



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:59 PM UTC

PDB ID : 8YUA / pdb_00008yua
Title : Tubulin-RB3-TTL in complex with compound SI10
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2024-03-27
Resolution : 2.37 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

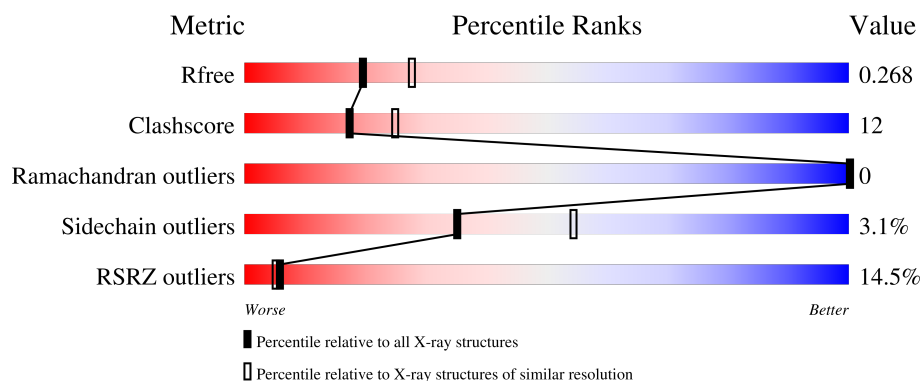
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	440	5% 81% 17% ..
1	C	440	3% 83% 17%
2	B	431	10% 77% 22% ..
2	D	431	26% 66% 29% ..
3	E	143	15% 63% 18% 16%

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Mol	Chain	Length	Quality of chain
4	F	380	28% 55% 23% • 18%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17194 atoms, of which 38 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	418	Total	C	N	O	S	0	0	0
			3281	2065	555	634	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			988	611	180	192	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

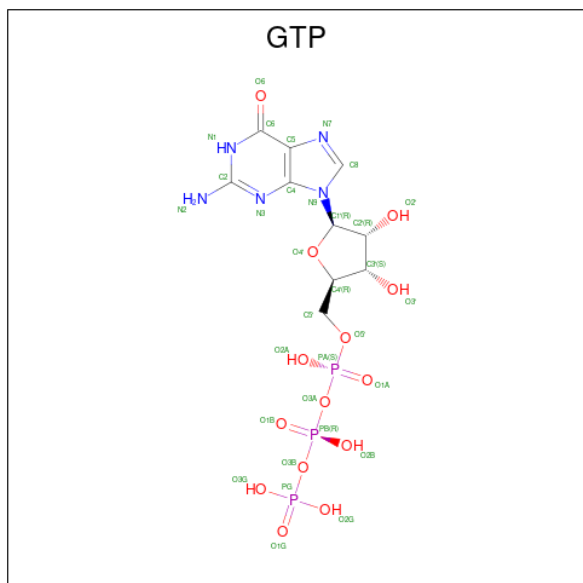
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	310	Total	C	N	O	S	0	0	0
			2476	1595	415	452	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1

- 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	32	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	32	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

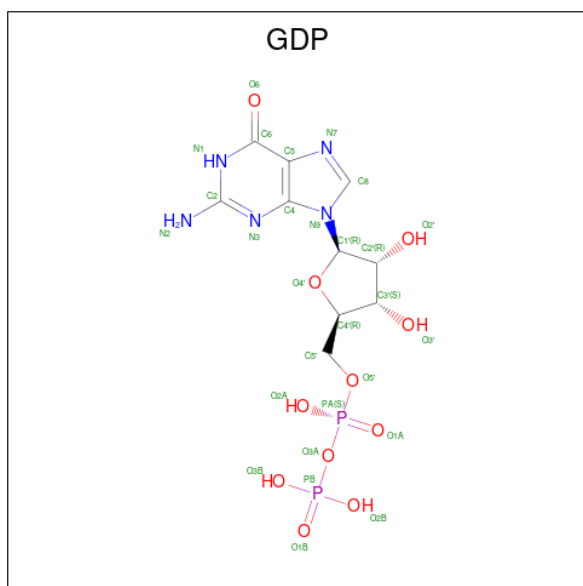
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

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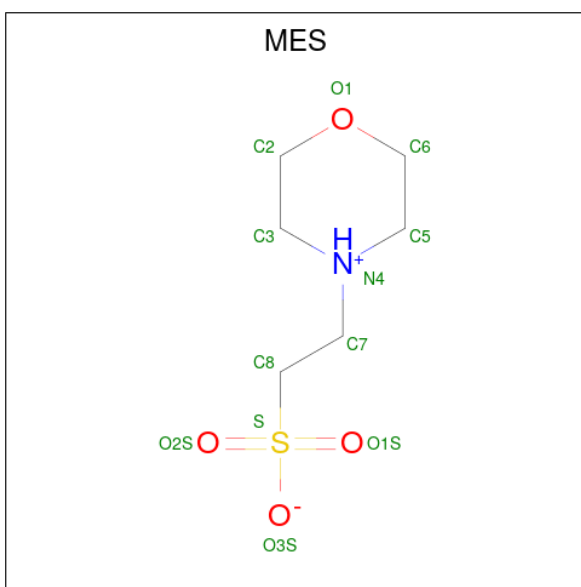
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



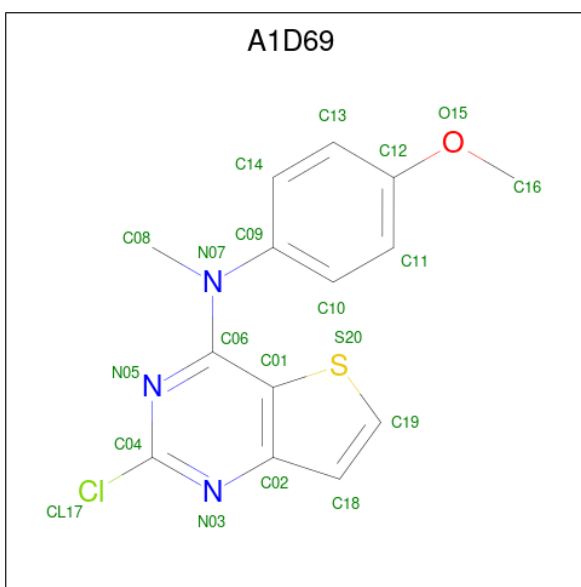
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	28	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	28	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is 2-chloranyl- {N}-(4-methoxyphenyl)- {N}-methyl-thieno[3,2-d]pyrimidin-4-amine (CCD ID: A1D69) (formula: $C_{14}H_{12}ClN_3OS$) (labeled as "Ligand of Interest" by depositor).



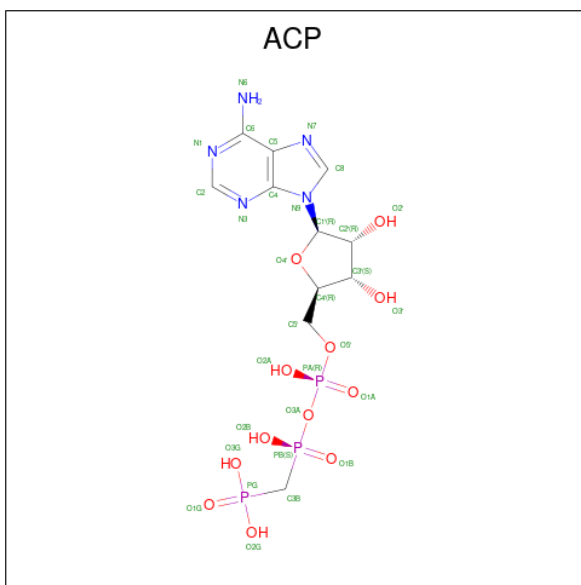
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	B	1	Total	C	Cl	H	N	O	S	0	0
			32	14	1	12	3	1	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	D	1	Total	C	Cl	H	N	O	S	0	0
			32	14	1	12	3	1	1		

- 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	H	N	O	P	45	0
			45	11	14	5	12	3		

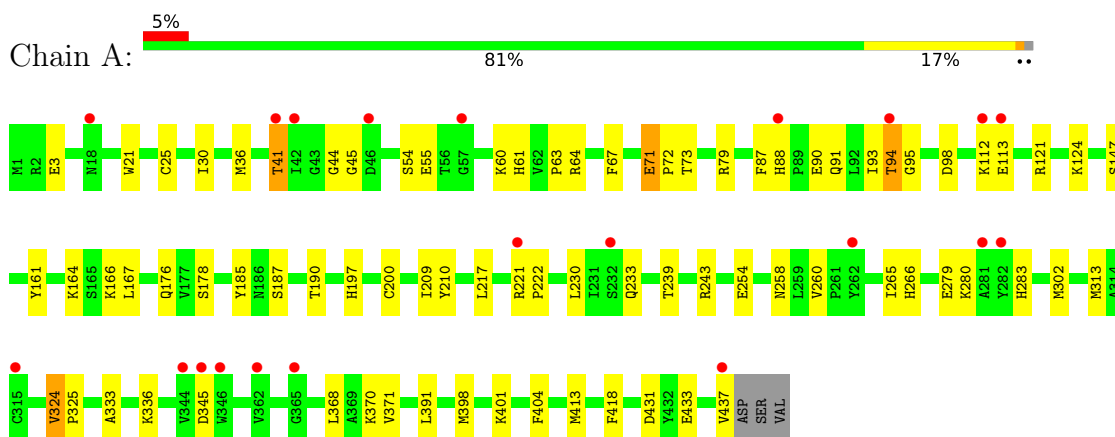
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O 1 1	0	0
12	D	1	Total O 1 1	0	0

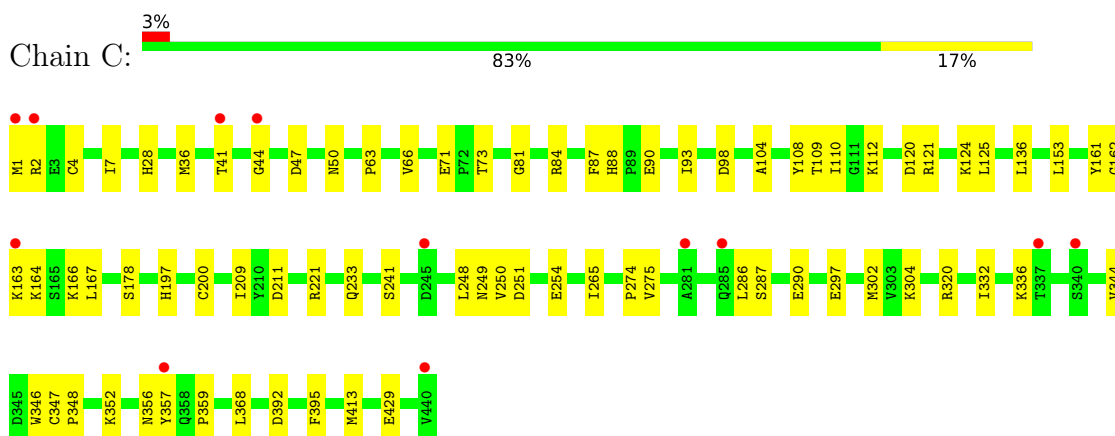
3 Residue-property plots

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.

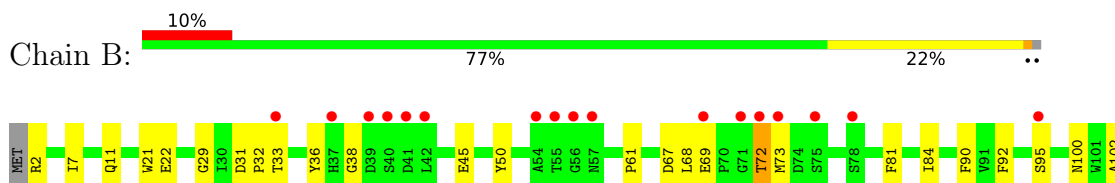
- Molecule 1: Detyrosinated tubulin alpha-1B chain

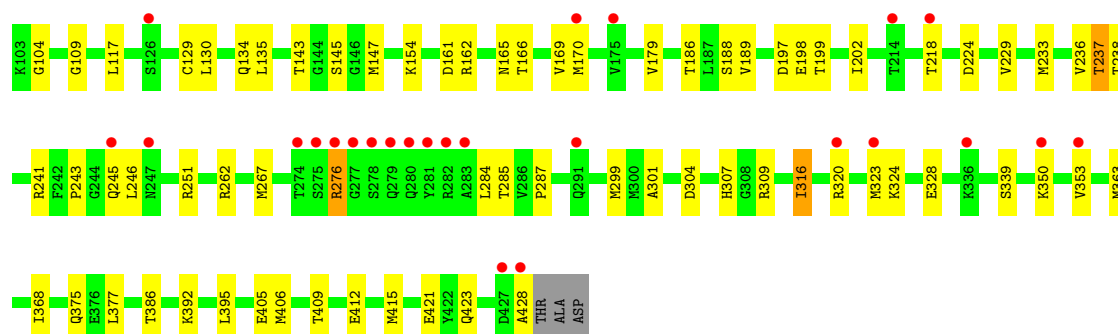


- Molecule 1: Detyrosinated tubulin alpha-1B chain

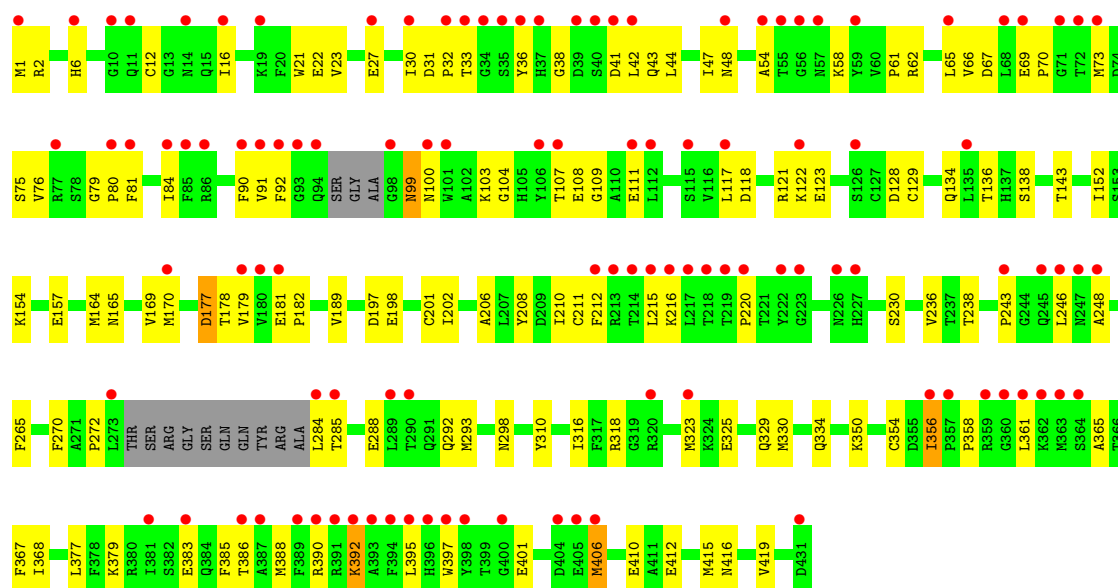


- Molecule 2: Tubulin beta chain

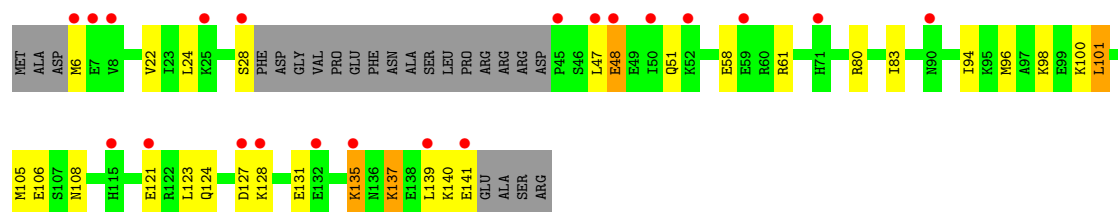




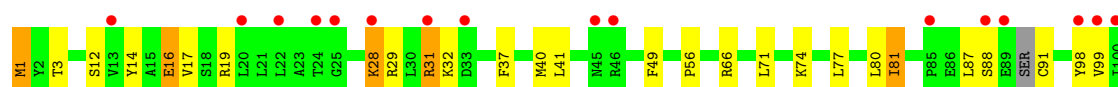
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase



E324	L325	K326	V327	I330	E331	V332	N333	G334	A335	C338	A339	Q340	K341	L342	Y343	D352	P360	LEU	ALA	ASP	THR	GLY	GLN	LYS	THR	SER	GLN	PRO	T372	S373	H379	H380	ASN	PHE	Q234	D235	K236	T237	C238	H239	L240	T241	N242	H243	C244	T245	GLN	LYS	GLU	TYR	SER	LYS	ASN	TYR	G254	ARG	Y256	E257	E258	G259	N260	E261	M262	F263	F264	L271	L275	M276	T277	T278	L279	E280	N281	M296	C297	L298	E299	H306	L307	Q310	S311	L314	M320	E323
																																	Y101	P102	T103	ASN	LEU	LYS	THR	PRO	VAL	ALA	PRO	ALA	GLN	ASN	GLY	ILE	ARG	HIS	LEU	ILE	ASN	ASN	THR	THR	THR	ASP	GLU	ARG	GLU	V130	F131	L132	A133	A134	Y135	N136	R137	R138	R139	GLU	GLY	ARG	GLU	G144	N145	V146	W147	I148	A149	LYS	SER	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 158.45Å 180.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.13 – 2.37 119.13 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.8 (119.13-2.37) 99.8 (119.13-2.37)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.229 , 0.254 (Not available) , 0.268	Depositor DCC
R_{free} test set	2000 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17194	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: A1D69, MES, MG, ACP, CA, 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	0.39	0/3482	0.58	0/4728
1	C	0.43	0/3511	0.63	0/4768
2	B	0.39	0/3426	0.57	0/4643
2	D	0.33	0/3353	0.53	0/4543
3	E	0.34	0/996	0.49	0/1320
4	F	0.31	0/2529	0.51	0/3424
All	All	0.38	0/17297	0.56	0/23426

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	3405	0	3312	67	0
1	C	3433	0	3337	56	0
2	B	3351	0	3214	80	1
2	D	3281	0	3150	114	0
3	E	988	0	1011	29	1
4	F	2476	0	2388	89	0
5	A	32	0	12	0	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	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	11	0	0
9	B	24	0	26	0	0
10	B	20	12	0	1	0
10	D	20	12	0	0	0
11	F	31	14	14	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
All	All	17156	38	16499	417	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (417) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.37	1.07
1:A:239:THR:OG1	1:A:243:ARG:NH1	1.96	0.98
2:D:54:ALA:HB3	2:D:58:LYS:HB2	1.50	0.93
4:F:98:TYR:O	4:F:181:VAL:HG23	1.75	0.86
4:F:256:TYR:HB2	4:F:257:GLU:OE1	1.74	0.86
2:D:318:ARG:HH21	2:D:356:ILE:HG12	1.41	0.85
1:A:71:GLU:OE2	1:A:73:THR:HB	1.77	0.84
2:B:68:LEU:HG	2:B:147:MET:HE1	1.60	0.84
3:E:121:GLU:HG3	3:E:124:GLN:HE21	1.45	0.81
4:F:1:MET:HE1	4:F:28:LYS:HB3	1.63	0.81
1:C:88:HIS:HD2	1:C:90:GLU:H	1.26	0.81
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.82	0.79
2:D:107:THR:O	2:D:111:GLU:HG3	1.83	0.78
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.65	0.78
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.64	0.78
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.66	0.77
2:B:11:GLN:HG3	2:B:72:THR:HG21	1.67	0.77
4:F:188:LYS:HD3	4:F:323:GLU:OE1	1.84	0.77
2:B:143:THR:HG23	2:B:147:MET:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:NZ	1:A:113:GLU:OE2	2.19	0.75
2:B:143:THR:HG23	2:B:147:MET:CE	2.18	0.74
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.70	0.74
2:D:179:VAL:O	2:D:388:MET:HE1	1.87	0.74
1:C:88:HIS:CD2	1:C:90:GLU:H	2.05	0.73
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.17	0.73
2:D:285:THR:HG23	2:D:288:GLU:H	1.53	0.72
4:F:149:ALA:CB	4:F:161:LEU:HB3	2.20	0.72
4:F:278:THR:HG23	4:F:281:ASN:H	1.54	0.71
2:B:68:LEU:HG	2:B:147:MET:CE	2.20	0.71
2:B:238:THR:HG21	2:B:316:ILE:HD11	1.72	0.70
2:B:262:ARG:NH1	2:B:421:GLU:OE2	2.24	0.70
4:F:149:ALA:HB3	4:F:161:LEU:HB3	1.71	0.70
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.25	0.70
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.72	0.70
4:F:186:LEU:CD1	4:F:320:MET:HG2	2.20	0.70
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.91	0.70
3:E:121:GLU:O	3:E:124:GLN:HG3	1.91	0.70
4:F:131:PHE:CZ	4:F:182:ILE:HD11	2.26	0.70
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.73	0.69
2:B:386:THR:HG22	2:B:412:GLU:OE2	1.93	0.69
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.28	0.69
2:D:104:GLY:O	2:D:109:GLY:HA3	1.91	0.69
1:A:336:LYS:HD3	3:E:24:LEU:CD1	2.22	0.69
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.75	0.69
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.74	0.67
3:E:101:LEU:O	3:E:105:MET:HG2	1.94	0.67
4:F:144:GLY:C	4:F:145:ASN:HD22	2.02	0.67
2:B:170:MET:HE2	2:B:377:LEU:CD2	2.25	0.67
4:F:148:ILE:HD12	4:F:161:LEU:HB2	1.77	0.67
2:B:189:VAL:CB	2:B:415:MET:HE2	2.25	0.66
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.78	0.65
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.26	0.65
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.78	0.65
1:C:108:TYR:O	1:C:112:LYS:HG2	1.97	0.65
1:C:178:SER:O	2:D:350:LYS:HE2	1.97	0.65
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.79	0.64
2:D:73:MET:HG3	2:D:90:PHE:CD2	2.32	0.64
2:B:170:MET:CE	2:B:377:LEU:HD21	2.28	0.64
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.22	0.63
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:121:GLU:HA	3:E:124:GLN:HG2	1.80	0.63
4:F:148:ILE:CD1	4:F:161:LEU:HB2	2.27	0.63
2:D:1:MET:HE3	2:D:128:ASP:CB	2.22	0.63
2:D:416:ASN:O	2:D:419:VAL:HG22	1.98	0.63
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.80	0.63
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.33	0.62
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.29	0.62
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.35	0.62
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.34	0.62
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.18	0.62
2:D:285:THR:HG22	2:D:288:GLU:HB2	1.81	0.62
4:F:144:GLY:O	4:F:145:ASN:ND2	2.24	0.62
4:F:257:GLU:OE1	4:F:257:GLU:N	2.33	0.62
2:B:189:VAL:HB	2:B:415:MET:CE	2.30	0.61
2:D:392:LYS:HG3	2:D:395:LEU:HD12	1.81	0.61
3:E:121:GLU:HG3	3:E:124:GLN:NE2	2.15	0.61
4:F:74:LYS:HE3	4:F:331:GLU:HG3	1.80	0.61
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.00	0.61
1:C:332:ILE:HG22	1:C:336:LYS:HE2	1.82	0.61
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.36	0.61
2:B:31:ASP:OD1	2:B:33:THR:HG22	2.00	0.61
2:D:23:VAL:O	2:D:27:GLU:HG3	2.00	0.60
2:B:81:PHE:O	2:B:84:ILE:HG22	2.01	0.60
2:D:330:MET:O	2:D:334:GLN:HG3	2.01	0.60
2:B:189:VAL:HG21	2:B:415:MET:HE2	1.84	0.60
1:A:398:MET:HE3	1:A:404:PHE:HD2	1.67	0.60
4:F:80:LEU:HD21	4:F:298:ILE:HG22	1.84	0.60
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.31	0.60
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.37	0.60
1:A:370:LYS:HD3	1:A:371:VAL:O	2.02	0.60
2:D:134:GLN:HA	2:D:165:ASN:O	2.00	0.60
4:F:338:CYS:O	4:F:343:TYR:HE1	1.85	0.60
2:D:285:THR:HG22	2:D:288:GLU:CG	2.32	0.59
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.84	0.59
2:D:42:LEU:HD22	2:D:243:PRO:HG2	1.85	0.59
2:B:233:MET:O	2:B:237:THR:OG1	2.21	0.59
4:F:161:LEU:HD23	4:F:172:PHE:CZ	2.37	0.59
1:C:41:THR:O	1:C:41:THR:OG1	2.21	0.59
1:C:41:THR:OG1	1:C:44:GLY:O	2.19	0.59
2:D:293:MET:CG	2:D:367:PHE:HB2	2.32	0.59
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.84	0.59
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.67	0.58
2:B:406:MET:HE3	2:B:409:THR:HB	1.85	0.58
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.38	0.58
4:F:29:ARG:HH21	4:F:31:ARG:HH22	1.51	0.58
4:F:171:ASP:O	4:F:175:GLU:HG3	2.03	0.58
1:A:71:GLU:HG2	1:A:72:PRO:N	2.18	0.58
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.27	0.58
2:D:170:MET:CE	2:D:377:LEU:HD21	2.33	0.58
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.84	0.58
4:F:80:LEU:HD21	4:F:298:ILE:CG2	2.33	0.58
4:F:202:ARG:HG3	4:F:203:SER:N	2.19	0.58
2:B:245:GLN:O	2:B:245:GLN:HG2	2.03	0.58
3:E:48:GLU:OE2	3:E:48:GLU:HA	2.04	0.58
2:B:324:LYS:HE2	2:B:328:GLU:OE2	2.04	0.57
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.85	0.57
1:A:25:CYS:HB3	1:A:30:ILE:O	2.05	0.57
2:D:189:VAL:HG21	2:D:415:MET:HE2	1.85	0.57
2:D:246:LEU:HD12	2:D:248:ALA:HB2	1.87	0.57
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.70	0.57
2:D:189:VAL:HG11	2:D:415:MET:HE2	1.87	0.57
2:D:30:ILE:HG21	2:D:84:ILE:HD11	1.87	0.56
2:D:386:THR:O	2:D:390:ARG:HG2	2.05	0.56
2:B:67:ASP:O	2:B:92:PHE:HA	2.06	0.56
2:B:145:SER:HG	2:B:188:SER:HG	1.52	0.56
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.87	0.56
2:D:1:MET:HG3	2:D:128:ASP:HB3	1.88	0.56
4:F:1:MET:HE1	4:F:28:LYS:CB	2.35	0.56
1:A:72:PRO:HA	1:A:94:THR:OG1	2.06	0.56
1:A:221:ARG:NH1	2:B:323:MET:HE2	2.21	0.56
1:C:221:ARG:NH1	2:D:323:MET:HB3	2.20	0.56
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.88	0.56
2:D:377:LEU:C	2:D:377:LEU:HD23	2.31	0.56
4:F:146:VAL:HG12	4:F:185:TYR:HB2	1.88	0.56
1:A:79:ARG:HH22	1:A:94:THR:HB	1.71	0.56
2:B:189:VAL:CG1	2:B:415:MET:HE2	2.36	0.56
2:B:285:THR:HB	2:B:287:PRO:HD2	1.86	0.56
2:D:285:THR:CG2	2:D:288:GLU:H	2.19	0.55
1:A:41:THR:HB	1:A:44:GLY:O	2.07	0.55
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.21	0.55
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.42	0.55
1:A:63:PRO:HG2	1:A:87:PHE:CE1	2.42	0.55
2:D:285:THR:HG22	2:D:288:GLU:CB	2.36	0.55
4:F:148:ILE:O	4:F:182:ILE:HA	2.06	0.55
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.42	0.55
2:D:31:ASP:OD1	2:D:33:THR:HG22	2.06	0.55
2:D:1:MET:CE	2:D:128:ASP:HB2	2.25	0.55
3:E:47:LEU:O	3:E:51:GLN:HG2	2.07	0.55
2:B:238:THR:HG21	2:B:316:ILE:CD1	2.35	0.55
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.89	0.55
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.88	0.55
1:A:336:LYS:HD3	3:E:24:LEU:HD12	1.89	0.55
1:C:88:HIS:HD2	1:C:90:GLU:N	2.03	0.55
3:E:106:GLU:HA	3:E:106:GLU:OE1	2.05	0.55
1:C:265:ILE:N	1:C:265:ILE:HD12	2.21	0.54
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.22	0.54
1:A:221:ARG:HH11	2:B:323:MET:HE2	1.73	0.54
2:D:318:ARG:NH2	2:D:356:ILE:HG12	2.18	0.54
3:E:47:LEU:O	3:E:47:LEU:HD23	2.07	0.54
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.43	0.54
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.72	0.54
2:D:73:MET:HG3	2:D:90:PHE:HD2	1.73	0.54
1:C:1:MET:O	1:C:2:ARG:HB2	2.08	0.54
1:C:221:ARG:CZ	2:D:323:MET:HB3	2.37	0.54
2:D:177:ASP:N	2:D:177:ASP:OD1	2.41	0.54
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.08	0.54
2:D:69:GLU:HG3	2:D:70:PRO:HD2	1.89	0.54
2:B:143:THR:CG2	2:B:147:MET:HE3	2.38	0.53
2:D:189:VAL:HB	2:D:415:MET:HE3	1.90	0.53
2:B:104:GLY:O	2:B:109:GLY:HA3	2.08	0.53
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.42	0.53
1:C:81:GLY:O	1:C:84:ARG:NH1	2.41	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.53
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.22	0.53
2:B:169:VAL:HA	2:B:202:ILE:O	2.08	0.53
2:D:386:THR:HG22	2:D:412:GLU:OE2	2.08	0.53
1:A:345:ASP:HB2	3:E:28:SER:HB2	1.91	0.53
3:E:127:ASP:O	3:E:131:GLU:HG2	2.09	0.53
1:A:178:SER:O	2:B:350:LYS:NZ	2.37	0.53
4:F:131:PHE:CE2	4:F:182:ILE:HD11	2.43	0.53
2:B:309:ARG:NH1	2:B:339:SER:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:192:LEU:HD21	4:F:262:MET:CE	2.38	0.53
1:C:320:ARG:HA	1:C:356:ASN:O	2.09	0.53
2:D:44:LEU:HA	2:D:47:ILE:HB	1.90	0.53
2:D:100:ASN:ND2	2:D:397:TRP:HB3	2.24	0.52
4:F:275:LEU:N	4:F:275:LEU:HD22	2.23	0.52
2:D:12:CYS:CB	2:D:138:SER:HB3	2.38	0.52
2:B:189:VAL:CG2	2:B:415:MET:HE2	2.39	0.52
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.90	0.52
2:D:212:PHE:O	2:D:216:LYS:HA	2.09	0.52
4:F:14:TYR:HA	4:F:17:VAL:HB	1.90	0.52
4:F:224:SER:OG	4:F:238:CYS:HA	2.09	0.52
2:D:65:LEU:N	2:D:65:LEU:HD12	2.25	0.52
2:D:236:VAL:HG12	2:D:368:ILE:HG12	1.92	0.52
2:B:29:GLY:O	2:B:36:TYR:HA	2.10	0.51
1:A:112:LYS:HE2	3:E:61:ARG:HH22	1.72	0.51
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.25	0.51
2:B:31:ASP:OD1	2:B:33:THR:CG2	2.58	0.51
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.46	0.51
2:D:416:ASN:O	2:D:419:VAL:CG2	2.59	0.51
1:C:357:TYR:O	1:C:359:PRO:HD3	2.10	0.51
2:D:118:ASP:HA	2:D:121:ARG:NH1	2.26	0.51
1:C:104:ALA:HB2	1:C:413:MET:SD	2.50	0.51
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.91	0.51
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.41	0.51
1:A:185:TYR:CZ	1:A:398:MET:HE2	2.46	0.51
1:A:265:ILE:HD12	1:A:265:ILE:N	2.25	0.51
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.26	0.51
2:B:50:TYR:OH	2:B:237:THR:CG2	2.59	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
1:A:71:GLU:HG2	1:A:73:THR:H	1.75	0.50
1:A:147:SER:HB2	1:A:190:THR:HB	1.93	0.50
2:B:237:THR:HB	2:B:241:ARG:HE	1.77	0.50
2:B:161:ASP:O	2:B:251:ARG:NH2	2.44	0.50
2:D:80:PRO:O	2:D:81:PHE:HB2	2.11	0.50
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.91	0.50
2:D:401:GLU:HA	3:E:137:LYS:HD3	1.94	0.50
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.93	0.50
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.92	0.50
2:B:284:LEU:N	2:B:284:LEU:HD12	2.26	0.50
4:F:271:LEU:O	4:F:275:LEU:O	2.30	0.50
1:A:94:THR:HG23	1:A:95:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:MET:HE3	2:B:353:VAL:HG11	1.94	0.49
1:A:88:HIS:N	1:A:91:GLN:OE1	2.38	0.49
2:B:189:VAL:CB	2:B:415:MET:CE	2.90	0.49
4:F:161:LEU:HD23	4:F:172:PHE:CE2	2.47	0.49
2:B:73:MET:HE3	2:B:90:PHE:CD2	2.47	0.49
2:B:284:LEU:O	2:B:363:MET:CE	2.61	0.49
2:D:170:MET:HE2	2:D:377:LEU:CD2	2.40	0.49
4:F:149:ALA:HB2	4:F:161:LEU:HB3	1.94	0.49
1:A:209:ILE:HD11	1:A:302:MET:SD	2.52	0.49
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.47	0.49
2:B:406:MET:HE3	2:B:406:MET:O	2.13	0.49
4:F:130:VAL:C	4:F:132:LEU:HD23	2.38	0.49
4:F:198:LYS:HG2	4:F:199:PHE:N	2.27	0.49
4:F:296:MET:HE2	4:F:380:HIS:HB2	1.95	0.49
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.95	0.49
1:A:401:LYS:HE3	2:B:428:ALA:HB1	1.95	0.49
1:C:71:GLU:OE1	1:C:73:THR:HB	2.13	0.49
4:F:148:ILE:HG13	4:F:149:ALA:N	2.28	0.49
2:B:134:GLN:HA	2:B:165:ASN:O	2.13	0.48
4:F:191:LEU:HA	4:F:197:ARG:O	2.12	0.48
2:B:130:LEU:HB3	2:B:162:ARG:HE	1.79	0.48
2:D:285:THR:HG22	2:D:288:GLU:CD	2.39	0.48
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.48	0.48
2:B:166:THR:OG1	2:B:199:THR:HB	2.13	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.48
1:C:287:SER:OG	1:C:290:GLU:HG3	2.14	0.48
2:B:236:VAL:HG12	2:B:368:ILE:HG12	1.96	0.48
4:F:102:PRO:HG3	4:F:178:GLN:O	2.14	0.48
4:F:326:LYS:HD2	4:F:327:VAL:N	2.28	0.48
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.96	0.48
3:E:135:LYS:HB3	3:E:135:LYS:HE3	1.39	0.48
1:A:280:LYS:NZ	1:A:283:HIS:HD2	2.12	0.48
2:D:169:VAL:HA	2:D:202:ILE:O	2.13	0.48
2:B:2:ARG:HA	2:B:129:CYS:O	2.14	0.47
2:B:7:ILE:O	2:B:135:LEU:HA	2.14	0.47
2:D:99:ASN:OD1	2:D:178:THR:HG21	2.15	0.47
2:B:117:LEU:HD11	2:B:154:LYS:HD3	1.96	0.47
4:F:165:GLU:HB2	4:F:168:GLU:HG3	1.96	0.47
1:C:286:LEU:N	1:C:286:LEU:HD12	2.29	0.47
2:D:325:GLU:O	2:D:329:GLN:HG2	2.14	0.47
2:D:379:LYS:O	2:D:383:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:ASP:C	2:B:198:GLU:HG3	2.40	0.47
4:F:275:LEU:HD22	4:F:275:LEU:H	1.79	0.47
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.97	0.47
2:D:189:VAL:HG21	2:D:415:MET:CE	2.44	0.47
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.32	0.47
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.97	0.47
2:D:238:THR:OG1	2:D:318:ARG:HD2	2.15	0.47
2:D:358:PRO:HG2	2:D:361:LEU:HD12	1.97	0.47
4:F:170:LEU:O	4:F:173:ILE:HG12	2.14	0.47
2:D:1:MET:CB	2:D:48:ASN:HD22	2.28	0.47
2:D:81:PHE:O	2:D:84:ILE:HG22	2.15	0.47
2:D:197:ASP:C	2:D:198:GLU:HG3	2.40	0.47
1:C:136:LEU:HD12	1:C:136:LEU:N	2.30	0.46
2:D:385:PHE:CE1	2:D:412:GLU:HB2	2.50	0.46
4:F:192:LEU:CD2	4:F:262:MET:CE	2.94	0.46
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.97	0.46
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.14	0.46
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.46
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.38	0.46
1:A:398:MET:HE3	1:A:404:PHE:CD2	2.49	0.46
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.97	0.46
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.49	0.46
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.46
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.96	0.46
2:D:272:PRO:HG3	2:D:284:LEU:HD13	1.98	0.46
2:D:406:MET:O	2:D:410:GLU:HG3	2.16	0.46
1:A:55:GLU:HA	1:A:60:LYS:O	2.16	0.46
2:D:208:TYR:CD1	2:D:220:PRO:HG2	2.50	0.46
1:A:324:VAL:HG13	1:A:325:PRO:CD	2.45	0.46
4:F:88:SER:HG	4:F:91:CYS:N	2.14	0.46
4:F:148:ILE:HD12	4:F:149:ALA:H	1.81	0.46
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.46	0.45
2:D:206:ALA:O	2:D:210:ILE:HG13	2.15	0.45
2:B:45:GLU:OE2	2:B:243:PRO:HG3	2.16	0.45
4:F:192:LEU:CD1	4:F:192:LEU:N	2.79	0.45
4:F:209:HIS:HA	4:F:311:SER:O	2.16	0.45
2:B:267:MET:HE1	2:B:299:MET:HG3	1.98	0.45
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.97	0.45
2:B:229:VAL:O	2:B:233:MET:HG3	2.16	0.45
1:C:395:PHE:CD1	1:C:395:PHE:C	2.94	0.45
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:PHE:O	2:D:298:ASN:HB3	2.16	0.45
4:F:162:ILE:HG22	4:F:163:SER:N	2.32	0.45
1:C:166:LYS:HE2	1:C:197:HIS:O	2.17	0.45
4:F:259:GLY:O	4:F:260:ASN:HB2	2.17	0.45
2:B:375:GLN:OE1	2:B:423:GLN:HG2	2.17	0.45
2:D:16:ILE:HD11	2:D:136:THR:HB	1.99	0.45
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.00	0.44
1:A:41:THR:HG21	1:A:45:GLY:CA	2.47	0.44
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.98	0.44
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.89	0.44
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.52	0.44
4:F:338:CYS:O	4:F:343:TYR:CE1	2.70	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.00	0.44
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.57	0.44
1:A:333:ALA:HA	3:E:6:MET:HE1	1.98	0.44
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.98	0.44
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.44
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.52	0.44
2:B:31:ASP:CG	2:B:33:THR:HG22	2.42	0.44
2:B:68:LEU:CD1	2:B:147:MET:HE2	2.47	0.44
2:D:288:GLU:O	2:D:292:GLN:HG3	2.18	0.44
1:C:274:PRO:HB3	1:C:286:LEU:HD22	1.99	0.44
1:A:370:LYS:HD3	1:A:371:VAL:N	2.31	0.44
2:D:354:CYS:SG	2:D:356:ILE:HG23	2.58	0.44
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.51	0.44
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.36	0.44
4:F:1:MET:HE2	4:F:1:MET:HB3	1.71	0.44
1:C:265:ILE:N	1:C:265:ILE:CD1	2.81	0.43
4:F:130:VAL:O	4:F:132:LEU:HD23	2.18	0.43
1:A:413:MET:CE	1:A:418:PHE:CE1	3.00	0.43
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.99	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.00	0.43
2:D:23:VAL:HG21	2:D:230:SER:HB2	2.01	0.43
1:A:41:THR:HG21	1:A:45:GLY:HA2	2.00	0.43
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.49	0.43
2:D:75:SER:O	2:D:79:GLY:N	2.49	0.43
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.99	0.43
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.53	0.43
2:B:100:ASN:OD1	2:B:102:ALA:HB3	2.19	0.43
10:B:505:A1D69:S20	10:B:505:A1D69:C09	3.06	0.43
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:ASP:OD1	2:D:33:THR:CG2	2.67	0.43
1:C:28:HIS:O	1:C:36:MET:HE3	2.18	0.43
1:C:47:ASP:O	1:C:50:ASN:HB2	2.18	0.43
2:D:66:VAL:HA	2:D:91:VAL:O	2.19	0.43
2:D:67:ASP:O	2:D:92:PHE:HA	2.18	0.43
2:D:181:GLU:HB2	2:D:182:PRO:HD3	2.00	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.42
2:D:152:ILE:HG23	2:D:164:MET:HG2	2.01	0.42
3:E:6:MET:HG3	3:E:24:LEU:CD2	2.48	0.42
4:F:49:PHE:CD2	4:F:66:ARG:HG3	2.54	0.42
4:F:29:ARG:NH2	4:F:31:ARG:HH22	2.16	0.42
1:C:88:HIS:NE2	1:C:90:GLU:HG3	2.34	0.42
4:F:74:LYS:HB3	4:F:181:VAL:HG11	2.01	0.42
4:F:178:GLN:N	4:F:178:GLN:OE1	2.53	0.42
4:F:199:PHE:HA	4:F:241:THR:HG21	2.01	0.42
1:C:161:TYR:O	1:C:162:GLY:C	2.63	0.42
2:D:41:ASP:C	2:D:43:GLN:N	2.77	0.42
2:D:350:LYS:HD2	2:D:350:LYS:HA	1.88	0.42
1:A:437:VAL:O	1:A:437:VAL:CG1	2.67	0.42
2:D:157:GLU:HA	3:E:123:LEU:HD13	2.01	0.42
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.50	0.42
2:D:293:MET:SD	2:D:365:ALA:HB1	2.60	0.42
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.55	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.42
2:B:377:LEU:C	2:B:377:LEU:HD23	2.45	0.42
1:A:437:VAL:O	1:A:437:VAL:HG12	2.20	0.41
1:C:164:LYS:HE2	1:C:164:LYS:HB2	1.70	0.41
4:F:71:LEU:HD12	4:F:77:LEU:HD13	2.02	0.41
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.83	0.41
4:F:16:GLU:OE2	4:F:19:ARG:HD3	2.21	0.41
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.55	0.41
2:D:285:THR:HG22	2:D:288:GLU:OE1	2.21	0.41
4:F:197:ARG:HB3	4:F:224:SER:O	2.21	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.50	0.41
4:F:81:ILE:O	4:F:87:LEU:O	2.39	0.41
4:F:296:MET:HE1	4:F:299:GLU:OE1	2.20	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.60	0.41
4:F:144:GLY:HA3	4:F:187:GLU:CD	2.45	0.41
1:A:54:SER:O	1:A:61:HIS:HA	2.21	0.41
2:B:395:LEU:HD23	2:B:395:LEU:HA	1.88	0.41
2:D:54:ALA:N	2:D:58:LYS:O	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.49	0.41
2:D:406:MET:HB3	2:D:406:MET:HE3	1.76	0.41
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.95	0.41
4:F:148:ILE:CG1	4:F:149:ALA:N	2.84	0.41
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.56	0.41
2:B:285:THR:CB	2:B:287:PRO:HD2	2.50	0.41
2:B:323:MET:HE3	2:B:353:VAL:CG1	2.51	0.41
1:C:71:GLU:CG	1:C:98:ASP:HB3	2.47	0.41
1:C:221:ARG:NH1	2:D:323:MET:CB	2.83	0.41
1:C:241:SER:HA	1:C:249:ASN:OD1	2.20	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.56	0.41
2:D:103:LYS:O	2:D:108:GLU:HB2	2.19	0.41
3:E:98:LYS:O	3:E:101:LEU:HD12	2.21	0.41
4:F:131:PHE:CZ	4:F:182:ILE:CD1	3.00	0.41
4:F:192:LEU:HD11	4:F:199:PHE:CD1	2.56	0.41
1:A:67:PHE:CD1	1:A:67:PHE:N	2.89	0.41
1:C:109:THR:HG22	1:C:110:ILE:HD13	2.03	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.02	0.40
3:E:47:LEU:HD23	3:E:51:GLN:HG2	2.03	0.40
4:F:186:LEU:HD13	4:F:320:MET:CG	2.51	0.40
2:B:50:TYR:OH	2:B:237:THR:HG21	2.22	0.40
2:D:401:GLU:HA	3:E:137:LYS:CD	2.51	0.40
1:C:120:ASP:O	1:C:124:LYS:HG2	2.21	0.40
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.51	0.40
2:D:67:ASP:HA	2:D:143:THR:HG21	2.04	0.40
2:D:189:VAL:HB	2:D:415:MET:CE	2.52	0.40
2:B:186:THR:HA	2:B:415:MET:CE	2.51	0.40
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.03	0.40
3:E:47:LEU:HD23	3:E:47:LEU:C	2.46	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ARG:NH2	3:E:131:GLU:OE2[4_545]	2.11	0.09

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	435/440 (99%)	428 (98%)	7 (2%)	0	100	100
1	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
2	B	425/431 (99%)	418 (98%)	7 (2%)	0	100	100
2	D	412/431 (96%)	405 (98%)	7 (2%)	0	100	100
3	E	116/143 (81%)	116 (100%)	0	0	100	100
4	F	293/380 (77%)	283 (97%)	10 (3%)	0	100	100
All	All	2119/2265 (94%)	2075 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	366/371 (99%)	361 (99%)	5 (1%)	59	77
1	C	370/371 (100%)	366 (99%)	4 (1%)	65	81
2	B	367/372 (99%)	359 (98%)	8 (2%)	45	65
2	D	360/372 (97%)	353 (98%)	7 (2%)	50	69
3	E	107/127 (84%)	95 (89%)	12 (11%)	6	8
4	F	266/338 (79%)	245 (92%)	21 (8%)	11	17
All	All	1836/1951 (94%)	1779 (97%)	57 (3%)	35	54

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	71	GLU
1	A	94	THR
1	A	324	VAL
1	A	433	GLU
2	B	69	GLU
2	B	72	THR
2	B	95	SER
2	B	218	THR
2	B	237	THR
2	B	246	LEU
2	B	276	ARG
2	B	316	ILE
1	C	163	LYS
1	C	251	ASP
1	C	297	GLU
1	C	347	CYS
2	D	99	ASN
2	D	122	LYS
2	D	177	ASP
2	D	316	ILE
2	D	356	ILE
2	D	392	LYS
2	D	406	MET
3	E	22	VAL
3	E	48	GLU
3	E	96	MET
3	E	100	LYS
3	E	101	LEU
3	E	108	ASN
3	E	128	LYS
3	E	135	LYS
3	E	137	LYS
3	E	139	LEU
3	E	140	LYS
3	E	141	GLU
4	F	1	MET
4	F	12	SER
4	F	16	GLU
4	F	28	LYS
4	F	31	ARG
4	F	81	ILE

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Mol	Chain	Res	Type
4	F	99	VAL
4	F	132	LEU
4	F	136	ASN
4	F	161	LEU
4	F	180	HIS
4	F	192	LEU
4	F	224	SER
4	F	234	GLN
4	F	237	THR
4	F	241	THR
4	F	243	HIS
4	F	257	GLU
4	F	279	LEU
4	F	307	LEU
4	F	310	GLN

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

Mol	Chain	Res	Type
1	A	258	ASN
1	A	283	HIS
1	A	285	GLN
1	A	301	GLN
1	A	393	HIS
2	B	15	GLN
2	B	165	ASN
2	B	423	GLN
1	C	88	HIS
1	C	133	GLN
1	C	372	GLN
1	C	393	HIS
1	C	406	HIS
2	D	37	HIS
2	D	165	ASN
2	D	329	GLN
3	E	115	HIS
3	E	124	GLN
3	E	129	HIS
4	F	26	GLN
4	F	145	ASN
4	F	183	GLN
4	F	212	ASN

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Mol	Chain	Res	Type
4	F	234	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	B	501	7	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
10	A1D69	B	505	-	21,22,22	0.98	1 (4%)	25,31,31	2.17	9 (36%)
5	GTP	A	501	7	33,34,34	0.95	2 (6%)	50,54,54	1.58	9 (18%)
5	GTP	C	501	7	33,34,34	0.97	1 (3%)	50,54,54	1.58	9 (18%)
10	A1D69	D	502	-	21,22,22	1.02	1 (4%)	25,31,31	2.46	8 (32%)
11	ACP	F	401	-	31,33,33	2.02	2 (6%)	47,52,52	0.98	3 (6%)
8	GDP	D	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.89	9 (20%)
9	MES	B	502	-	12,12,12	1.25	1 (8%)	15,16,16	0.62	0
9	MES	B	503	-	12,12,12	1.18	1 (8%)	15,16,16	0.69	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	B	501	7	-	3/16/32/32	0/3/3/3
10	A1D69	B	505	-	-	0/10/16/16	0/3/3/3
5	GTP	A	501	7	-	9/22/38/38	0/3/3/3
5	GTP	C	501	7	-	6/22/38/38	0/3/3/3
10	A1D69	D	502	-	-	0/10/16/16	0/3/3/3
11	ACP	F	401	-	-	1/19/38/38	0/3/3/3
8	GDP	D	501	-	-	4/16/32/32	0/3/3/3
9	MES	B	502	-	-	5/6/14/14	0/1/1/1
9	MES	B	503	-	-	3/6/14/14	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	10.15	1.69	1.58
10	D	502	A1D69	C06-N07	3.38	1.46	1.39
9	B	502	MES	C8-S	3.34	1.82	1.77
8	B	501	GDP	C5-C4	3.20	1.47	1.38
9	B	503	MES	C8-S	3.14	1.82	1.77
8	D	501	GDP	C5-C4	3.03	1.47	1.38
10	B	505	A1D69	C02-C01	-2.47	1.37	1.40
8	B	501	GDP	C6-N1	-2.40	1.34	1.38
5	C	501	GTP	C2-N3	2.19	1.38	1.33
8	D	501	GDP	C6-N1	-2.15	1.34	1.38
11	F	401	ACP	PB-O2B	-2.10	1.51	1.56
5	A	501	GTP	C2-N3	2.09	1.38	1.33
8	D	501	GDP	PA-O3A	2.09	1.61	1.59
8	B	501	GDP	C5-N7	-2.02	1.35	1.39
5	A	501	GTP	PA-O3A	2.00	1.61	1.59

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-6.44	118.14	128.39
10	D	502	A1D69	C02-C01-S20	-6.27	104.30	110.75
8	B	501	GDP	C5-C4-N3	-6.16	118.58	128.39
8	D	501	GDP	C2-N3-C4	5.68	122.08	112.30
5	C	501	GTP	C5-C4-N3	-5.05	120.36	128.39
8	B	501	GDP	C2-N3-C4	5.04	120.98	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C4-N3	-4.98	120.46	128.39
10	D	502	A1D69	C01-S20-C19	4.72	97.48	91.24
10	B	505	A1D69	C02-N03-C04	4.70	119.00	114.58
5	C	501	GTP	C2-N3-C4	4.65	120.30	112.30
8	B	501	GDP	N9-C4-N3	4.60	135.15	125.95
5	A	501	GTP	C2-N3-C4	4.58	120.19	112.30
8	D	501	GDP	N9-C4-N3	4.53	135.00	125.95
10	B	505	A1D69	CL17-C04-N03	4.25	121.15	115.17
10	D	502	A1D69	C02-N03-C04	3.88	118.22	114.58
10	D	502	A1D69	C01-C06-N05	-3.80	117.80	122.33
10	D	502	A1D69	C04-N05-C06	3.66	121.35	110.98
10	D	502	A1D69	C18-C19-S20	-3.64	106.41	113.90
10	B	505	A1D69	N05-C06-N07	3.64	119.92	116.12
10	B	505	A1D69	N05-C04-N03	-3.53	123.07	129.52
8	D	501	GDP	C6-C5-N7	3.48	136.62	130.29
10	D	502	A1D69	N05-C04-N03	-3.24	123.60	129.52
10	B	505	A1D69	C18-C19-S20	-3.24	107.25	113.90
5	C	501	GTP	N9-C4-N3	3.21	132.38	125.95
8	B	501	GDP	C6-C5-N7	3.18	136.09	130.29
11	F	401	ACP	O2B-PB-O1B	3.17	120.26	109.95
5	A	501	GTP	N9-C4-N3	3.11	132.17	125.95
10	B	505	A1D69	C01-S20-C19	3.09	95.32	91.24
10	B	505	A1D69	C04-N05-C06	2.97	119.39	110.98
5	A	501	GTP	C2-N1-C6	-2.94	119.79	125.11
5	C	501	GTP	C2-N1-C6	-2.90	119.84	125.11
8	D	501	GDP	C4-C5-N7	-2.76	106.30	110.67
11	F	401	ACP	PB-O3A-PA	-2.75	123.39	132.37
10	D	502	A1D69	CL17-C04-N03	2.66	118.92	115.17
11	F	401	ACP	O1G-PG-C3B	-2.65	105.58	111.37
10	B	505	A1D69	C02-C01-S20	-2.64	108.04	110.75
5	A	501	GTP	N9-C8-N7	-2.63	108.53	113.40
5	C	501	GTP	N9-C8-N7	-2.58	108.62	113.40
8	B	501	GDP	C4-C5-N7	-2.54	106.65	110.67
5	A	501	GTP	C8-N7-C5	2.51	108.73	104.26
5	C	501	GTP	C5-C6-N1	2.50	119.61	113.25
5	C	501	GTP	C8-N7-C5	2.48	108.68	104.26
5	A	501	GTP	C5-C6-N1	2.46	119.52	113.25
5	C	501	GTP	O6-C6-C5	-2.37	120.26	126.53
5	A	501	GTP	O6-C6-C5	-2.36	120.31	126.53
8	B	501	GDP	C3'-C2'-C1'	2.32	105.86	101.46
10	B	505	A1D69	C01-C06-N07	-2.29	119.11	122.14
8	D	501	GDP	O6-C6-C5	-2.17	120.79	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C3'-C2'-C1'	2.16	105.56	101.46
5	C	501	GTP	C3'-C2'-C1'	2.15	105.52	101.46
8	D	501	GDP	C3'-C2'-C1'	2.13	105.49	101.46
8	B	501	GDP	O6-C6-C5	-2.10	121.00	126.53
8	D	501	GDP	N2-C2-N1	2.07	121.13	116.76
8	D	501	GDP	C5-C6-N1	2.05	118.46	113.25

There are no chirality outliers.

All (31) torsion outliers are listed below:

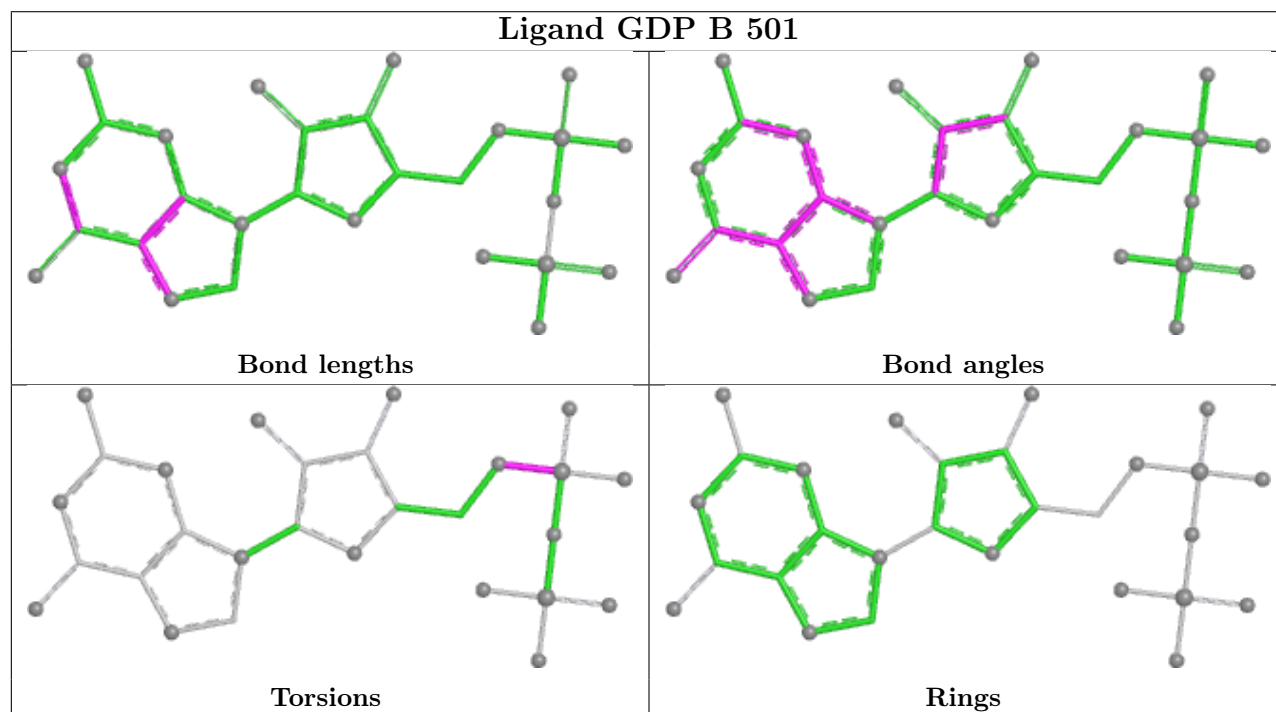
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	502	MES	C7-C8-S-O1S
9	B	502	MES	C7-C8-S-O2S
9	B	502	MES	C7-C8-S-O3S
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
9	B	502	MES	C8-C7-N4-C3
9	B	502	MES	C8-C7-N4-C5
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
8	D	501	GDP	C3'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
8	D	501	GDP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3B-PG-O1G

There are no ring outliers.

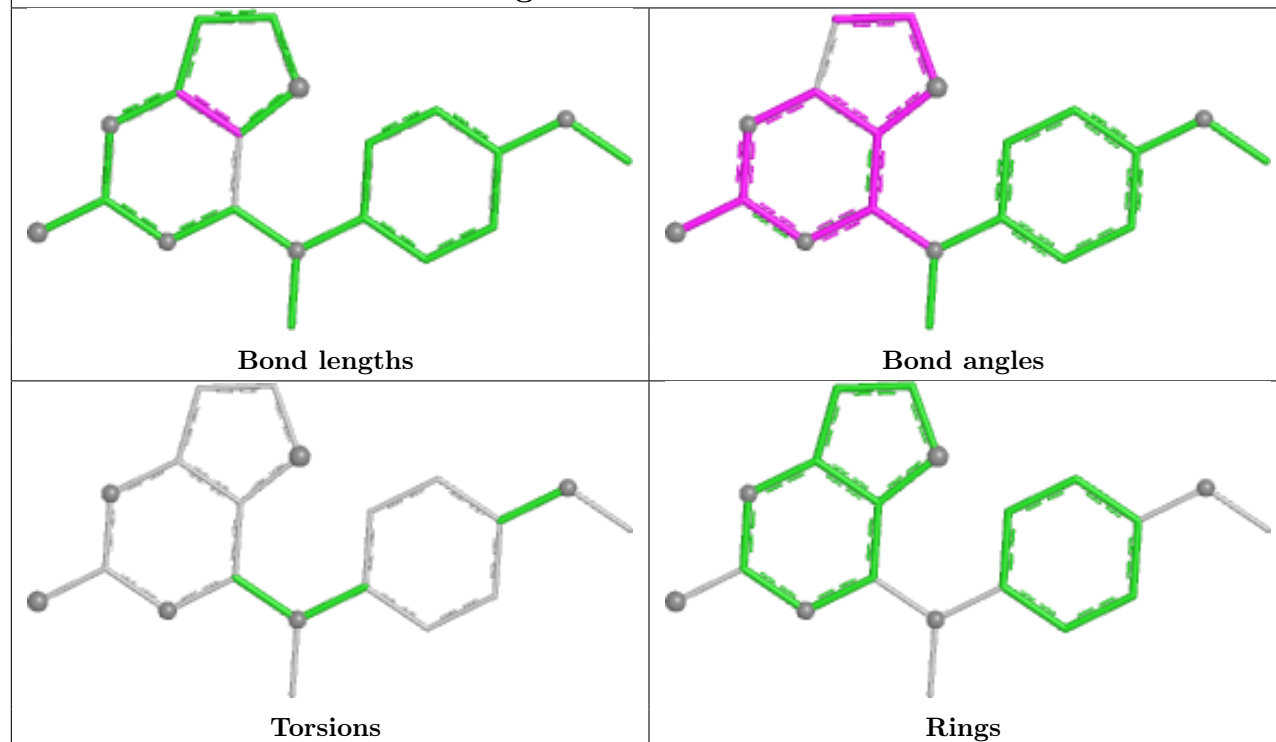
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	A1D69	1	0

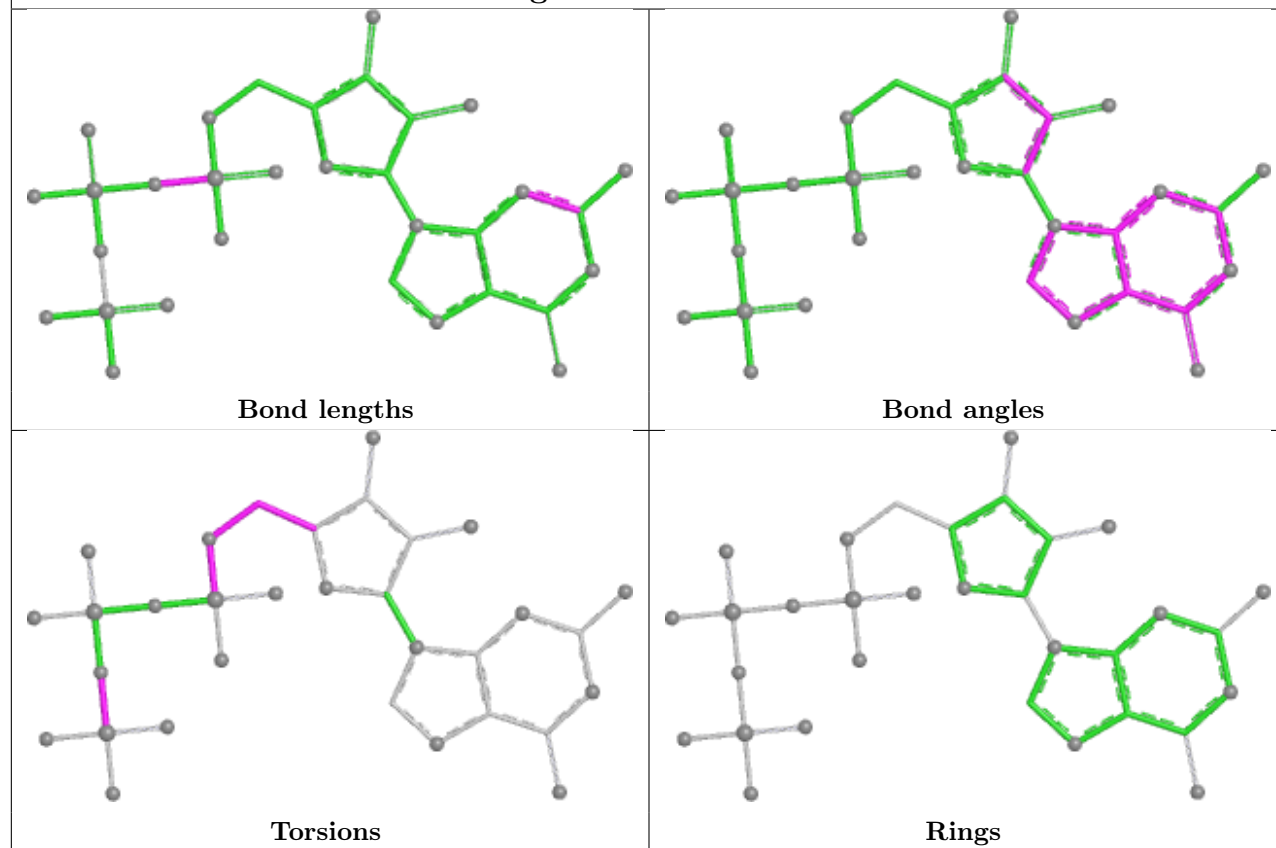
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

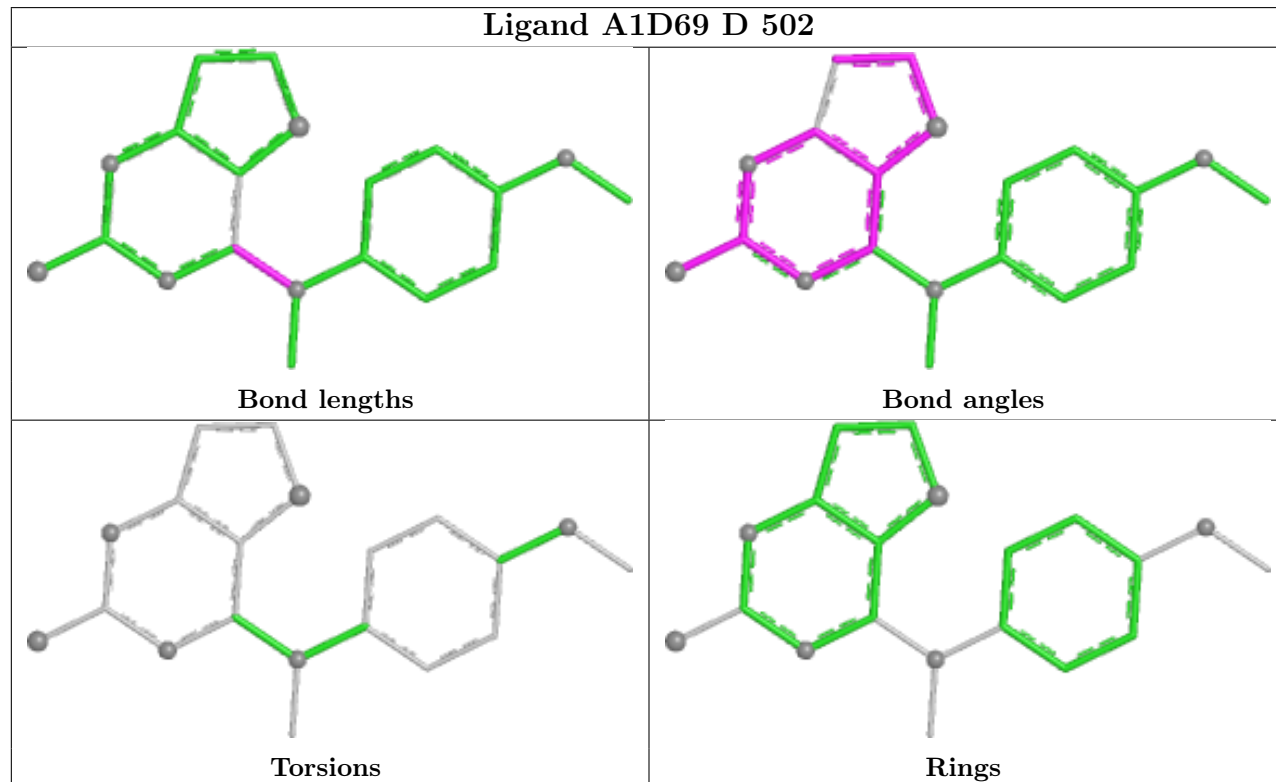
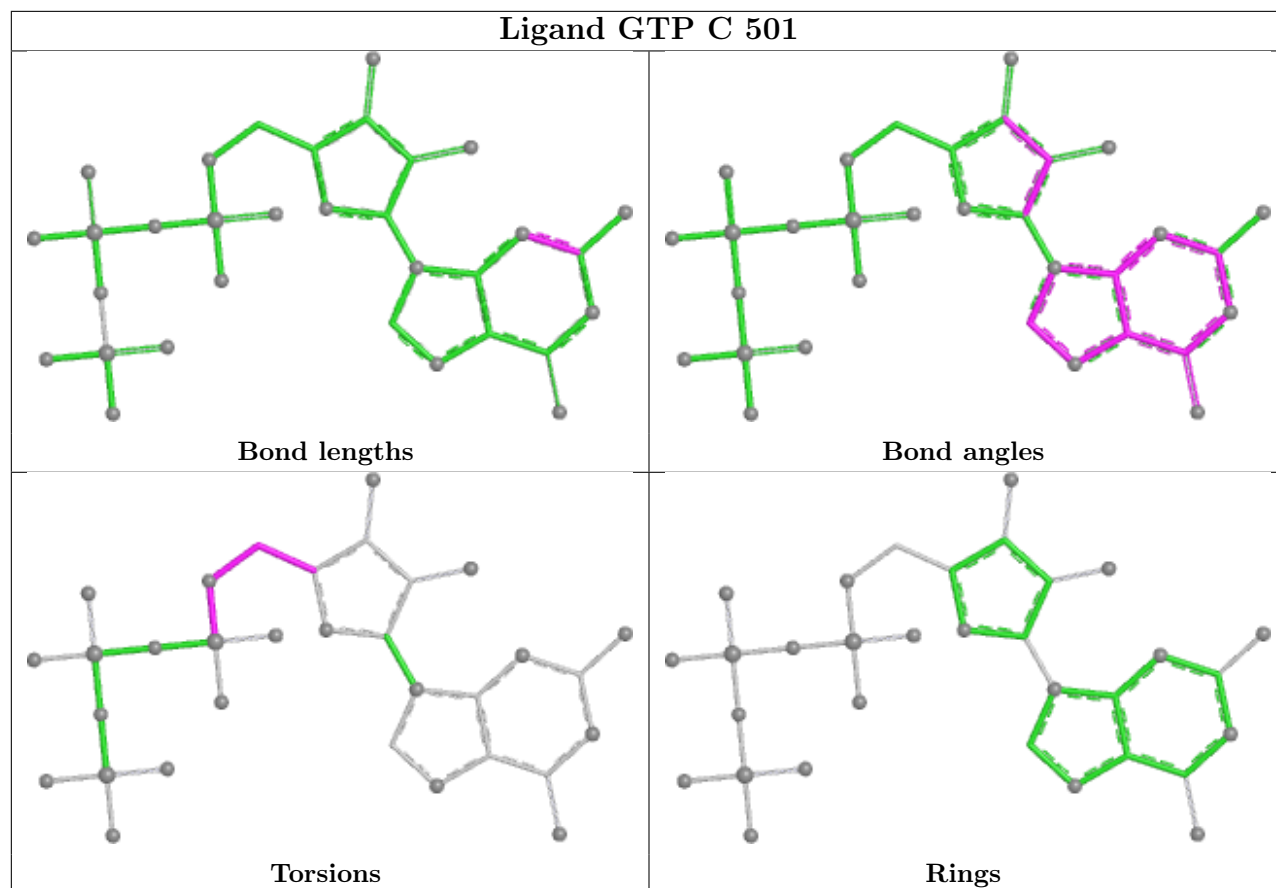


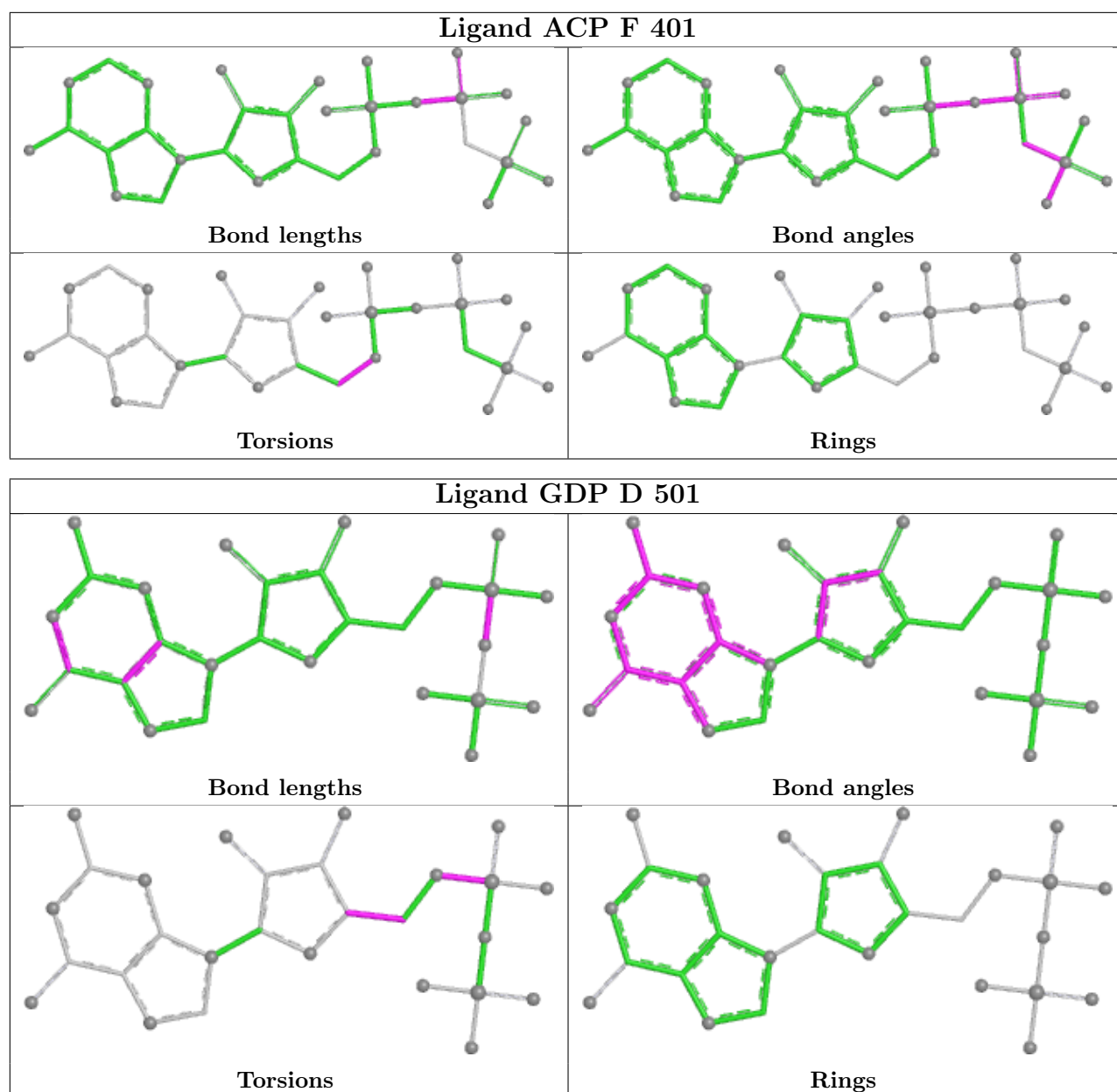
Ligand A1D69 B 505



Ligand GTP A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/440 (99%)	0.53	21 (4%) 35 35	36, 51, 77, 97	0
1	C	440/440 (100%)	0.25	12 (2%) 56 56	29, 42, 63, 100	0
2	B	427/431 (99%)	0.69	42 (9%) 13 12	31, 50, 86, 146	0
2	D	418/431 (96%)	1.37	110 (26%) 1 1	40, 68, 103, 142	0
3	E	120/143 (83%)	1.21	21 (17%) 4 3	44, 63, 97, 105	0
4	F	310/380 (81%)	1.93	105 (33%) 1 1	44, 69, 133, 170	0
All	All	2152/2265 (95%)	0.91	311 (14%) 6 5	29, 55, 99, 170	0

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	148	ILE	9.3
4	F	162	ILE	9.2
4	F	245	ILE	9.2
4	F	130	VAL	8.9
4	F	146	VAL	7.9
4	F	169	LEU	7.0
4	F	161	LEU	6.8
4	F	254	GLY	6.7
4	F	149	ALA	6.5
4	F	99	VAL	6.4
4	F	103	THR	6.3
1	A	437	VAL	6.2
2	D	247	ASN	6.2
4	F	166	ALA	6.2
4	F	186	LEU	6.1
4	F	240	LEU	6.0
4	F	180	HIS	6.0
4	F	134	ALA	5.9
4	F	239	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
2	D	73	MET	5.8
4	F	256	TYR	5.7
4	F	184	LYS	5.7
2	B	428	ALA	5.6
4	F	170	LEU	5.6
4	F	172	PHE	5.6
4	F	147	TRP	5.6
4	F	182	ILE	5.5
4	F	173	ILE	5.5
4	F	98	TYR	5.3
4	F	101	TYR	5.3
2	D	72	THR	5.3
3	E	45	PRO	5.2
4	F	179	VAL	5.2
2	D	92	PHE	5.1
4	F	132	LEU	5.0
2	D	397	TRP	4.9
2	D	55	THR	4.9
4	F	181	VAL	4.8
4	F	238	CYS	4.8
3	E	139	LEU	4.8
2	D	284	LEU	4.7
4	F	135	TYR	4.7
4	F	131	PHE	4.6
2	B	72	THR	4.6
2	D	42	LEU	4.6
4	F	89	GLU	4.6
4	F	164	SER	4.5
2	D	219	THR	4.4
4	F	236	LYS	4.4
4	F	185	TYR	4.4
2	D	11	GLN	4.4
4	F	163	SER	4.4
4	F	100	ILE	4.3
4	F	243	HIS	4.3
4	F	380	HIS	4.2
4	F	225	SER	4.2
2	B	280	GLN	4.2
2	D	32	PRO	4.2
2	D	1	MET	4.1
2	D	98	GLY	4.1
4	F	244	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	440	VAL	4.1
2	D	394	PHE	4.1
3	E	141	GLU	4.1
2	D	246	LEU	4.0
2	D	37	HIS	4.0
4	F	194	PRO	4.0
1	A	282	TYR	4.0
2	D	245	GLN	3.9
2	D	56	GLY	3.9
4	F	237	THR	3.9
1	C	357	TYR	3.9
1	C	41	THR	3.9
3	E	28	SER	3.9
2	D	81	PHE	3.9
4	F	139	ARG	3.9
2	B	218	THR	3.9
2	B	279	GLN	3.8
2	B	55	THR	3.8
4	F	133	ALA	3.8
1	C	340	SER	3.8
1	A	112	LYS	3.7
2	B	277	GLY	3.7
1	C	1	MET	3.7
2	D	80	PRO	3.7
4	F	138	ARG	3.6
4	F	277	THR	3.6
2	D	170	MET	3.6
4	F	242	ASN	3.5
4	F	102	PRO	3.5
2	B	276	ARG	3.5
3	E	6	MET	3.5
2	D	395	LEU	3.5
2	D	222	TYR	3.5
4	F	379	HIS	3.5
2	B	427	ASP	3.4
4	F	241	THR	3.4
4	F	372	THR	3.4
2	D	94	GLN	3.4
2	D	57	ASN	3.4
4	F	224	SER	3.4
2	D	391	ARG	3.3
2	B	278	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	33	THR	3.3
2	D	248	ALA	3.3
2	B	247	ASN	3.3
4	F	145	ASN	3.3
2	D	390	ARG	3.3
2	B	281	TYR	3.2
2	B	41	ASP	3.2
2	D	389	PHE	3.2
1	C	245	ASP	3.2
2	D	115	SER	3.1
4	F	263	PHE	3.1
2	D	91	VAL	3.1
2	D	217	LEU	3.1
2	B	37	HIS	3.1
2	B	40	SER	3.1
4	F	167	SER	3.1
4	F	183	GLN	3.1
2	D	405	GLU	3.1
1	A	46	ASP	3.1
2	D	387	ALA	3.1
1	A	42	ILE	3.0
1	A	365	GLY	3.0
2	D	404	ASP	3.0
4	F	33	ASP	3.0
4	F	320	MET	3.0
2	D	356	ILE	3.0
2	D	386	THR	3.0
2	B	245	GLN	3.0
2	D	362	LYS	3.0
1	A	262	TYR	3.0
2	D	431	ASP	3.0
4	F	341	LYS	2.9
1	A	41	THR	2.9
2	D	323	MET	2.9
4	F	28	LYS	2.9
4	F	46	ARG	2.9
2	D	285	THR	2.9
4	F	187	GLU	2.9
2	B	56	GLY	2.9
2	D	39	ASP	2.9
4	F	88	SER	2.9
1	C	163	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	361	LEU	2.9
2	B	275	SER	2.8
2	D	215	LEU	2.8
2	D	69	GLU	2.8
2	D	218	THR	2.8
2	D	68	LEU	2.8
4	F	221	LEU	2.8
2	D	100	ASN	2.8
4	F	334	GLY	2.8
1	A	113	GLU	2.8
3	E	7	GLU	2.8
4	F	165	GLU	2.8
2	D	393	ALA	2.8
2	B	336	LYS	2.8
2	D	406	MET	2.8
4	F	197	ARG	2.8
2	D	398	TYR	2.8
2	D	90	PHE	2.8
2	D	180	VAL	2.8
2	D	84	ILE	2.7
4	F	235	ASP	2.7
4	F	175	GLU	2.7
2	B	282	ARG	2.7
2	D	30	ILE	2.7
4	F	136	ASN	2.7
4	F	333	ASN	2.7
1	A	346	TRP	2.7
4	F	20	LEU	2.7
4	F	234	GLN	2.6
2	D	212	PHE	2.6
1	A	362	VAL	2.6
3	E	8	VAL	2.6
4	F	330	ILE	2.6
3	E	115	HIS	2.6
2	D	392	LYS	2.6
3	E	52	LYS	2.6
2	D	290	THR	2.6
4	F	191	LEU	2.6
2	D	383	GLU	2.6
3	E	59	GLU	2.6
2	D	36	TYR	2.6
4	F	177	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	223	THR	2.6
4	F	85	PRO	2.6
2	B	69	GLU	2.6
1	A	281	ALA	2.6
4	F	259	GLY	2.6
2	D	179	VAL	2.6
2	B	42	LEU	2.5
2	D	273	LEU	2.5
2	D	289	LEU	2.5
2	D	77	ARG	2.5
2	D	359	ARG	2.5
2	B	323	MET	2.5
2	D	101	TRP	2.5
4	F	24	THR	2.5
2	D	16	ILE	2.5
2	D	35	SER	2.5
2	D	216	LYS	2.5
4	F	306	HIS	2.5
4	F	178	GLN	2.5
3	E	48	GLU	2.5
4	F	335	ALA	2.5
2	D	122	LYS	2.5
2	D	360	GLY	2.5
3	E	25	LYS	2.5
1	C	337	THR	2.5
2	D	227	HIS	2.5
1	C	2	ARG	2.5
2	B	54	ALA	2.5
2	D	54	ALA	2.5
2	B	71	GLY	2.5
2	B	214	THR	2.5
2	D	40	SER	2.5
2	D	135	LEU	2.5
4	F	314	LEU	2.5
4	F	198	LYS	2.5
2	B	283	ALA	2.5
2	D	71	GLY	2.5
2	D	400	GLY	2.5
4	F	25	GLY	2.5
3	E	121	GLU	2.4
4	F	190	LEU	2.4
2	B	57	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	176	GLN	2.4
4	F	144	GLY	2.4
2	B	175	VAL	2.4
4	F	340	GLN	2.4
2	B	291	GLN	2.4
1	A	345	ASP	2.4
2	D	34	GLY	2.4
1	A	232	SER	2.4
2	B	78	SER	2.4
3	E	50	ILE	2.4
2	D	213	ARG	2.4
1	C	285	GLN	2.4
2	D	111	GLU	2.4
2	D	14	ASN	2.3
2	D	223	GLY	2.3
2	B	33	THR	2.3
2	D	107	THR	2.3
4	F	22	LEU	2.3
2	D	93	GLY	2.3
2	D	6	HIS	2.3
3	E	128	LYS	2.3
2	D	357	PRO	2.3
1	A	221	ARG	2.3
1	C	281	ALA	2.3
3	E	132	GLU	2.3
3	E	47	LEU	2.2
2	B	39	ASP	2.2
2	D	41	ASP	2.2
2	B	320	ARG	2.2
2	D	10	GLY	2.2
2	D	181	GLU	2.2
2	D	214	THR	2.2
4	F	188	LYS	2.2
4	F	13	VAL	2.2
4	F	192	LEU	2.2
2	D	85	PHE	2.2
2	D	86	ARG	2.2
2	B	95	SER	2.2
2	D	59	TYR	2.2
1	A	344	VAL	2.2
4	F	31	ARG	2.2
4	F	45	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	360	PRO	2.2
2	D	126	SER	2.2
2	D	106	TYR	2.2
1	A	18	ASN	2.2
2	D	363	MET	2.2
3	E	90	ASN	2.2
3	E	127	ASP	2.2
2	B	274	THR	2.2
2	D	320	ARG	2.1
1	A	88	HIS	2.1
4	F	373	SER	2.1
2	B	73	MET	2.1
1	A	94	THR	2.1
2	B	75	SER	2.1
2	B	170	MET	2.1
2	D	27	GLU	2.1
4	F	137	ARG	2.1
3	E	71	HIS	2.1
2	D	381	ILE	2.1
2	D	220	PRO	2.1
4	F	220	VAL	2.1
1	C	44	GLY	2.1
2	B	350	LYS	2.0
2	D	19	LYS	2.0
2	B	126	SER	2.0
2	D	364	SER	2.0
1	A	315	CYS	2.0
4	F	323	GLU	2.0
2	D	48	ASN	2.0
2	D	65	LEU	2.0
2	D	226	ASN	2.0
2	B	353	VAL	2.0
1	A	57	GLY	2.0
2	D	396	HIS	2.0
2	D	112	LEU	2.0
2	D	117	LEU	2.0
4	F	171	ASP	2.0
4	F	352	ASP	2.0
2	D	243	PRO	2.0
3	E	135	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

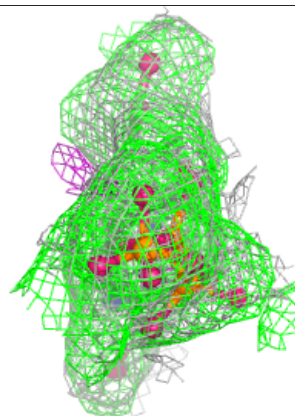
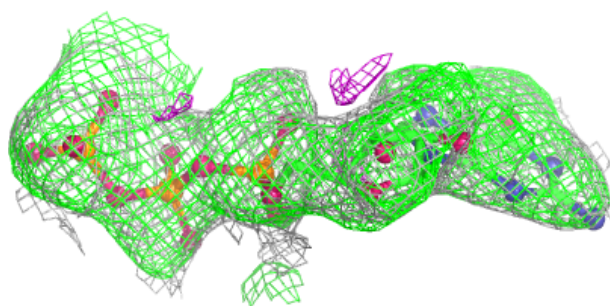
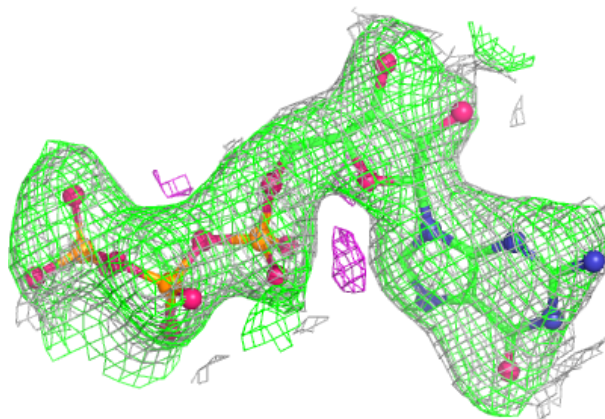
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	-	-	39,40,42,44	32
5	GTP	C	501	32/32	-	-	34,37,39,39	32
6	CA	A	502	1/1	-	-	80,80,80,80	1
6	CA	C	502	1/1	-	-	54,54,54,54	1
7	MG	A	503	1/1	-	-	44,44,44,44	1
7	MG	B	504	1/1	-	-	47,47,47,47	1
7	MG	C	503	1/1	-	-	39,39,39,39	1
8	GDP	B	501	28/28	-	-	37,42,43,44	28
8	GDP	D	501	28/28	-	-	68,72,74,75	28
9	MES	B	502	12/12	-	-	43,45,47,48	12
9	MES	B	503	12/12	-	-	56,57,57,58	12
10	A1D69	D	502	20/20	0.93	0.09	39,50,64,65	0
10	A1D69	B	505	20/20	0.96	0.08	36,43,51,51	0
11	ACP	F	401	31/31	-	-	75,88,106,110	45

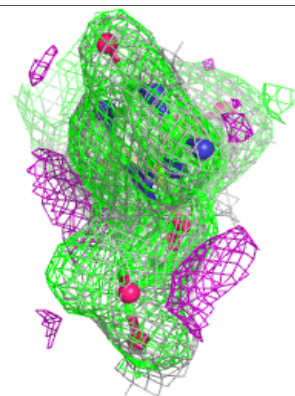
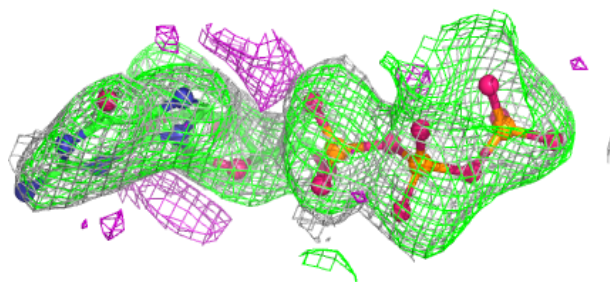
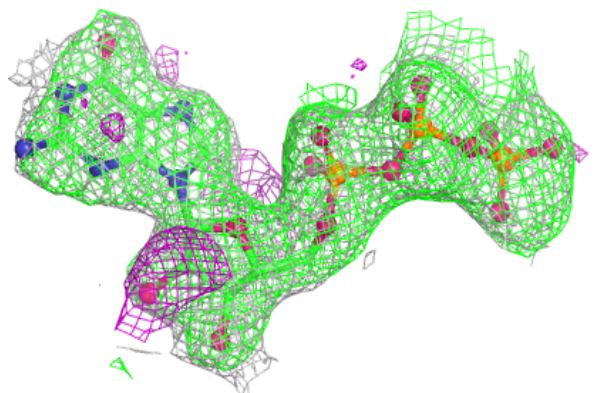
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP A 501:

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

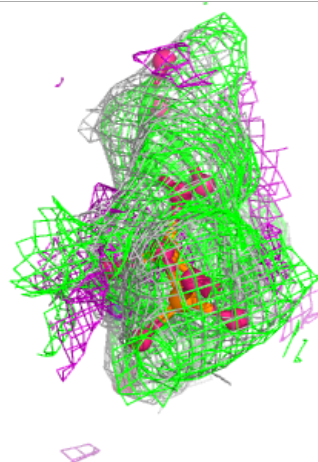
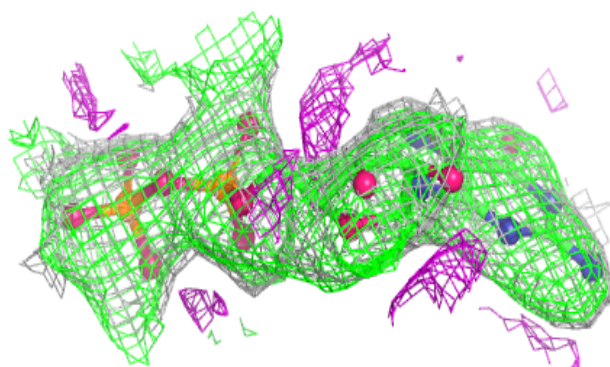
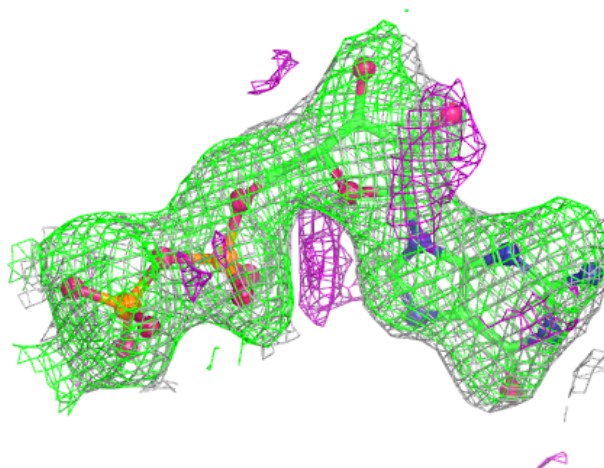
**Electron density around GTP C 501:**

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



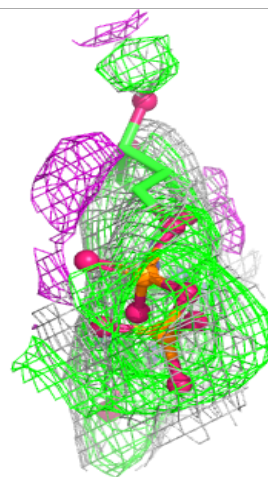
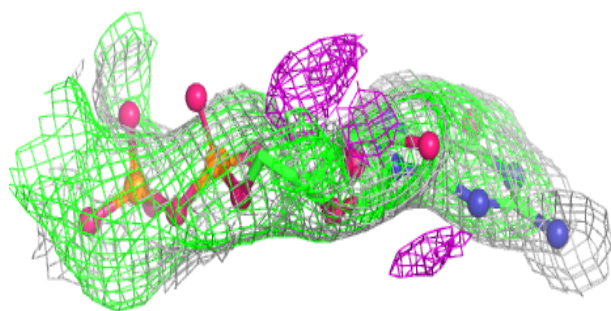
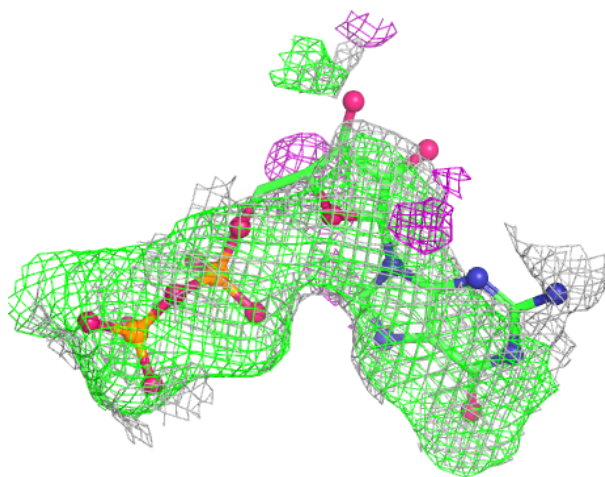
Electron density around GDP B 501:

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



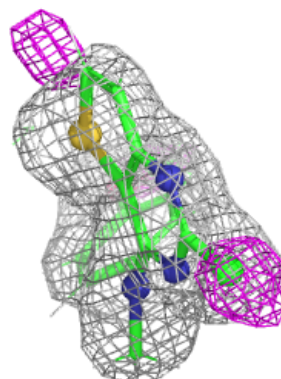
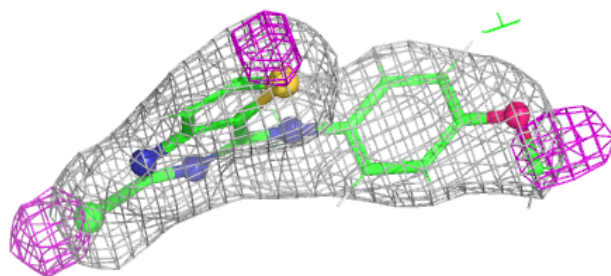
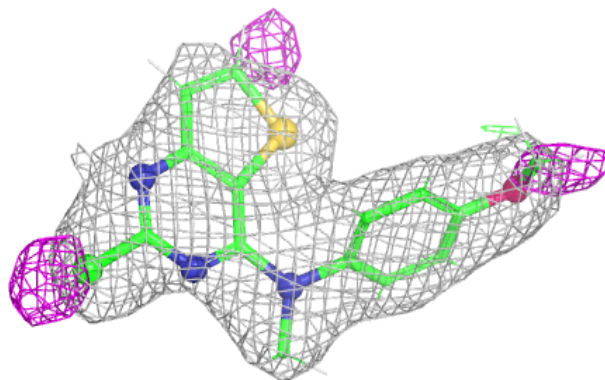
Electron density around GDP D 501:

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

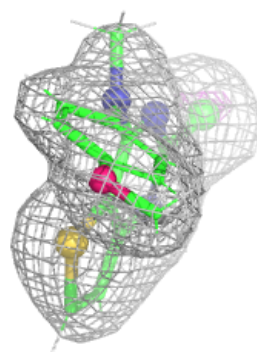
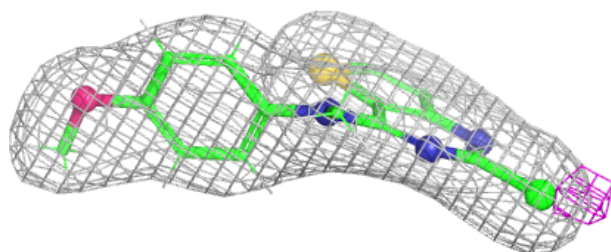
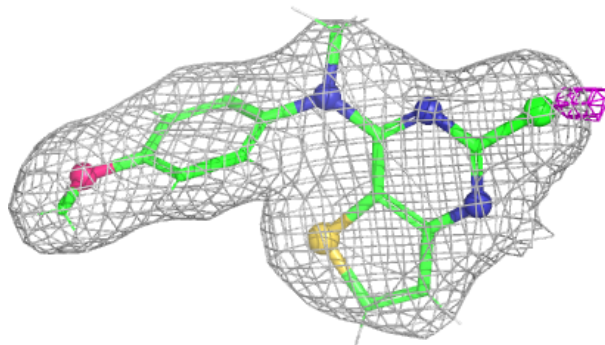


Electron density around A1D69 D 502:

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

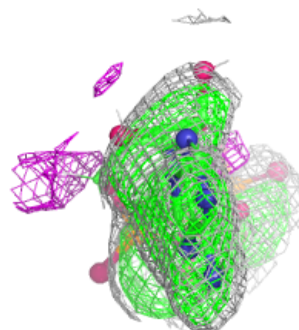
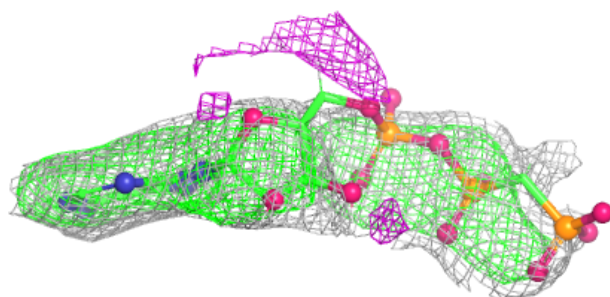
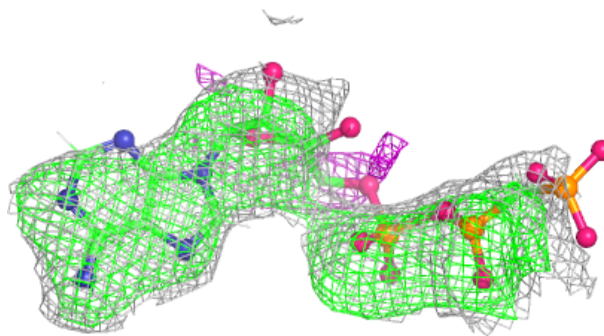
**Electron density around A1D69 B 505:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.