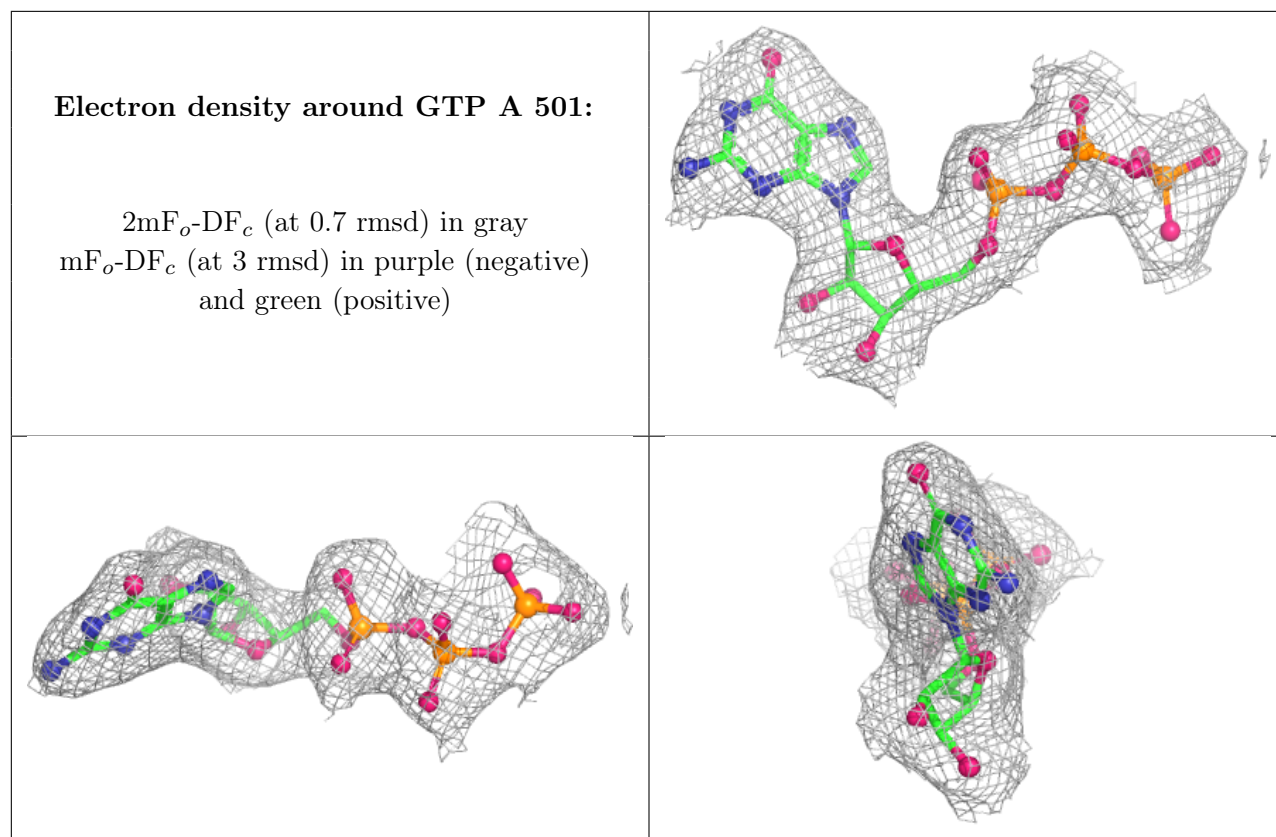
Electron density around GTP C 501:

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

**Electron density around GDP B 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.