



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2026 – 09:13 PM JST

PDB ID : 9VYP / pdb_00009vyp
Title : Crystal structure of T2R-TTL-TZ2 complex
Authors : Lun, T.; Chengyong, W.
Deposited on : 2025-07-21
Resolution : 2.52 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

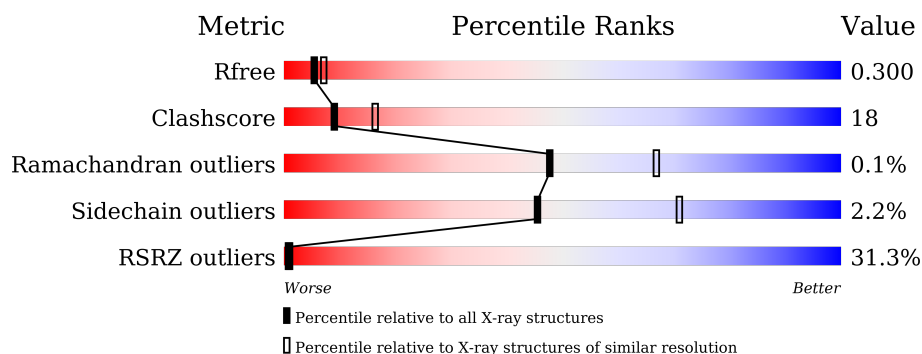
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	25% 67% 32% .
1	C	440	5% 73% 26% .
2	B	431	12% 65% 33% ..
2	D	431	71% 62% 35% ..
3	E	136	35% 57% 32% 11%
4	F	380	38% 49% 38% . 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	A1EU1	D	502	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17464 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	421	Total	C	N	O	S	0	0	0
			3300	2076	559	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2713	1740	466	493	14			

There are 35 discrepancies between the modelled and reference sequences:

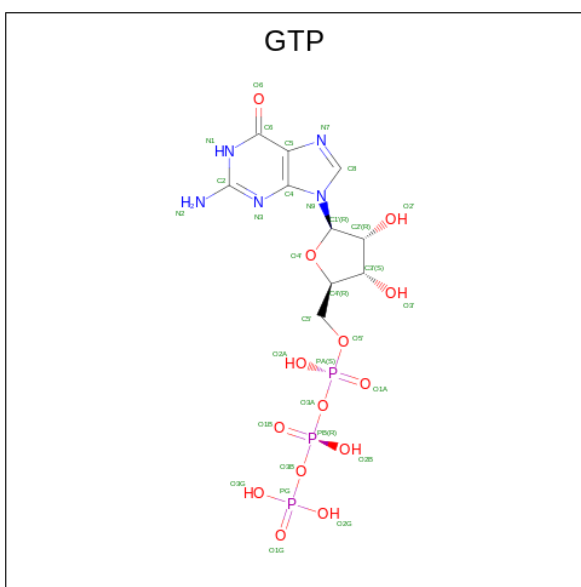
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0

- 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		

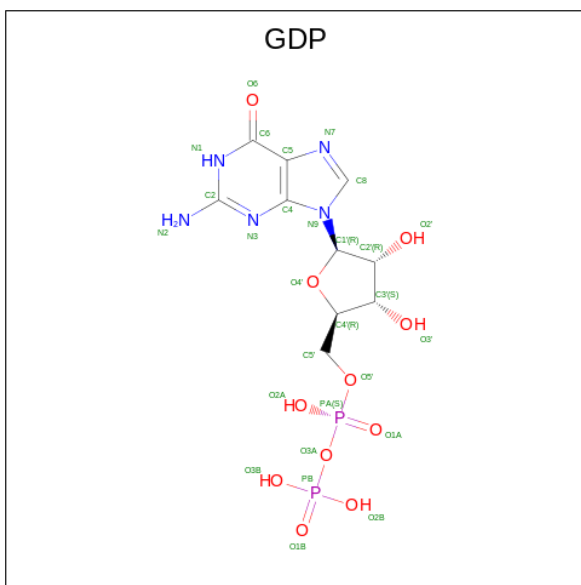
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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).

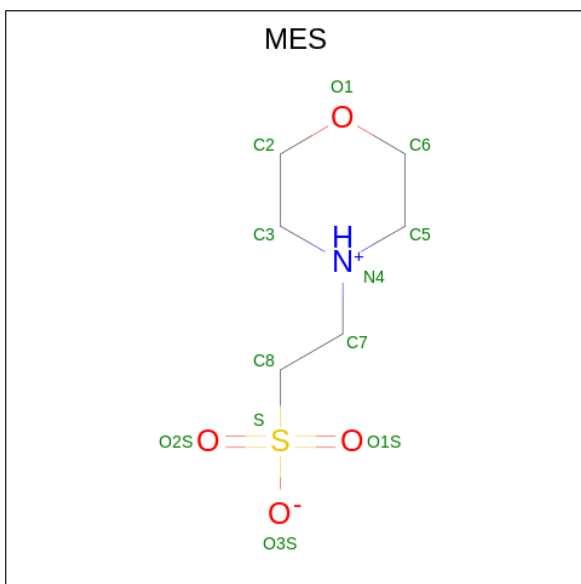
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		
7	C	1	Total	Mg	1	0
			1	1		

- 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	28	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	28	0

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



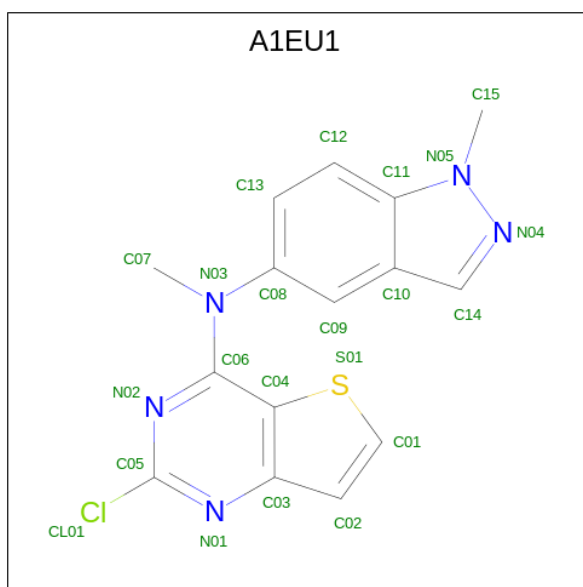
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

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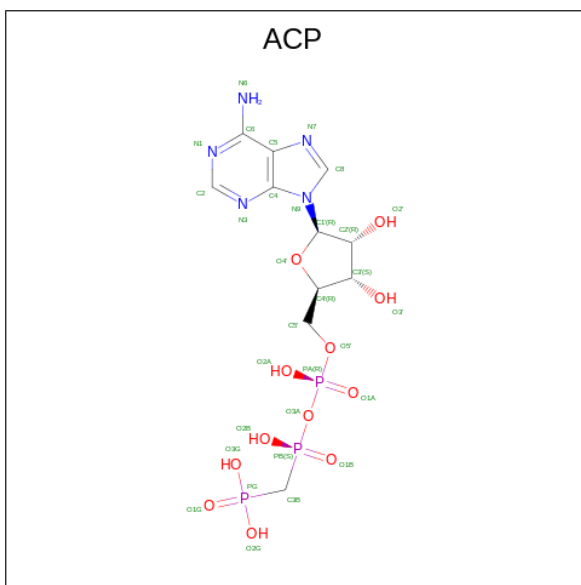
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

- Molecule 10 is 2-chloranyl- {N}-methyl- {N}-(1-methylindazol-5-yl)thieno[3,2-d]pyrimidin-4-amine (CCD ID: A1EU1) (formula: C₁₅H₁₂ClN₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	Cl	H	N	S	0	0
			34	15	1	12	5	1		
10	D	1	Total	C	Cl	H	N	S	0	0
			34	15	1	12	5	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

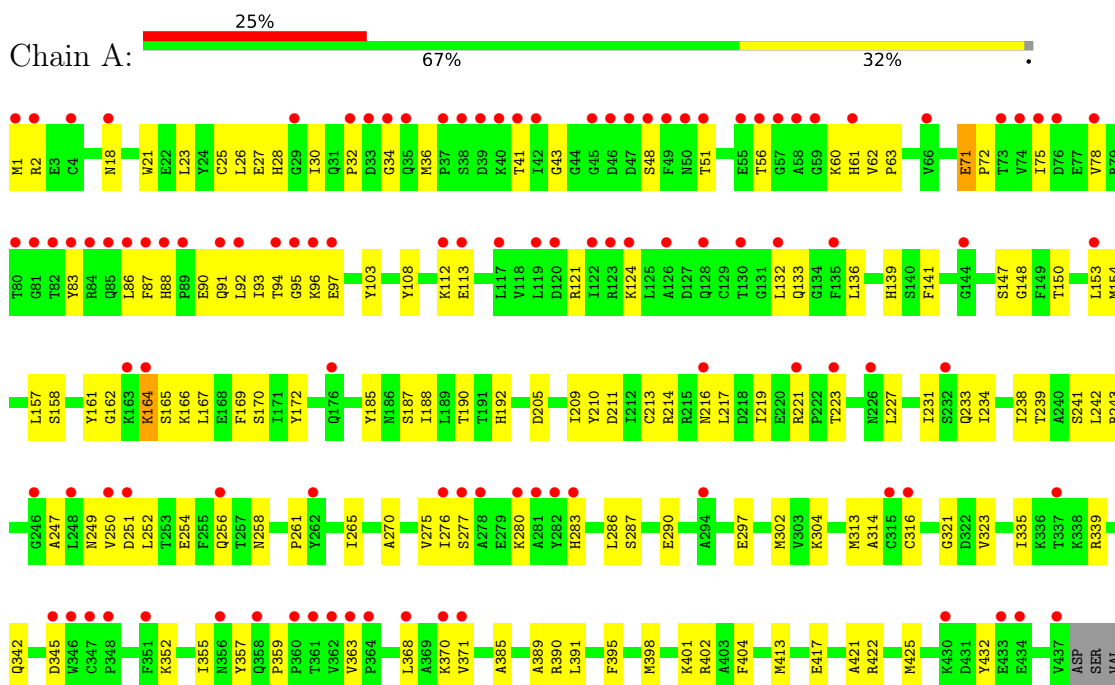


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		

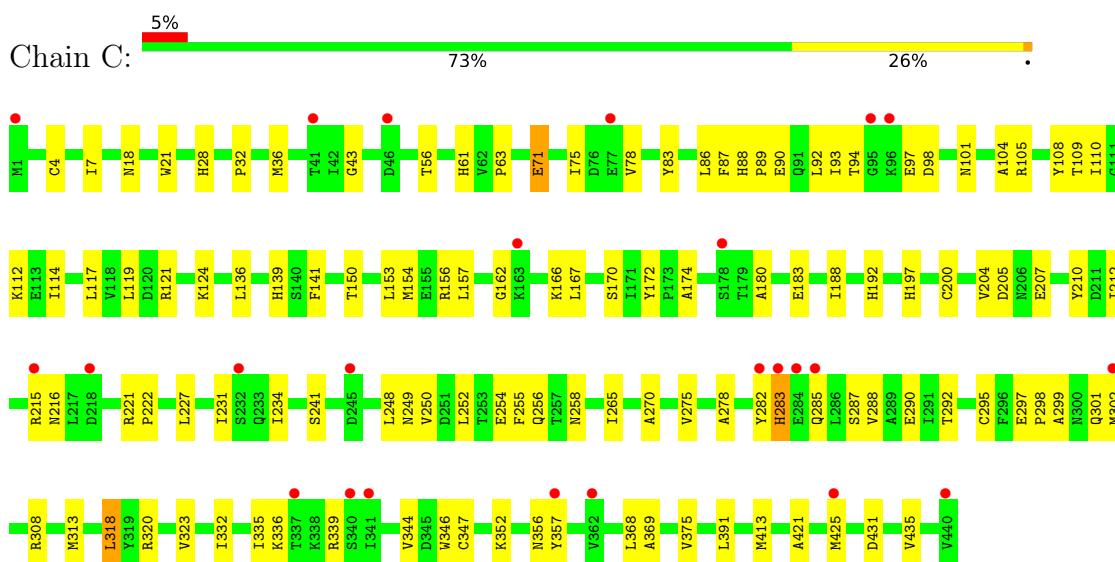
3 Residue-property plots [i](#)

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

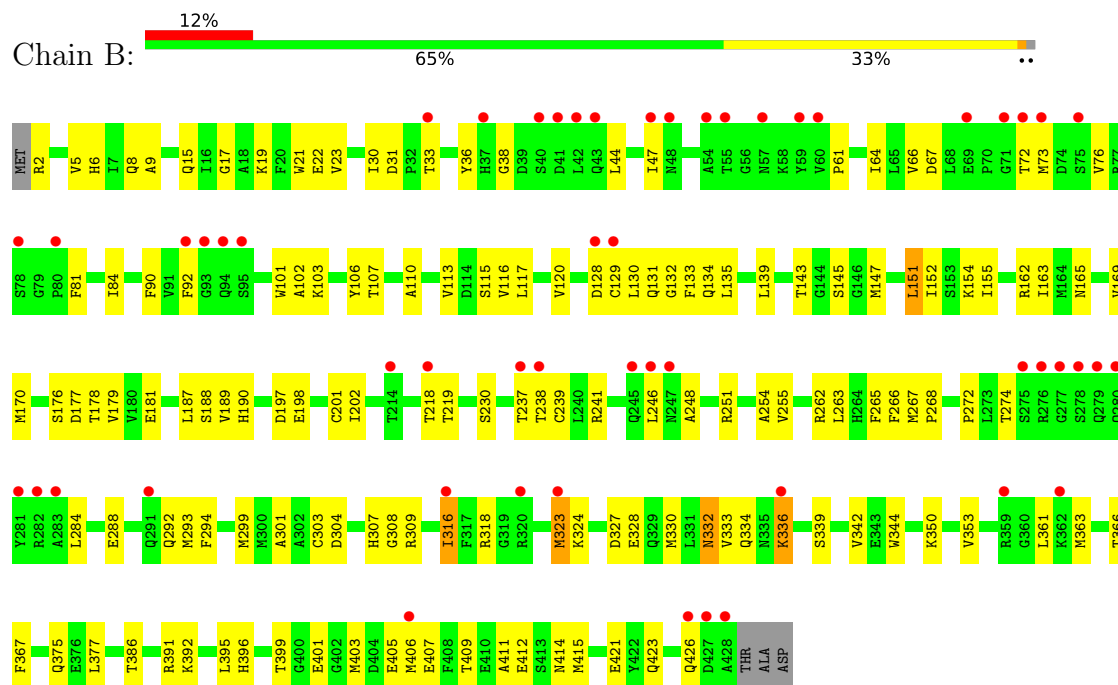
• Molecule 1: Detyrosinated tubulin alpha-1B chain



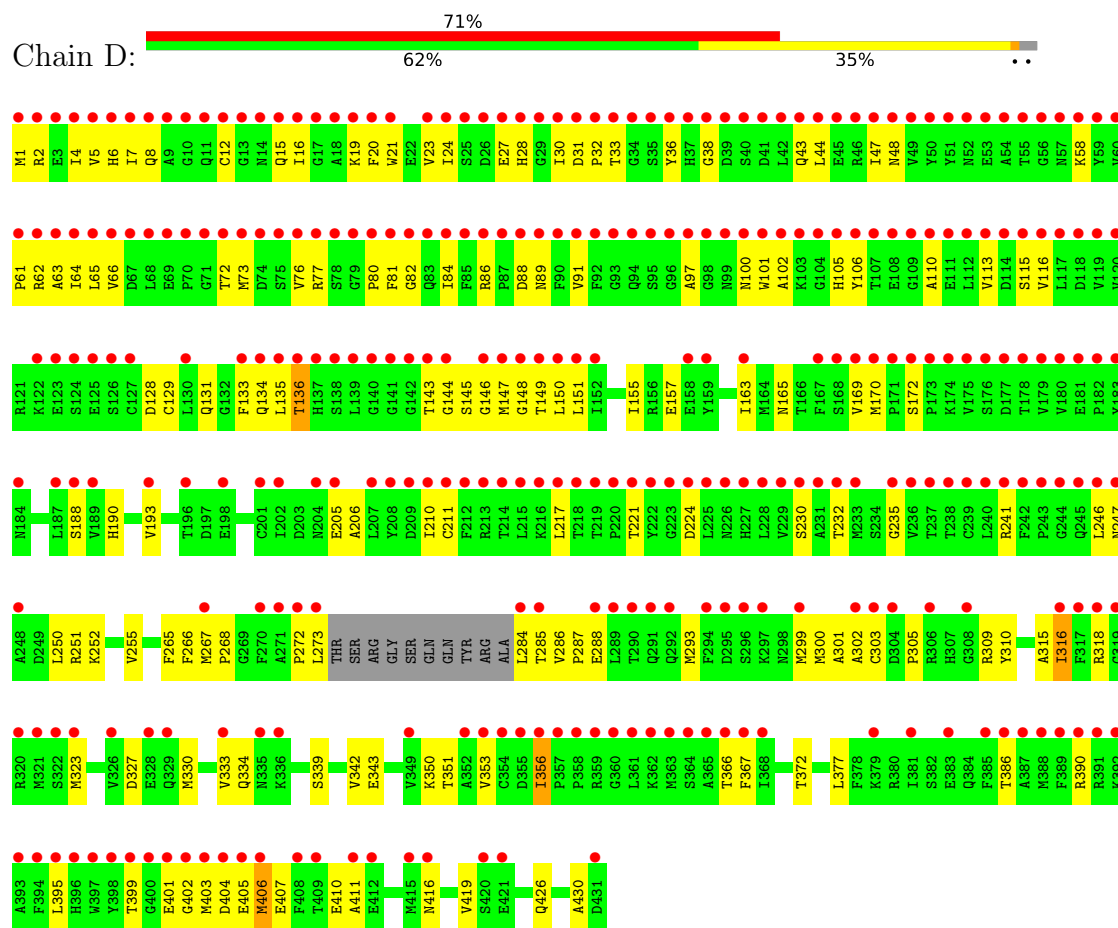
• Molecule 1: Detyrosinated tubulin alpha-1B chain



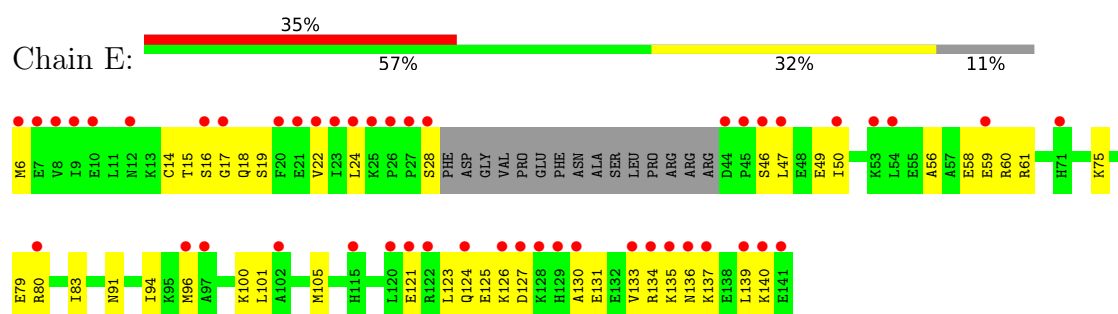
- Molecule 2: Tubulin beta chain



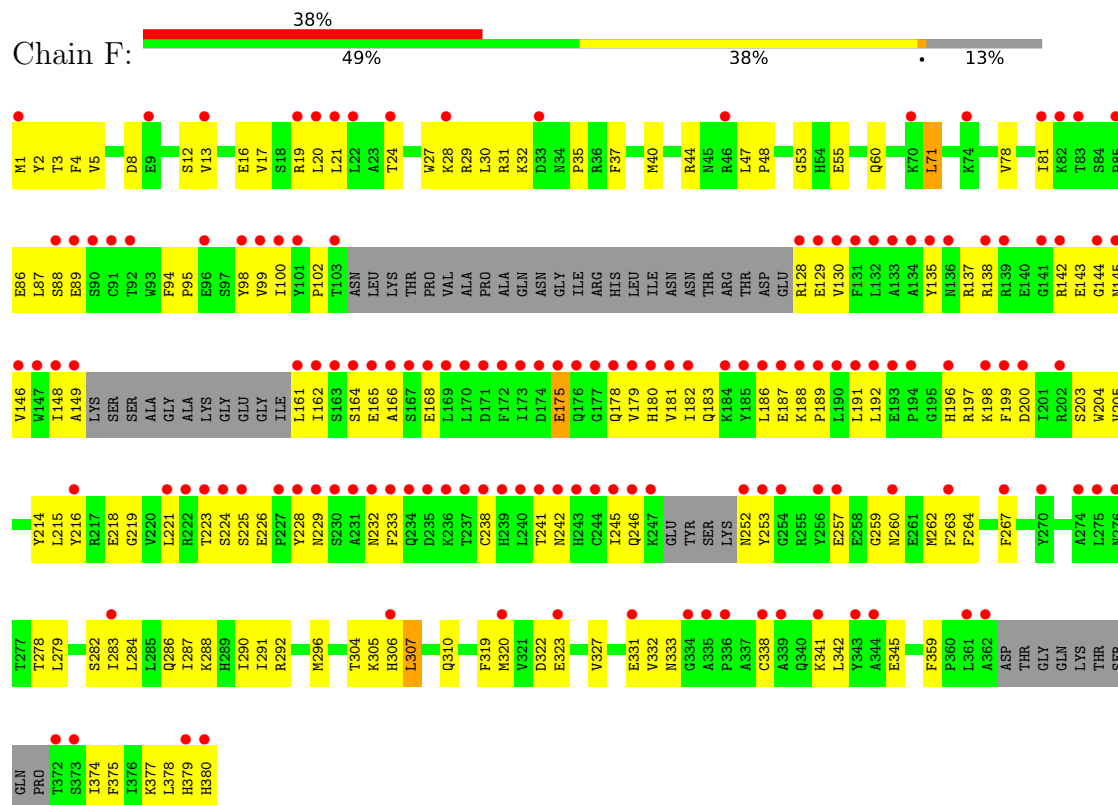
- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.74Å 157.26Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.05 – 2.52 56.05 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.05-2.52) 99.8 (56.05-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.268 , 0.300 0.269 , 0.300	Depositor DCC
R_{free} test set	5121 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17464	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACP, GDP, A1EU1, MG, MES, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3482	0.44	0/4728
1	C	0.23	0/3511	0.42	0/4768
2	B	0.34	3/3426 (0.1%)	0.45	1/4643 (0.0%)
2	D	0.23	0/3373	0.40	0/4570
3	E	0.18	0/1008	0.33	0/1337
4	F	0.18	0/2775	0.34	0/3752
All	All	0.25	3/17575 (0.0%)	0.41	1/23798 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	323	MET	SD-CE	11.49	2.08	1.79
2	B	332	ASN	CB-CG	-6.26	1.36	1.52
2	B	336	LYS	CD-CE	-5.20	1.36	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	323	MET	CG-SD-CE	-8.42	82.37	100.90

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	121	0
1	C	3433	0	3337	98	2
2	B	3351	0	3216	128	1
2	D	3300	0	3176	139	0
3	E	1000	0	1018	40	1
4	F	2713	0	2659	124	0
5	A	32	0	12	0	0
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	12	0	0
9	B	24	0	26	0	0
10	B	22	12	0	5	0
10	D	22	12	0	5	0
11	F	31	14	14	0	0
All	All	17426	38	16806	626	2

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 18.

All (626) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:MET:SD	2:B:323:MET:CE	2.08	1.41
1:A:209:ILE:HD11	1:A:302:MET:HE1	1.12	1.12
3:E:46:SER:HB3	3:E:49:GLU:HG3	1.44	0.98
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.44	0.98
2:D:350:LYS:HB2	10:D:502:A1EU1:C14	1.94	0.97
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.47	0.95
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.47	0.95
2:B:350:LYS:HB2	10:B:505:A1EU1:C14	1.98	0.92
1:A:132:LEU:HD23	1:A:164:LYS:HE2	1.54	0.90
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.05	0.90
2:B:262:ARG:NH1	2:B:421:GLU:OE1	2.06	0.89
2:B:308:GLY:HA2	2:B:426:GLN:HE21	1.38	0.89
1:A:72:PRO:HB3	1:A:94:THR:HG21	1.56	0.88
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.06	0.88
2:D:134:GLN:HA	2:D:165:ASN:O	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD11	1:A:302:MET:CE	2.01	0.87
4:F:16:GLU:O	4:F:20:LEU:HD12	1.74	0.87
2:B:323:MET:CE	2:B:323:MET:CG	2.54	0.86
2:D:145:SER:OG	2:D:188:SER:OG	1.88	0.85
3:E:96:MET:HE3	3:E:100:LYS:HE2	1.60	0.83
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.59	0.83
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.78	0.82
1:C:234:ILE:HD13	1:C:302:MET:SD	2.20	0.81
2:D:401:GLU:HA	3:E:137:LYS:HD2	1.62	0.80
2:B:307:HIS:O	2:B:426:GLN:NE2	2.15	0.80
2:D:66:VAL:HG12	2:D:147:MET:HE1	1.63	0.80
3:E:131:GLU:OE1	3:E:134:ARG:NH2	2.14	0.79
1:A:63:PRO:CD	1:A:86:LEU:HG	2.13	0.78
2:D:5:VAL:HB	2:D:133:PHE:HD2	1.48	0.78
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.64	0.78
1:A:133:GLN:OE1	1:A:251:ASP:HA	1.84	0.77
1:A:62:VAL:HG13	1:A:86:LEU:O	1.85	0.76
2:D:350:LYS:CB	10:D:502:A1EU1:C14	2.62	0.76
4:F:135:TYR:CD2	4:F:166:ALA:HB2	2.20	0.76
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.68	0.76
4:F:100:ILE:HD12	4:F:128:ARG:N	1.99	0.76
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.68	0.76
2:D:1:MET:HG3	2:D:128:ASP:HB3	1.68	0.75
2:B:66:VAL:HG12	2:B:147:MET:HE1	1.68	0.75
2:B:323:MET:SD	2:B:353:VAL:HG11	2.26	0.75
4:F:188:LYS:HD3	4:F:323:GLU:OE1	1.87	0.75
2:D:285:THR:HG23	2:D:288:GLU:H	1.51	0.74
2:B:177:ASP:O	1:C:352:LYS:HE2	1.86	0.74
2:D:66:VAL:CG1	2:D:147:MET:HE1	2.17	0.74
4:F:197:ARG:HH22	4:F:257:GLU:CD	1.96	0.73
2:B:81:PHE:O	2:B:84:ILE:HG22	1.89	0.73
1:C:234:ILE:HG21	1:C:302:MET:SD	2.28	0.73
4:F:31:ARG:HH21	4:F:32:LYS:HG3	1.54	0.72
2:D:350:LYS:HB2	10:D:502:A1EU1:N04	2.03	0.72
2:D:5:VAL:HB	2:D:133:PHE:CD2	2.24	0.72
2:D:110:ALA:O	2:D:113:VAL:HG12	1.90	0.72
2:D:330:MET:HG3	2:D:351:THR:HG21	1.70	0.72
2:D:16:ILE:HD11	2:D:136:THR:HG22	1.71	0.71
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.20	0.71
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.25	0.71
1:A:97:GLU:HG3	2:B:2:ARG:NH1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLN:HA	2:B:165:ASN:O	1.90	0.71
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.71	0.71
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.72	0.70
2:D:72:THR:O	2:D:76:VAL:HG23	1.90	0.70
1:C:215:ARG:NH2	1:C:299:ALA:O	2.23	0.70
1:A:187:SER:CB	1:A:391:LEU:HD21	2.22	0.70
3:E:101:LEU:O	3:E:105:MET:HG2	1.92	0.70
2:B:324:LYS:O	2:B:328:GLU:HG3	1.92	0.69
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.74	0.69
2:D:190:HIS:ND1	2:D:411:ALA:HA	2.07	0.69
4:F:137:ARG:O	4:F:137:ARG:NH1	2.17	0.69
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.28	0.68
1:A:161:TYR:HD2	1:A:164:LYS:HE3	1.56	0.68
2:B:330:MET:O	2:B:333:VAL:HG12	1.93	0.68
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.74	0.68
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.29	0.68
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.29	0.67
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.29	0.67
2:B:316:ILE:HG23	2:B:366:THR:HB	1.76	0.67
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.77	0.67
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.67
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.75	0.67
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.76	0.67
2:B:308:GLY:CA	2:B:426:GLN:HE21	2.08	0.67
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.77	0.66
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.76	0.66
2:D:221:THR:HG22	2:D:224:ASP:OD2	1.95	0.66
1:C:90:GLU:OE1	1:C:124:LYS:NZ	2.28	0.66
2:B:350:LYS:CB	10:B:505:A1EU1:C14	2.71	0.66
1:A:210:TYR:OH	1:A:221:ARG:HG3	1.95	0.66
2:D:309:ARG:HH21	2:D:342:VAL:HA	1.60	0.66
1:A:43:GLY:HA2	1:A:56:THR:O	1.96	0.66
4:F:296:MET:HE2	4:F:380:HIS:HB2	1.78	0.66
1:C:265:ILE:HG22	1:C:265:ILE:O	1.97	0.65
2:D:330:MET:O	2:D:334:GLN:HG3	1.95	0.65
1:A:187:SER:HB2	1:A:391:LEU:HD21	1.79	0.65
2:B:309:ARG:HH21	2:B:342:VAL:HA	1.61	0.65
2:B:323:MET:CE	2:B:323:MET:HG3	2.25	0.65
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.70	0.65
2:D:63:ALA:O	2:D:64:ILE:HD13	1.96	0.65
4:F:186:LEU:HD12	4:F:320:MET:CG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:TYR:OH	2:B:407:GLU:OE2	2.09	0.65
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.77	0.65
1:A:96:LYS:HE3	2:B:128:ASP:OD1	1.98	0.64
2:D:1:MET:HB3	2:D:48:ASN:ND2	2.12	0.64
2:B:330:MET:O	2:B:334:GLN:HG3	1.96	0.64
2:D:267:MET:HG2	2:D:301:ALA:HB3	1.78	0.64
1:A:88:HIS:N	1:A:91:GLN:OE1	2.29	0.64
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.33	0.63
2:B:189:VAL:HB	2:B:415:MET:CE	2.28	0.63
2:D:19:LYS:O	2:D:23:VAL:HG23	1.97	0.63
3:E:46:SER:O	3:E:50:ILE:HG12	1.97	0.63
2:D:323:MET:SD	2:D:353:VAL:HG11	2.38	0.63
3:E:130:ALA:O	3:E:133:VAL:HG12	1.98	0.63
4:F:149:ALA:HB3	4:F:161:LEU:HD23	1.79	0.63
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.28	0.63
2:D:211:CYS:HB3	2:D:217:LEU:HD12	1.79	0.63
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.32	0.63
1:A:216:ASN:HB3	1:A:275:VAL:O	1.99	0.62
1:C:43:GLY:HA2	1:C:56:THR:O	2.00	0.62
2:D:221:THR:HG23	2:D:224:ASP:H	1.62	0.62
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.34	0.62
3:E:96:MET:HE3	3:E:100:LYS:CE	2.27	0.62
2:D:330:MET:HE2	2:D:351:THR:CG2	2.29	0.62
2:B:176:SER:HB2	2:B:181:GLU:OE1	1.99	0.62
2:D:105:HIS:O	2:D:150:LEU:HD22	1.99	0.62
2:B:237:THR:HG22	2:B:241:ARG:HG3	1.82	0.62
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.81	0.62
1:A:234:ILE:HD13	1:A:302:MET:SD	2.40	0.61
1:C:227:LEU:O	1:C:231:ILE:HG13	2.00	0.61
4:F:98:TYR:O	4:F:181:VAL:HG23	2.00	0.61
4:F:135:TYR:OH	4:F:164:SER:O	2.15	0.61
2:D:80:PRO:O	2:D:81:PHE:HB2	2.00	0.61
4:F:135:TYR:HE1	4:F:145:ASN:HB3	1.64	0.61
2:D:86:ARG:NE	2:D:88:ASP:HB2	2.15	0.61
1:A:112:LYS:NZ	1:A:113:GLU:OE2	2.30	0.61
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.35	0.61
2:D:301:ALA:O	2:D:303:CYS:N	2.32	0.61
2:B:145:SER:HG	2:B:188:SER:HG	1.42	0.61
4:F:292:ARG:O	4:F:296:MET:HG2	2.01	0.61
2:B:170:MET:CE	2:B:377:LEU:HD21	2.30	0.60
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:HB2	1:A:190:THR:HB	1.83	0.60
1:C:431:ASP:O	1:C:435:VAL:HG13	2.01	0.60
2:D:23:VAL:O	2:D:27:GLU:HG3	2.01	0.60
2:D:395:LEU:HD21	2:D:405:GLU:HG2	1.82	0.60
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.36	0.60
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.81	0.60
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.36	0.60
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.02	0.60
1:A:72:PRO:HB3	1:A:94:THR:CG2	2.30	0.60
2:D:44:LEU:HA	2:D:47:ILE:HB	1.82	0.60
1:A:345:ASP:HB2	3:E:28:SER:HB2	1.83	0.60
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.17	0.60
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.37	0.60
1:A:270:ALA:O	1:A:302:MET:HG2	2.02	0.59
2:B:169:VAL:HA	2:B:202:ILE:O	2.02	0.59
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.20	0.59
4:F:192:LEU:HD21	4:F:262:MET:CE	2.27	0.59
4:F:203:SER:HB3	4:F:215:LEU:HD11	1.84	0.59
4:F:216:TYR:CE1	4:F:374:ILE:HD12	2.38	0.59
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.32	0.59
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.85	0.59
4:F:305:LYS:HE3	4:F:306:HIS:NE2	2.18	0.59
4:F:87:LEU:O	4:F:88:SER:OG	2.18	0.59
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.18	0.59
2:B:170:MET:HE2	2:B:377:LEU:CD2	2.32	0.59
4:F:13:VAL:O	4:F:17:VAL:HG23	2.03	0.59
1:A:2:ARG:O	1:A:51:THR:HG22	2.02	0.58
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.03	0.58
4:F:95:PRO:HB2	4:F:183:GLN:HG2	1.85	0.58
4:F:286:GLN:O	4:F:290:ILE:HG13	2.04	0.58
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.83	0.58
4:F:128:ARG:N	4:F:128:ARG:HD2	2.18	0.58
1:A:71:GLU:HG2	1:A:72:PRO:N	2.18	0.58
2:B:61:PRO:HD3	2:B:84:ILE:HG12	1.83	0.58
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.58
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.39	0.58
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.68	0.58
4:F:138:ARG:HD2	4:F:143:GLU:HB2	1.85	0.58
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.03	0.58
1:A:227:LEU:O	1:A:231:ILE:HG13	2.04	0.58
2:B:189:VAL:HB	2:B:415:MET:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:THR:HB	2:B:241:ARG:HE	1.67	0.58
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.39	0.58
1:A:167:LEU:HD22	1:A:252:LEU:HD22	1.86	0.58
2:B:19:LYS:O	2:B:23:VAL:HG23	2.04	0.58
2:B:113:VAL:HG21	2:B:154:LYS:HD2	1.85	0.58
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.85	0.58
4:F:20:LEU:O	4:F:24:THR:HG23	2.04	0.57
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.87	0.57
2:B:139:LEU:HD22	2:B:188:SER:HB3	1.87	0.57
2:D:206:ALA:O	2:D:210:ILE:HG13	2.04	0.57
4:F:191:LEU:HA	4:F:197:ARG:O	2.05	0.57
3:E:96:MET:O	3:E:100:LYS:HD3	2.05	0.57
4:F:138:ARG:HB3	4:F:145:ASN:OD1	2.05	0.57
1:C:221:ARG:HD2	2:D:327:ASP:OD2	2.05	0.57
1:A:72:PRO:CB	1:A:94:THR:HG21	2.33	0.57
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.40	0.57
4:F:191:LEU:HD21	4:F:228:TYR:HB3	1.85	0.57
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.23	0.56
1:A:185:TYR:CZ	1:A:398:MET:HE2	2.39	0.56
2:D:232:THR:OG1	2:D:300:MET:HE3	2.05	0.56
2:B:350:LYS:HB2	10:B:505:A1EU1:N04	2.19	0.56
2:D:1:MET:HB3	2:D:48:ASN:HD22	1.69	0.56
2:D:12:CYS:O	2:D:16:ILE:HG23	2.05	0.56
2:D:266:PHE:O	2:D:268:PRO:HD3	2.04	0.56
2:D:102:ALA:HB2	2:D:403:MET:SD	2.45	0.56
1:A:94:THR:HG22	1:A:95:GLY:O	2.06	0.56
1:A:345:ASP:O	3:E:28:SER:N	2.36	0.56
2:B:117:LEU:HD11	2:B:154:LYS:HD3	1.88	0.56
2:B:135:LEU:HD22	2:B:152:ILE:HD11	1.87	0.56
2:B:31:ASP:CG	2:B:33:THR:HG22	2.31	0.56
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.21	0.56
4:F:189:PRO:HA	4:F:322:ASP:HA	1.88	0.56
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.87	0.55
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.87	0.55
1:A:169:PHE:HE1	1:A:238:ILE:HD12	1.70	0.55
1:C:83:TYR:CD1	1:C:86:LEU:HD22	2.41	0.55
4:F:99:VAL:O	4:F:100:ILE:HD13	2.06	0.55
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.88	0.55
2:D:1:MET:HG3	2:D:128:ASP:CB	2.35	0.55
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.24	0.55
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.21	0.55
2:D:86:ARG:HE	2:D:88:ASP:HB2	1.70	0.55
4:F:149:ALA:HB3	4:F:161:LEU:HB3	1.88	0.55
1:A:161:TYR:CD2	1:A:164:LYS:HE3	2.39	0.55
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.42	0.55
1:C:282:TYR:O	1:C:283:HIS:HB2	2.05	0.55
2:D:91:VAL:HG11	2:D:116:VAL:HG22	1.89	0.55
1:C:117:LEU:HD11	1:C:121:ARG:CZ	2.37	0.55
4:F:135:TYR:CE1	4:F:145:ASN:HB3	2.41	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.55
2:B:395:LEU:HD21	2:B:405:GLU:HG2	1.89	0.55
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.89	0.55
4:F:199:PHE:CE2	4:F:221:LEU:HD23	2.41	0.55
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.37	0.54
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.90	0.54
1:C:204:VAL:HG22	1:C:302:MET:CE	2.37	0.54
4:F:47:LEU:HD23	4:F:48:PRO:N	2.22	0.54
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.89	0.54
4:F:1:MET:HE2	4:F:28:LYS:HD2	1.89	0.54
1:A:164:LYS:HB3	1:A:164:LYS:HZ2	1.73	0.54
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.89	0.54
2:B:5:VAL:HB	2:B:133:PHE:CD2	2.43	0.54
4:F:253:TYR:CE1	4:F:259:GLY:HA2	2.42	0.54
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.43	0.54
4:F:229:ASN:ND2	4:F:232:ASN:OD1	2.40	0.54
1:A:136:LEU:HD23	1:A:167:LEU:HB2	1.90	0.54
2:B:190:HIS:CE1	2:B:414:ASN:HD22	2.26	0.54
2:B:198:GLU:OE2	2:B:254:ALA:HB2	2.08	0.54
1:A:165:SER:OG	1:A:256:GLN:OE1	2.26	0.54
1:A:25:CYS:HB3	1:A:30:ILE:O	2.09	0.53
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.90	0.53
2:B:406:MET:HE3	2:B:409:THR:HB	1.90	0.53
2:B:73:MET:CE	2:B:90:PHE:HB3	2.38	0.53
4:F:278:THR:O	4:F:282:SER:OG	2.26	0.53
1:A:34:GLY:O	1:A:61:HIS:N	2.30	0.53
2:D:285:THR:HG22	2:D:288:GLU:OE1	2.08	0.53
1:A:214:ARG:HG2	1:A:219:ILE:O	2.09	0.53
2:B:67:ASP:O	2:B:92:PHE:HA	2.08	0.53
2:B:238:THR:OG1	2:B:318:ARG:HD2	2.09	0.53
1:C:212:ILE:HG12	1:C:215:ARG:NH2	2.23	0.53
4:F:263:PHE:HE2	4:F:342:LEU:HD21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ASN:HD21	2:B:336:LYS:NZ	2.06	0.53
1:A:164:LYS:HZ2	1:A:164:LYS:CB	2.23	0.52
1:C:166:LYS:HE2	1:C:197:HIS:O	2.09	0.52
2:D:395:LEU:CD2	2:D:405:GLU:HG2	2.39	0.52
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.91	0.52
2:B:377:LEU:C	2:B:377:LEU:HD23	2.34	0.52
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.09	0.52
1:A:247:ALA:HB3	3:E:19:SER:OG	2.09	0.52
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.75	0.52
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.92	0.52
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.44	0.52
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.91	0.52
2:D:1:MET:HE3	2:D:128:ASP:CB	2.36	0.52
1:A:398:MET:HE3	1:A:404:PHE:HD2	1.75	0.52
2:B:350:LYS:CB	10:B:505:A1EU1:C10	2.88	0.52
4:F:221:LEU:HD22	4:F:262:MET:CE	2.40	0.52
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.40	0.52
4:F:191:LEU:HD22	4:F:196:HIS:CD2	2.45	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.52
2:B:267:MET:HE3	2:B:299:MET:HG3	1.92	0.52
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.92	0.52
4:F:135:TYR:HD2	4:F:166:ALA:HB2	1.73	0.52
2:B:308:GLY:HA2	2:B:426:GLN:NE2	2.16	0.51
2:D:251:ARG:O	2:D:255:VAL:HG23	2.10	0.51
1:A:241:SER:HB2	1:A:249:ASN:O	2.10	0.51
2:B:116:VAL:CG1	2:B:151:LEU:HD21	2.40	0.51
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.93	0.51
2:B:423:GLN:NE2	2:B:426:GLN:OE1	2.43	0.51
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.45	0.51
1:C:162:GLY:CA	3:E:94:ILE:HD11	2.39	0.51
2:D:97:ALA:HB2	2:D:143:THR:OG1	2.10	0.51
2:D:151:LEU:O	2:D:155:ILE:HG13	2.11	0.51
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.25	0.51
4:F:191:LEU:HD23	4:F:196:HIS:C	2.35	0.51
2:B:304:ASP:HB3	2:B:307:HIS:CG	2.45	0.51
2:D:1:MET:CE	2:D:128:ASP:HB2	2.39	0.51
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.92	0.51
3:E:130:ALA:HA	3:E:133:VAL:HG12	1.93	0.51
2:D:12:CYS:SG	2:D:169:VAL:HG21	2.51	0.51
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.93	0.51
4:F:102:PRO:HG3	4:F:178:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.92	0.51
1:A:265:ILE:O	1:A:265:ILE:HG22	2.11	0.50
1:C:241:SER:HB2	1:C:250:VAL:O	2.10	0.50
2:D:330:MET:O	2:D:333:VAL:HG12	2.11	0.50
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.93	0.50
2:B:44:LEU:HA	2:B:47:ILE:HB	1.91	0.50
1:C:28:HIS:O	1:C:36:MET:HE3	2.11	0.50
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.94	0.50
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.47	0.50
2:B:2:ARG:O	2:B:131:GLN:NE2	2.33	0.50
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.93	0.50
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.44	0.50
2:D:33:THR:OG1	2:D:58:LYS:HE3	2.12	0.50
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.42	0.50
1:A:213:CYS:O	1:A:217:LEU:HB2	2.12	0.50
1:A:234:ILE:HD13	1:A:302:MET:CE	2.42	0.50
2:B:294:PHE:CZ	2:B:330:MET:HE1	2.46	0.50
1:C:192:HIS:CG	1:C:421:ALA:HA	2.47	0.50
2:D:2:ARG:CB	2:D:131:GLN:HE21	2.25	0.50
1:C:221:ARG:NE	2:D:323:MET:HB3	2.27	0.50
3:E:22:VAL:HG13	3:E:22:VAL:O	2.12	0.50
1:A:192:HIS:CG	1:A:421:ALA:HA	2.46	0.50
4:F:225:SER:CB	4:F:252:ASN:HB3	2.42	0.50
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.47	0.50
4:F:35:PRO:O	4:F:55:GLU:HG3	2.11	0.50
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.42	0.50
1:A:112:LYS:HE2	3:E:61:ARG:NH2	2.26	0.49
1:A:133:GLN:OE1	1:A:252:LEU:N	2.45	0.49
1:A:97:GLU:HG3	2:B:2:ARG:HH12	1.76	0.49
4:F:148:ILE:O	4:F:182:ILE:HA	2.12	0.49
4:F:198:LYS:HG2	4:F:199:PHE:N	2.28	0.49
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.42	0.49
1:C:252:LEU:O	1:C:256:GLN:HG3	2.13	0.49
4:F:31:ARG:HG3	4:F:32:LYS:N	2.27	0.49
2:B:151:LEU:O	2:B:155:ILE:HG13	2.13	0.49
2:D:77:ARG:O	2:D:82:GLY:HA3	2.12	0.49
2:D:386:THR:O	2:D:390:ARG:HG2	2.11	0.49
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.77	0.49
4:F:130:VAL:HG12	4:F:130:VAL:O	2.11	0.49
1:A:270:ALA:HB3	1:A:302:MET:CG	2.42	0.49
2:D:210:ILE:HG23	2:D:273:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:VAL:CG1	2:B:147:MET:HE1	2.39	0.49
2:B:238:THR:HG21	2:B:316:ILE:HD11	1.94	0.49
1:C:101:ASN:ND2	2:D:252:LYS:HE2	2.27	0.49
1:A:221:ARG:HD2	2:B:327:ASP:OD2	2.13	0.49
1:A:258:ASN:O	1:A:314:ALA:HB1	2.13	0.49
1:C:32:PRO:HA	1:C:83:TYR:CE1	2.48	0.49
3:E:139:LEU:O	3:E:139:LEU:HG	2.13	0.49
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.47	0.49
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.93	0.49
1:A:32:PRO:HA	1:A:83:TYR:CD1	2.47	0.48
2:B:288:GLU:O	2:B:292:GLN:HG3	2.13	0.48
2:D:157:GLU:HA	3:E:123:LEU:HD13	1.95	0.48
3:E:47:LEU:HD12	3:E:47:LEU:O	2.13	0.48
3:E:123:LEU:O	3:E:126:LYS:HB2	2.13	0.48
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.32	0.48
2:D:395:LEU:HD21	2:D:405:GLU:CG	2.43	0.48
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.48	0.48
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.49	0.48
2:D:63:ALA:C	2:D:64:ILE:HD13	2.38	0.48
1:C:287:SER:OG	1:C:290:GLU:HG3	2.14	0.48
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.48	0.48
2:D:285:THR:HG22	2:D:288:GLU:CD	2.39	0.48
2:D:285:THR:OG1	2:D:287:PRO:HD2	2.14	0.48
2:D:293:MET:CG	2:D:367:PHE:HB2	2.44	0.48
3:E:137:LYS:O	3:E:140:LYS:HB3	2.14	0.48
1:C:105:ARG:HA	1:C:109:THR:HB	1.96	0.48
1:C:241:SER:HA	1:C:249:ASN:OD1	2.14	0.48
1:C:254:GLU:HG2	1:C:352:LYS:HE3	1.95	0.48
2:D:285:THR:HG22	2:D:288:GLU:HB2	1.96	0.48
4:F:200:ASP:HB3	4:F:320:MET:HE1	1.94	0.48
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.48	0.48
2:D:7:ILE:HG21	2:D:151:LEU:CD2	2.44	0.48
2:B:267:MET:HE3	2:B:299:MET:CG	2.44	0.47
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.41	0.47
1:C:88:HIS:ND1	1:C:89:PRO:HD2	2.29	0.47
2:D:28:HIS:ND1	2:D:43:GLN:O	2.42	0.47
1:A:401:LYS:HG3	2:B:344:TRP:CE3	2.49	0.47
2:D:65:LEU:HD23	2:D:76:VAL:HG11	1.96	0.47
2:B:5:VAL:HG23	2:B:130:LEU:CD1	2.44	0.47
2:D:2:ARG:O	2:D:131:GLN:NE2	2.44	0.47
1:A:63:PRO:HG2	1:A:87:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.15	0.47
2:B:189:VAL:CB	2:B:415:MET:CE	2.92	0.47
2:B:239:CYS:HB3	2:B:248:ALA:HB3	1.96	0.47
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.44	0.47
3:E:140:LYS:O	3:E:140:LYS:HG2	2.14	0.47
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.45	0.47
2:B:72:THR:O	2:B:76:VAL:HG23	2.15	0.47
3:E:75:LYS:O	3:E:79:GLU:HG3	2.15	0.47
4:F:138:ARG:HB3	4:F:145:ASN:HD21	1.80	0.47
1:A:321:GLY:HA2	1:A:359:PRO:HA	1.97	0.47
2:D:81:PHE:O	2:D:84:ILE:HG22	2.15	0.47
2:D:318:ARG:HH21	2:D:356:ILE:HG12	1.80	0.47
1:A:265:ILE:HD12	1:A:265:ILE:N	2.30	0.46
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.50	0.46
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.97	0.46
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.98	0.46
1:C:332:ILE:HG22	1:C:336:LYS:HE2	1.96	0.46
1:C:139:HIS:CE1	1:C:150:THR:HG21	2.50	0.46
4:F:16:GLU:OE2	4:F:19:ARG:HD2	2.14	0.46
4:F:287:ILE:HG23	4:F:319:PHE:CE1	2.50	0.46
2:D:286:VAL:HB	2:D:287:PRO:HD3	1.97	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.46
1:A:276:ILE:HD11	1:A:280:LYS:NZ	2.31	0.46
2:B:8:GLN:OE1	2:B:17:GLY:HA3	2.16	0.46
2:B:251:ARG:O	2:B:255:VAL:HG23	2.15	0.46
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.49	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.46
1:C:97:GLU:O	1:C:110:ILE:HG21	2.16	0.46
1:C:270:ALA:O	1:C:302:MET:HG3	2.15	0.46
2:D:402:GLY:HA2	3:E:136:ASN:HB3	1.97	0.46
2:D:404:ASP:CG	2:D:406:MET:HG2	2.40	0.46
4:F:165:GLU:HB2	4:F:168:GLU:HG3	1.97	0.46
1:A:28:HIS:O	1:A:36:MET:HE3	2.15	0.46
1:A:276:ILE:CD1	1:A:283:HIS:CD2	2.98	0.46
4:F:288:LYS:HG2	4:F:378:LEU:HD21	1.97	0.46
1:A:401:LYS:HG3	2:B:344:TRP:CD2	2.51	0.46
2:B:101:TRP:HD1	2:B:145:SER:OG	1.98	0.46
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.46	0.46
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.50	0.46
2:D:406:MET:HE3	2:D:406:MET:HB3	1.69	0.46
4:F:142:ARG:O	4:F:142:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HA	1:A:94:THR:HG23	1.99	0.45
2:B:309:ARG:NH2	2:B:342:VAL:HA	2.28	0.45
2:D:377:LEU:C	2:D:377:LEU:HD23	2.42	0.45
4:F:138:ARG:NH1	4:F:144:GLY:O	2.49	0.45
4:F:148:ILE:HG13	4:F:149:ALA:N	2.32	0.45
10:B:505:A1EU1:C08	10:B:505:A1EU1:S01	3.04	0.45
2:D:235:GLY:HA3	2:D:366:THR:OG1	2.17	0.45
1:C:313:MET:HA	1:C:347:CYS:SG	2.57	0.45
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.51	0.45
2:D:267:MET:HE3	2:D:299:MET:CG	2.47	0.45
2:B:301:ALA:O	2:B:303:CYS:N	2.48	0.45
2:D:86:ARG:HD3	2:D:89:ASN:OD1	2.17	0.45
2:D:172:SER:OG	2:D:205:GLU:HB2	2.17	0.45
3:E:127:ASP:O	3:E:131:GLU:HG2	2.16	0.45
2:B:9:ALA:HA	2:B:66:VAL:O	2.16	0.45
4:F:226:GLU:OE2	4:F:252:ASN:HB2	2.17	0.45
1:A:158:SER:OG	1:A:166:LYS:HE2	2.17	0.45
1:A:287:SER:OG	1:A:290:GLU:HG3	2.17	0.45
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.52	0.45
2:B:241:ARG:HH22	2:B:318:ARG:HH12	1.64	0.45
3:E:125:GLU:OE1	3:E:125:GLU:HA	2.17	0.45
4:F:161:LEU:N	4:F:161:LEU:HD12	2.32	0.45
1:A:150:THR:O	1:A:154:MET:HG2	2.17	0.45
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.99	0.45
2:D:241:ARG:HH22	2:D:318:ARG:HH12	1.64	0.45
2:B:67:ASP:HA	2:B:143:THR:HG21	1.98	0.45
1:A:75:ILE:CG2	1:A:92:LEU:HB3	2.46	0.45
2:B:30:ILE:HD12	2:B:30:ILE:N	2.32	0.44
2:B:36:TYR:CE2	2:B:44:LEU:HD11	2.52	0.44
2:B:267:MET:CE	2:B:299:MET:HG3	2.47	0.44
2:B:274:THR:HG21	2:B:361:LEU:HD21	2.00	0.44
1:C:180:ALA:O	1:C:183:GLU:HG3	2.17	0.44
2:D:23:VAL:HG21	2:D:230:SER:HB2	1.99	0.44
2:D:406:MET:O	2:D:410:GLU:HG3	2.17	0.44
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.99	0.44
4:F:47:LEU:HD23	4:F:47:LEU:C	2.42	0.44
1:A:286:LEU:HA	1:A:290:GLU:OE1	2.16	0.44
1:A:402:ARG:HG3	1:A:402:ARG:NH1	2.32	0.44
1:C:88:HIS:NE2	1:C:90:GLU:HG3	2.32	0.44
2:D:66:VAL:HG11	2:D:147:MET:HE1	1.99	0.44
1:A:321:GLY:CA	1:A:359:PRO:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.32	0.44
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.47	0.44
2:D:402:GLY:C	3:E:133:VAL:HG23	2.42	0.44
4:F:232:ASN:OD1	4:F:232:ASN:N	2.48	0.44
4:F:263:PHE:CE2	4:F:342:LEU:HD21	2.52	0.44
1:A:26:LEU:HD12	1:A:363:VAL:HG22	2.00	0.44
2:D:31:ASP:CG	2:D:33:THR:HG22	2.43	0.44
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.53	0.44
2:D:267:MET:HE3	2:D:299:MET:HG3	2.00	0.44
4:F:8:ASP:OD2	4:F:44:ARG:HG3	2.18	0.44
4:F:146:VAL:HG11	4:F:233:PHE:CE1	2.53	0.44
4:F:198:LYS:HG2	4:F:199:PHE:H	1.81	0.44
1:A:234:ILE:O	1:A:238:ILE:HG13	2.18	0.44
2:B:266:PHE:O	2:B:268:PRO:HD3	2.18	0.44
2:B:294:PHE:HZ	2:B:330:MET:HE1	1.82	0.44
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.82	0.44
3:E:121:GLU:O	3:E:124:GLN:HG3	2.17	0.44
1:A:23:LEU:O	1:A:27:GLU:HG3	2.18	0.43
2:D:32:PRO:O	2:D:84:ILE:HB	2.18	0.43
4:F:21:LEU:O	4:F:27:TRP:HB2	2.18	0.43
4:F:47:LEU:HD23	4:F:48:PRO:CD	2.48	0.43
4:F:86:GLU:C	4:F:87:LEU:HD23	2.43	0.43
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.51	0.43
4:F:377:LYS:HD3	4:F:379:HIS:NE2	2.33	0.43
2:B:132:GLY:HA2	2:B:162:ARG:HB3	2.00	0.43
2:B:165:ASN:HA	2:B:198:GLU:O	2.18	0.43
4:F:197:ARG:NH2	4:F:223:THR:OG1	2.51	0.43
4:F:225:SER:HB3	4:F:252:ASN:HB3	2.00	0.43
2:B:2:ARG:HA	2:B:129:CYS:O	2.19	0.43
1:C:75:ILE:HB	1:C:94:THR:CG2	2.48	0.43
1:C:216:ASN:HB3	1:C:275:VAL:O	2.18	0.43
2:D:210:ILE:CG2	2:D:273:LEU:HD13	2.48	0.43
2:D:267:MET:HE1	2:D:305:PRO:HG3	1.99	0.43
4:F:47:LEU:HD23	4:F:48:PRO:HD2	2.00	0.43
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.53	0.43
2:B:66:VAL:HG12	2:B:147:MET:CE	2.41	0.43
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.01	0.43
1:A:132:LEU:HD23	1:A:164:LYS:CE	2.35	0.43
2:D:193:VAL:HG22	2:D:265:PHE:CE2	2.53	0.43
2:D:403:MET:HE3	2:D:407:GLU:CD	2.43	0.43
4:F:135:TYR:HE1	4:F:145:ASN:CB	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CD2	1:A:90:GLU:HG3	2.54	0.43
2:B:375:GLN:HE22	2:B:423:GLN:HG2	1.83	0.43
4:F:204:TRP:CZ2	4:F:338:CYS:HA	2.54	0.43
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.57	0.43
1:C:136:LEU:HD12	1:C:136:LEU:N	2.34	0.43
1:C:288:VAL:HG22	1:C:323:VAL:HG22	2.01	0.43
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.00	0.43
4:F:216:TYR:OH	4:F:345:GLU:OE1	2.33	0.43
1:A:223:THR:O	1:A:227:LEU:HG	2.19	0.43
2:B:110:ALA:O	2:B:113:VAL:HG12	2.19	0.43
1:C:174:ALA:HB2	1:C:207:GLU:N	2.34	0.43
1:C:298:PRO:HA	1:C:301:GLN:HG3	2.00	0.43
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.75	0.43
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.49	0.43
1:A:316:CYS:HA	1:A:352:LYS:O	2.18	0.43
1:C:139:HIS:NE2	1:C:150:THR:HG21	2.33	0.43
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.54	0.43
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.53	0.43
2:B:64:ILE:HD12	2:B:120:VAL:HG22	2.00	0.42
1:C:150:THR:O	1:C:154:MET:HG2	2.18	0.42
2:D:16:ILE:CD1	2:D:136:THR:HG22	2.45	0.42
2:B:5:VAL:HB	2:B:133:PHE:HD2	1.84	0.42
1:C:108:TYR:O	1:C:112:LYS:HG2	2.19	0.42
1:C:318:LEU:N	1:C:318:LEU:CD1	2.82	0.42
2:D:416:ASN:O	2:D:419:VAL:CG2	2.67	0.42
4:F:99:VAL:O	4:F:99:VAL:HG23	2.19	0.42
2:D:268:PRO:HA	2:D:367:PHE:O	2.19	0.42
2:D:416:ASN:O	2:D:419:VAL:HG22	2.20	0.42
4:F:3:THR:HG22	4:F:28:LYS:CG	2.43	0.42
2:D:272:PRO:HB3	2:D:284:LEU:HD21	2.01	0.42
2:D:285:THR:HG22	2:D:288:GLU:CG	2.50	0.42
4:F:81:ILE:HD12	4:F:94:PHE:CD2	2.53	0.42
4:F:242:ASN:HB2	4:F:245:ILE:HB	2.01	0.42
1:A:280:LYS:HB3	1:A:280:LYS:HE2	1.83	0.42
1:A:370:LYS:HD3	1:A:371:VAL:N	2.34	0.42
1:A:389:ALA:O	1:A:390:ARG:C	2.63	0.42
2:B:218:THR:HG23	2:B:219:THR:N	2.34	0.42
2:B:116:VAL:HG11	2:B:151:LEU:HD21	2.01	0.42
2:B:396:HIS:HA	2:B:399:THR:OG1	2.19	0.42
1:C:295:CYS:SG	1:C:375:VAL:HG13	2.60	0.42
2:D:4:ILE:O	2:D:62:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:225:SER:HB2	4:F:252:ASN:HB3	2.01	0.42
2:B:391:ARG:HA	2:B:391:ARG:HD2	1.81	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.42
2:D:7:ILE:O	2:D:135:LEU:HD12	2.20	0.42
2:D:145:SER:O	2:D:149:THR:HG23	2.20	0.42
4:F:138:ARG:HB3	4:F:145:ASN:ND2	2.35	0.42
4:F:283:ILE:HG23	4:F:327:VAL:HG22	2.02	0.42
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.50	0.42
1:A:153:LEU:O	1:A:157:LEU:HG	2.20	0.42
1:C:153:LEU:O	1:C:157:LEU:HG	2.20	0.42
4:F:99:VAL:C	4:F:100:ILE:HD13	2.45	0.42
1:A:133:GLN:OE1	1:A:251:ASP:CA	2.64	0.42
1:A:251:ASP:OD1	1:A:254:GLU:N	2.53	0.42
2:D:2:ARG:HB3	2:D:131:GLN:CG	2.49	0.42
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.55	0.42
2:B:102:ALA:HB2	2:B:403:MET:SD	2.60	0.41
1:C:212:ILE:HG12	1:C:215:ARG:HH22	1.85	0.41
3:E:58:GLU:HA	3:E:61:ARG:NH2	2.35	0.41
4:F:53:GLY:N	4:F:60:GLN:OE1	2.28	0.41
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.02	0.41
2:B:73:MET:HE1	2:B:92:PHE:HD1	1.84	0.41
2:B:130:LEU:O	2:B:162:ARG:NE	2.53	0.41
1:C:265:ILE:N	1:C:265:ILE:HD12	2.35	0.41
2:D:66:VAL:HA	2:D:91:VAL:O	2.20	0.41
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.55	0.41
1:A:261:PRO:HG3	1:A:313:MET:HB3	2.02	0.41
1:C:255:PHE:CD1	1:C:352:LYS:HD3	2.55	0.41
2:D:30:ILE:HD12	2:D:30:ILE:N	2.36	0.41
1:A:242:LEU:HD23	1:A:250:VAL:O	2.20	0.41
2:B:5:VAL:HG23	2:B:130:LEU:HD11	2.03	0.41
2:B:284:LEU:O	2:B:363:MET:CE	2.69	0.41
2:D:44:LEU:O	2:D:47:ILE:HG22	2.20	0.41
1:A:398:MET:HE3	1:A:404:PHE:CD2	2.56	0.41
2:B:73:MET:SD	2:B:92:PHE:HB3	2.61	0.41
2:B:103:LYS:HA	2:B:107:THR:OG1	2.20	0.41
2:B:332:ASN:HD21	2:B:336:LYS:HZ1	1.68	0.41
2:D:267:MET:CE	2:D:299:MET:HG3	2.51	0.41
2:D:395:LEU:HG	2:D:399:THR:HG23	2.03	0.41
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.89	0.41
4:F:71:LEU:HD23	4:F:332:VAL:HG11	2.03	0.41
2:B:178:THR:O	2:B:181:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.41
2:D:33:THR:O	2:D:58:LYS:HD2	2.21	0.41
2:D:221:THR:HG22	2:D:224:ASP:CG	2.44	0.41
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.56	0.41
2:D:372:THR:HG21	2:D:426:GLN:HB2	2.02	0.41
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.47	0.41
1:C:167:LEU:HA	1:C:200:CYS:O	2.21	0.41
2:D:106:TYR:CD1	3:E:133:VAL:HG11	2.55	0.41
2:D:144:GLY:O	2:D:148:GLY:HA3	2.21	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.56	0.41
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.56	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.41
2:D:350:LYS:HG2	10:D:502:A1EU1:C10	2.51	0.41
2:B:189:VAL:CB	2:B:415:MET:HE2	2.51	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.40
1:C:298:PRO:HG2	1:C:308:ARG:CZ	2.51	0.40
4:F:186:LEU:O	4:F:189:PRO:HD3	2.21	0.40
1:A:1:MET:HE3	1:A:1:MET:HB3	1.97	0.40
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.56	0.40
2:D:350:LYS:CG	10:D:502:A1EU1:C14	2.99	0.40
4:F:197:ARG:HB3	4:F:224:SER:O	2.22	0.40
2:B:163:ILE:HA	2:B:197:ASP:OD2	2.22	0.40
2:D:316:ILE:N	2:D:316:ILE:HD12	2.36	0.40
2:B:23:VAL:HG21	2:B:230:SER:HB2	2.03	0.40
2:B:116:VAL:O	2:B:120:VAL:HG23	2.20	0.40
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.61	0.40
1:C:174:ALA:HB2	1:C:207:GLU:H	1.87	0.40
2:D:66:VAL:HG11	2:D:147:MET:CE	2.52	0.40
3:E:135:LYS:HE2	3:E:135:LYS:HB3	1.89	0.40
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.86	0.40
2:B:263:LEU:HD21	2:B:421:GLU:HG2	2.03	0.40
1:C:75:ILE:CG2	1:C:92:LEU:HB3	2.51	0.40
1:C:88:HIS:CD2	1:C:90:GLU:H	2.39	0.40
1:C:221:ARG:CZ	2:D:323:MET:HB3	2.52	0.40
3:E:130:ALA:C	3:E:133:VAL:HG12	2.47	0.40
4:F:175:GLU:HG2	4:F:175:GLU:O	2.21	0.40
4:F:331:GLU:HG2	4:F:332:VAL:N	2.37	0.40

All (2) 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:401:GLU:OE1	1:C:282:TYR:OH[4_445]	2.06	0.14
1:C:285:GLN:NE2	3:E:91:ASN:OD1[4_545]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/440 (99%)	426 (98%)	8 (2%)	1 (0%)	43	62
1	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
2	B	425/431 (99%)	417 (98%)	8 (2%)	0	100	100
2	D	417/431 (97%)	408 (98%)	8 (2%)	1 (0%)	43	62
3	E	117/136 (86%)	114 (97%)	3 (3%)	0	100	100
4	F	322/380 (85%)	305 (95%)	16 (5%)	1 (0%)	36	53
All	All	2154/2258 (95%)	2095 (97%)	56 (3%)	3 (0%)	48	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
2	D	302	ALA
4	F	129	GLU

5.3.2 Protein sidechains [i](#)

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%)	359 (98%)	7 (2%)	50	74
1	C	370/371 (100%)	366 (99%)	4 (1%)	65	83
2	B	367/372 (99%)	361 (98%)	6 (2%)	55	78
2	D	362/372 (97%)	350 (97%)	12 (3%)	33	58
3	E	109/122 (89%)	105 (96%)	4 (4%)	30	54
4	F	295/338 (87%)	286 (97%)	9 (3%)	35	60
All	All	1869/1946 (96%)	1827 (98%)	42 (2%)	45	71

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	71	GLU
1	A	164	LYS
1	A	277	SER
1	A	297	GLU
1	A	342	GLN
2	B	15	GLN
2	B	115	SER
2	B	151	LEU
2	B	246	LEU
2	B	316	ILE
2	B	339	SER
1	C	71	GLU
1	C	283	HIS
1	C	297	GLU
1	C	318	LEU
2	D	8	GLN
2	D	15	GLN
2	D	73	MET
2	D	100	ASN
2	D	115	SER
2	D	136	THR
2	D	246	LEU
2	D	247	ASN
2	D	316	ILE
2	D	339	SER
2	D	356	ILE
2	D	406	MET
3	E	14	CYS

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Mol	Chain	Res	Type
3	E	15	THR
3	E	16	SER
3	E	18	GLN
4	F	12	SER
4	F	71	LEU
4	F	89	GLU
4	F	175	GLU
4	F	179	VAL
4	F	180	HIS
4	F	307	LEU
4	F	310	GLN
4	F	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	332	ASN
2	B	423	GLN
2	B	426	GLN
2	D	298	ASN
4	F	180	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 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
10	A1EU1	D	502	-	25,25,25	3.66	14 (56%)	34,37,37	6.27	16 (47%)
10	A1EU1	B	505	-	25,25,25	3.68	15 (60%)	34,37,37	6.32	13 (38%)
5	GTP	C	501	7	30,34,34	0.83	1 (3%)	46,54,54	1.74	10 (21%)
9	MES	B	503	-	12,12,12	1.11	1 (8%)	14,16,16	0.85	0
8	GDP	D	501	-	28,30,30	1.14	3 (10%)	44,47,47	1.84	8 (18%)
9	MES	B	502	-	12,12,12	1.13	1 (8%)	14,16,16	0.91	2 (14%)
8	GDP	B	501	7	28,30,30	1.14	3 (10%)	44,47,47	1.80	7 (15%)
11	ACP	F	401	-	30,33,33	1.90	2 (6%)	45,52,52	1.14	3 (6%)
5	GTP	A	501	7	30,34,34	0.85	1 (3%)	46,54,54	1.76	10 (21%)

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
10	A1EU1	D	502	-	-	0/8/8/8	0/4/4/4
10	A1EU1	B	505	-	-	0/8/8/8	0/4/4/4
5	GTP	C	501	7	-	6/22/38/38	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
8	GDP	D	501	-	-	3/16/32/32	0/3/3/3
9	MES	B	502	-	-	3/6/14/14	0/1/1/1
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
11	ACP	F	401	-	-	4/19/38/38	0/3/3/3
5	GTP	A	501	7	-	6/22/38/38	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	A1EU1	N05-N04	-11.09	1.31	1.37
10	B	505	A1EU1	N05-N04	-10.75	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	9.37	1.68	1.58
10	D	502	A1EU1	C04-S01	8.75	1.88	1.73
10	B	505	A1EU1	C04-S01	8.71	1.88	1.73
10	D	502	A1EU1	C06-N03	4.72	1.49	1.39
10	B	505	A1EU1	C10-C11	4.43	1.47	1.41
10	B	505	A1EU1	C10-C14	4.16	1.47	1.42
10	D	502	A1EU1	C10-C11	3.97	1.47	1.41
10	D	502	A1EU1	C03-C04	3.79	1.43	1.40
10	D	502	A1EU1	C10-C14	3.72	1.46	1.42
10	B	505	A1EU1	C06-N03	3.50	1.46	1.39
10	B	505	A1EU1	C11-N05	3.36	1.44	1.36
10	B	505	A1EU1	C04-C06	-3.33	1.36	1.42
10	B	505	A1EU1	C14-N04	-3.33	1.28	1.32
10	B	505	A1EU1	C03-C02	-3.27	1.38	1.42
8	B	501	GDP	C5-C4	3.08	1.47	1.38
8	D	501	GDP	C5-C4	3.06	1.47	1.38
10	D	502	A1EU1	C11-N05	3.05	1.43	1.36
9	B	502	MES	C8-S	3.00	1.81	1.77
9	B	503	MES	C8-S	2.91	1.81	1.77
10	B	505	A1EU1	C08-N03	2.71	1.48	1.42
10	B	505	A1EU1	C03-C04	2.71	1.42	1.40
10	D	502	A1EU1	C08-N03	2.70	1.48	1.42
10	B	505	A1EU1	C09-C08	2.65	1.44	1.39
10	D	502	A1EU1	C05-N02	2.65	1.37	1.32
10	D	502	A1EU1	C14-N04	-2.61	1.29	1.32
10	D	502	A1EU1	C09-C08	2.53	1.44	1.39
8	B	501	GDP	C6-N1	-2.45	1.34	1.38
10	B	505	A1EU1	C03-N01	-2.44	1.32	1.35
10	B	505	A1EU1	C13-C08	2.42	1.44	1.39
10	D	502	A1EU1	C03-C02	-2.40	1.39	1.42
8	D	501	GDP	C6-N1	-2.36	1.34	1.38
11	F	401	ACP	PB-O2B	-2.34	1.50	1.56
10	D	502	A1EU1	C13-C08	2.26	1.43	1.39
5	A	501	GTP	C2-N3	2.25	1.38	1.33
5	C	501	GTP	C2-N3	2.17	1.38	1.33
8	B	501	GDP	C5-N7	-2.13	1.35	1.39
10	B	505	A1EU1	C05-CL01	2.13	1.79	1.73
8	D	501	GDP	C5-N7	-2.12	1.35	1.39
10	D	502	A1EU1	C05-CL01	2.09	1.79	1.73

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	A1EU1	C10-C11-N05	-23.00	98.35	106.68
10	D	502	A1EU1	C10-C11-N05	-21.25	98.99	106.68
10	B	505	A1EU1	C11-N05-N04	19.78	122.47	111.62
10	D	502	A1EU1	C11-N05-N04	19.73	122.44	111.62
10	D	502	A1EU1	C10-C14-N04	10.92	120.34	112.06
10	D	502	A1EU1	C14-N04-N05	-10.66	97.79	106.42
10	B	505	A1EU1	C10-C14-N04	10.54	120.05	112.06
10	B	505	A1EU1	C14-N04-N05	-10.02	98.31	106.42
10	D	502	A1EU1	C15-N05-C11	-8.22	117.86	128.39
10	B	505	A1EU1	C15-N05-C11	-6.92	119.51	128.39
10	D	502	A1EU1	C11-C10-C14	-6.75	100.42	104.48
10	B	505	A1EU1	C11-C10-C14	-6.09	100.81	104.48
8	B	501	GDP	C5-C4-N3	-5.91	118.87	128.46
8	D	501	GDP	C5-C4-N3	-5.88	118.92	128.46
10	D	502	A1EU1	C03-C02-C01	5.43	122.44	108.14
10	B	505	A1EU1	C12-C11-N05	5.21	139.12	132.07
10	B	505	A1EU1	N02-C06-N03	5.20	121.55	116.12
5	A	501	GTP	C5-C4-N3	-5.04	120.28	128.46
5	C	501	GTP	C5-C4-N3	-4.98	120.39	128.46
10	B	505	A1EU1	C03-C02-C01	4.97	121.21	108.14
10	D	502	A1EU1	N02-C06-N03	4.95	121.29	116.12
8	B	501	GDP	C2-N3-C4	4.78	120.82	112.30
8	D	501	GDP	C2-N3-C4	4.78	120.81	112.30
11	F	401	ACP	PB-O3A-PA	-4.54	118.18	132.56
8	D	501	GDP	N9-C4-N3	4.52	135.01	125.94
10	D	502	A1EU1	C12-C11-N05	4.46	138.10	132.07
5	C	501	GTP	C2-N3-C4	4.45	120.23	112.30
8	B	501	GDP	N9-C4-N3	4.43	134.83	125.94
5	A	501	GTP	C2-N3-C4	4.41	120.15	112.30
10	D	502	A1EU1	C04-C06-N02	-3.96	119.34	122.57
10	B	505	A1EU1	C04-C06-N03	-3.95	116.91	122.19
10	B	505	A1EU1	C09-C10-C14	3.91	141.87	135.50
10	D	502	A1EU1	C09-C10-C14	3.78	141.66	135.50
5	A	501	GTP	PB-O3B-PG	-3.78	119.87	132.83
8	D	501	GDP	PA-O3A-PB	-3.72	120.07	132.83
5	C	501	GTP	PA-O3A-PB	-3.68	120.19	132.83
5	C	501	GTP	PB-O3B-PG	-3.62	120.39	132.83
8	B	501	GDP	PA-O3A-PB	-3.44	121.02	132.83
5	A	501	GTP	PA-O3A-PB	-3.41	121.12	132.83
10	D	502	A1EU1	C07-N03-C08	3.32	124.29	117.90
5	C	501	GTP	N9-C4-N3	3.30	132.57	125.94
5	A	501	GTP	N9-C4-N3	3.25	132.47	125.94
8	B	501	GDP	C6-C5-N7	3.19	136.18	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C6-C5-N7	3.14	136.09	130.25
11	F	401	ACP	O2B-PB-O1B	3.05	120.24	110.07
5	A	501	GTP	C2-N1-C6	-2.90	119.81	125.10
5	C	501	GTP	C2-N1-C6	-2.76	120.07	125.10
5	A	501	GTP	N9-C8-N7	-2.72	108.26	113.39
5	C	501	GTP	N9-C8-N7	-2.66	108.37	113.39
5	A	501	GTP	C8-N7-C5	2.64	109.02	104.24
5	C	501	GTP	C8-N7-C5	2.55	108.85	104.24
11	F	401	ACP	O1G-PG-C3B	-2.55	105.76	111.24
8	B	501	GDP	C4-C5-N7	-2.54	106.70	110.72
5	A	501	GTP	C5-C6-N1	2.50	119.53	113.19
8	D	501	GDP	C4-C5-N7	-2.45	106.85	110.72
5	C	501	GTP	C5-C6-N1	2.42	119.34	113.19
5	A	501	GTP	O6-C6-C5	-2.39	120.25	126.60
10	D	502	A1EU1	C02-C01-S01	-2.39	108.96	113.96
10	D	502	A1EU1	C08-N03-C06	-2.37	115.39	120.28
10	D	502	A1EU1	C05-N02-C06	2.36	117.57	110.86
5	C	501	GTP	O6-C6-C5	-2.28	120.54	126.60
10	B	505	A1EU1	C09-C10-C11	-2.21	117.31	119.51
10	D	502	A1EU1	C04-C06-N03	-2.19	119.26	122.19
9	B	502	MES	O1S-S-C8	-2.18	104.29	106.92
8	B	501	GDP	O6-C6-C5	-2.15	120.90	126.60
8	D	501	GDP	O6-C6-C5	-2.15	120.91	126.60
9	B	502	MES	O2S-S-C8	-2.04	104.46	106.92
10	B	505	A1EU1	C05-N02-C06	2.03	116.65	110.86
8	D	501	GDP	C2'-C3'-C4'	2.01	106.54	102.64

There are no chirality outliers.

All (25) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	502	MES	C7-C8-S-O2S

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

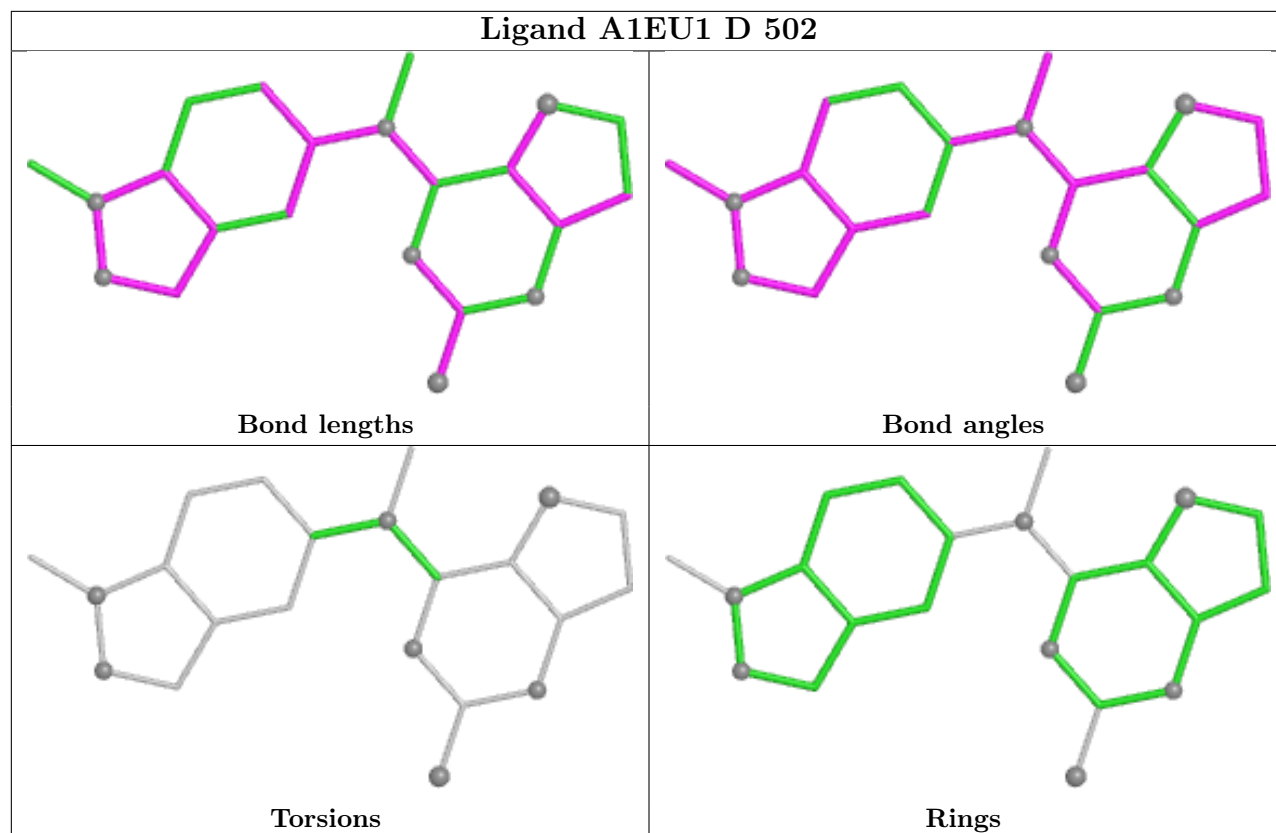
There are no ring outliers.

2 monomers are involved in 10 short contacts:

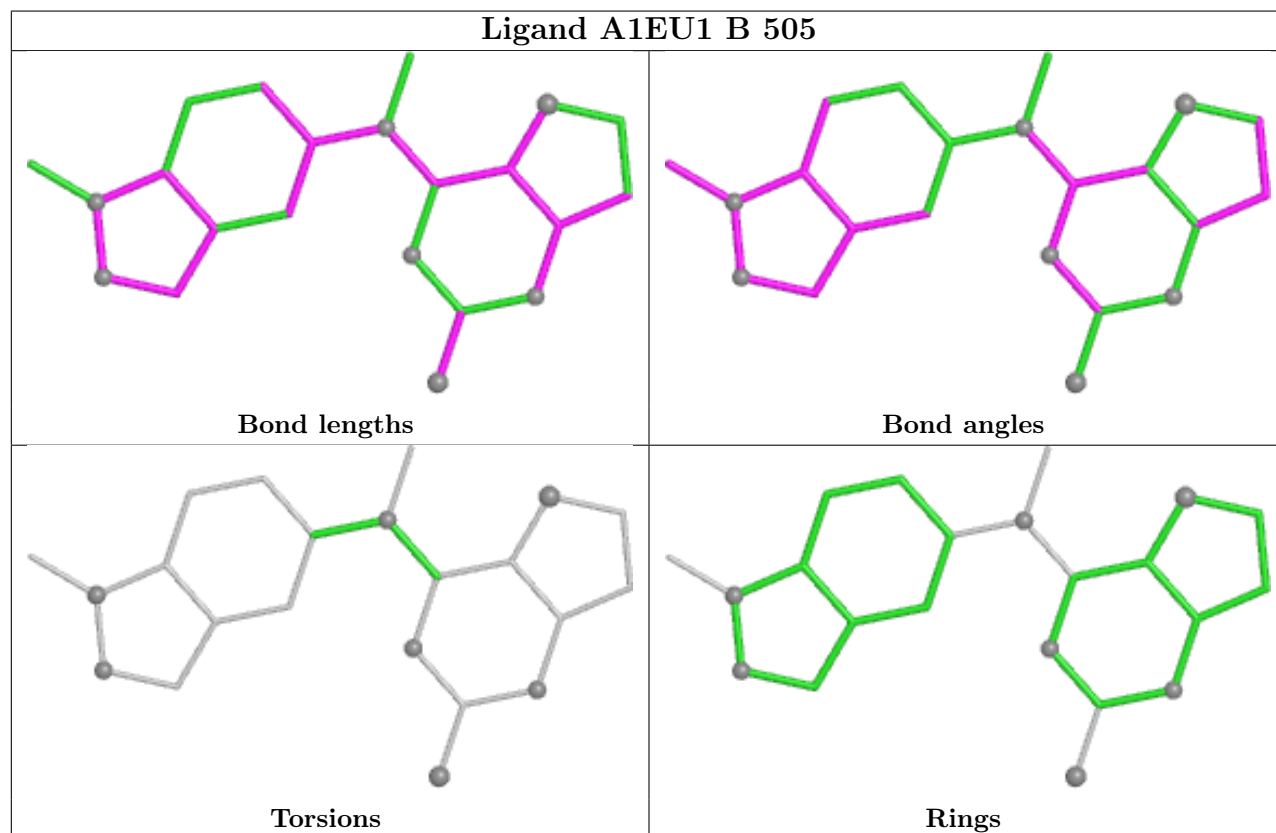
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	A1EU1	5	0
10	B	505	A1EU1	5	0

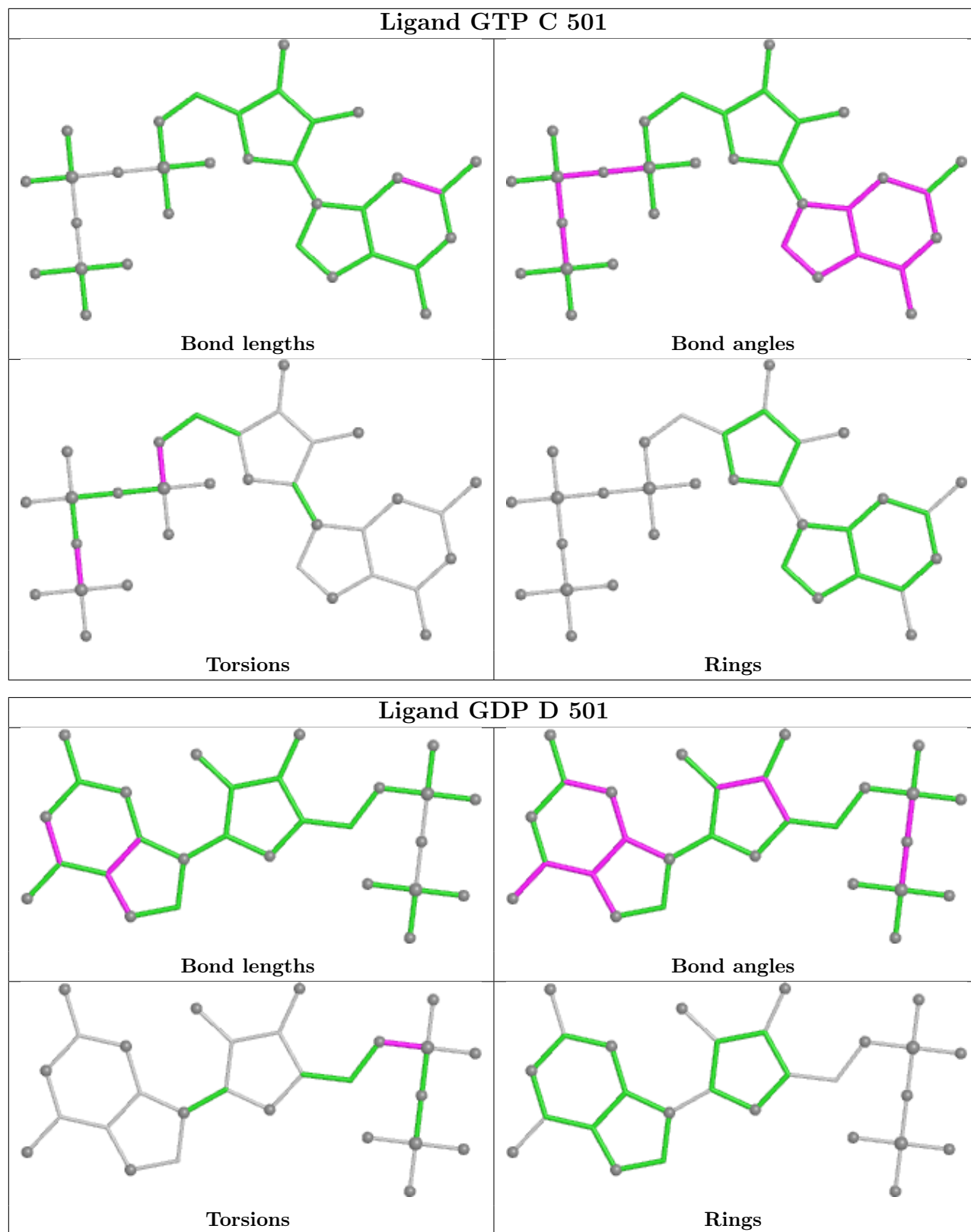
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

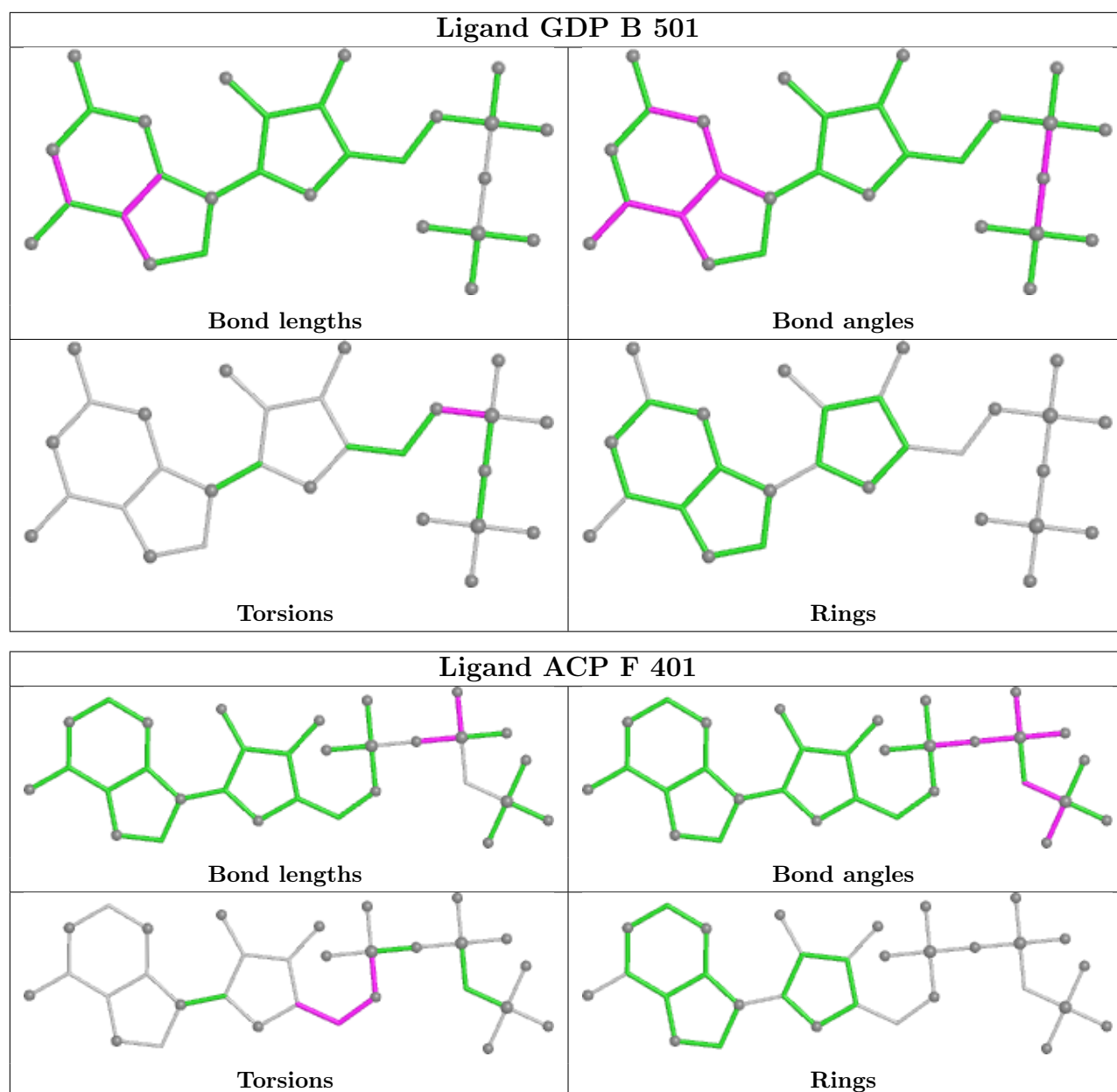
Ligand A1EU1 D 502

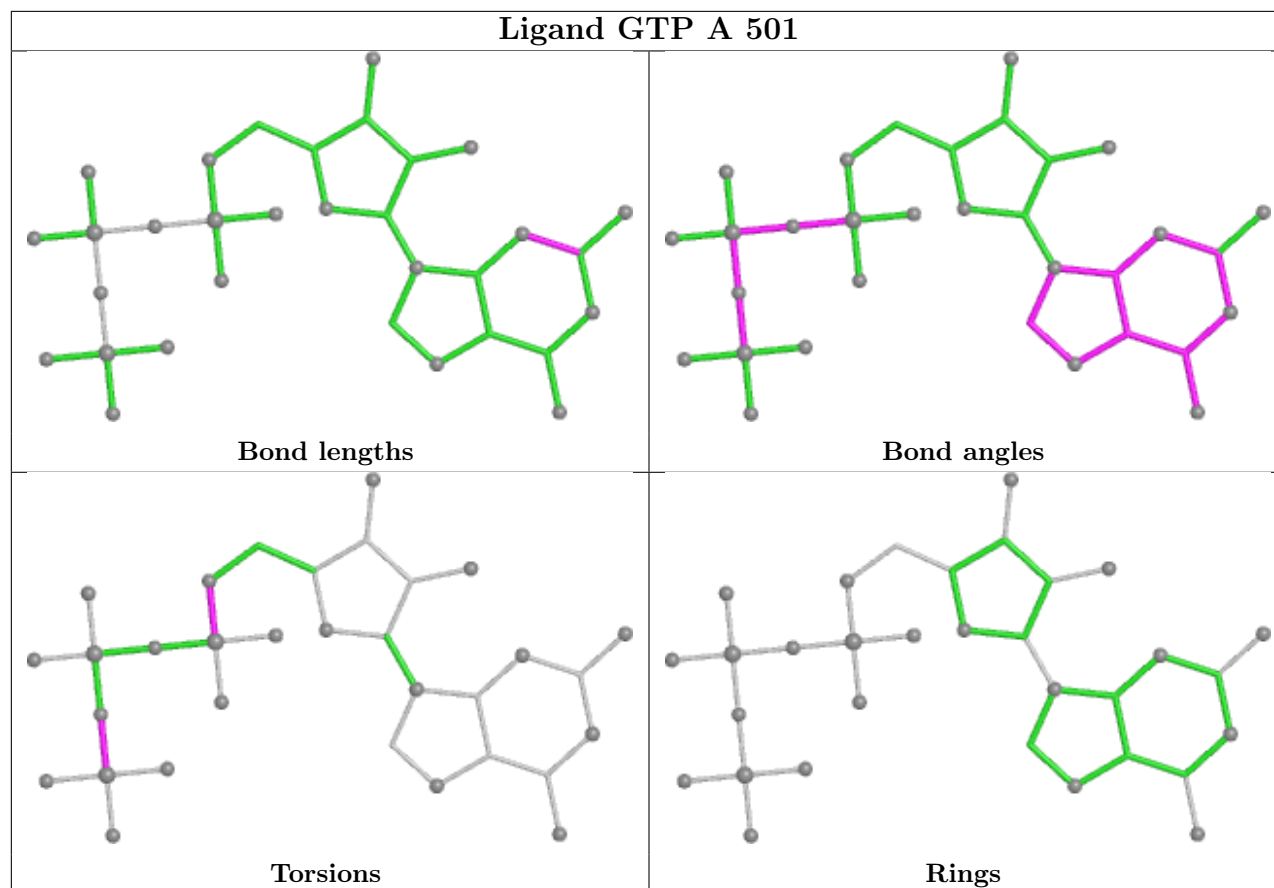


Ligand A1EU1 B 505









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	437/440 (99%)	1.34	109 (24%) 2 1	42, 58, 84, 125	0
1	C	440/440 (100%)	0.52	24 (5%) 30 27	34, 49, 67, 87	0
2	B	427/431 (99%)	1.01	53 (12%) 8 7	39, 56, 86, 138	0
2	D	421/431 (97%)	2.91	305 (72%) 0 0	47, 84, 119, 137	0
3	E	121/136 (88%)	1.71	48 (39%) 1 0	49, 71, 102, 119	0
4	F	332/380 (87%)	2.04	143 (43%) 0 0	49, 81, 153, 169	0
All	All	2178/2258 (96%)	1.54	682 (31%) 1 1	34, 63, 116, 169	0

All (682) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	GLY	7.8
2	D	42	LEU	6.8
2	D	85	PHE	6.8
2	D	273	LEU	6.7
4	F	148	ILE	6.6
2	D	71	GLY	6.5
2	D	73	MET	6.4
2	D	360	GLY	6.4
2	D	212	PHE	6.3
4	F	162	ILE	6.3
2	D	91	VAL	6.2
4	F	253	TYR	6.2
2	D	32	PRO	6.1
2	D	179	VAL	6.1
4	F	161	LEU	6.1
2	D	395	LEU	6.0
4	F	132	LEU	5.9
2	D	80	PRO	5.9
2	D	361	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
2	D	284	LEU	5.7
2	D	397	TRP	5.7
2	D	362	LYS	5.7
2	D	215	LEU	5.6
2	D	394	PHE	5.6
2	D	46	ARG	5.6
4	F	173	ILE	5.4
2	D	178	THR	5.4
2	D	180	VAL	5.4
4	F	149	ALA	5.4
2	D	92	PHE	5.3
1	A	83	TYR	5.3
2	D	359	ARG	5.3
2	D	236	VAL	5.3
4	F	362	ALA	5.3
2	D	23	VAL	5.2
2	D	60	VAL	5.2
4	F	233	PHE	5.2
2	D	245	GLN	5.2
2	D	61	PRO	5.2
2	D	227	HIS	5.2
2	D	216	LYS	5.2
2	D	431	ASP	5.1
2	D	5	VAL	5.1
2	D	6	HIS	5.0
2	D	54	ALA	4.9
2	B	72	THR	4.9
2	D	116	VAL	4.9
2	D	140	GLY	4.9
2	D	70	PRO	4.9
2	D	68	LEU	4.9
2	D	82	GLY	4.9
1	A	282	TYR	4.9
2	D	72	THR	4.8
4	F	172	PHE	4.8
4	F	244	CYS	4.8
2	D	326	VAL	4.8
2	B	428	ALA	4.8
2	D	243	PRO	4.8
4	F	131	PHE	4.8
1	A	86	LEU	4.8
4	F	146	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	47	ILE	4.8
2	D	1	MET	4.8
4	F	103	THR	4.8
1	A	82	THR	4.7
2	D	43	GLN	4.7
4	F	245	ILE	4.7
2	D	65	LEU	4.7
2	D	222	TYR	4.7
2	D	242	PHE	4.7
4	F	181	VAL	4.6
1	A	276	ILE	4.6
2	D	84	ILE	4.6
2	D	142	GLY	4.6
2	D	90	PHE	4.6
2	D	229	VAL	4.6
2	D	107	THR	4.6
2	D	171	PRO	4.5
4	F	74	LYS	4.5
2	D	217	LEU	4.5
2	B	218	THR	4.5
2	D	81	PHE	4.5
2	D	356	ILE	4.5
2	D	208	TYR	4.5
4	F	134	ALA	4.5
2	D	96	GLY	4.5
1	C	440	VAL	4.5
4	F	101	TYR	4.4
2	D	220	PRO	4.4
1	A	85	GLN	4.4
2	B	128	ASP	4.4
2	D	51	TYR	4.4
2	D	223	GLY	4.4
1	A	42	ILE	4.4
4	F	133	ALA	4.4
2	D	29	GLY	4.4
4	F	263	PHE	4.4
4	F	182	ILE	4.4
2	D	44	LEU	4.4
2	D	98	GLY	4.3
2	D	16	ILE	4.3
4	F	130	VAL	4.3
4	F	166	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	283	HIS	4.3
4	F	185	TYR	4.3
2	B	282	ARG	4.3
2	B	55	THR	4.3
2	D	7	ILE	4.3
1	A	37	PRO	4.3
4	F	99	VAL	4.3
2	D	36	TYR	4.3
2	D	115	SER	4.3
2	D	94	GLN	4.2
2	D	20	PHE	4.2
2	D	244	GLY	4.2
4	F	169	LEU	4.2
2	D	247	ASN	4.2
4	F	240	LEU	4.2
2	D	52	ASN	4.2
2	D	304	ASP	4.1
2	D	117	LEU	4.1
4	F	170	LEU	4.1
2	D	321	MET	4.1
2	D	49	VAL	4.1
2	D	102	ALA	4.1
2	D	226	ASN	4.1
2	D	170	MET	4.1
4	F	180	HIS	4.1
2	D	83	GLN	4.1
2	D	24	ILE	4.1
4	F	372	THR	4.1
2	D	138	SER	4.0
2	D	30	ILE	4.0
2	D	323	MET	4.0
1	A	362	VAL	4.0
1	A	437	VAL	4.0
2	D	201	CYS	4.0
2	D	97	ALA	4.0
2	D	231	ALA	4.0
2	D	241	ARG	4.0
2	D	55	THR	4.0
2	D	63	ALA	4.0
2	D	391	ARG	4.0
3	E	6	MET	4.0
2	D	387	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	247	ASN	4.0
2	D	64	ILE	4.0
4	F	98	TYR	4.0
2	D	69	GLU	3.9
4	F	231	ALA	3.9
2	D	211	CYS	3.9
1	A	45	GLY	3.9
2	B	42	LEU	3.9
2	D	87	PRO	3.9
4	F	198	LYS	3.9
2	B	277	GLY	3.9
2	D	127	CYS	3.9
2	D	28	HIS	3.9
4	F	239	HIS	3.9
2	D	213	ARG	3.9
4	F	186	LEU	3.9
1	A	74	VAL	3.9
2	D	175	VAL	3.9
2	D	367	PHE	3.9
2	D	112	LEU	3.9
4	F	20	LEU	3.9
2	D	239	CYS	3.9
2	B	279	GLN	3.9
1	A	89	PRO	3.9
4	F	247	LYS	3.8
1	A	41	THR	3.8
1	A	281	ALA	3.8
2	B	281	TYR	3.8
2	D	59	TYR	3.8
2	D	12	CYS	3.8
2	D	120	VAL	3.8
2	D	271	ALA	3.8
2	D	401	GLU	3.8
2	B	280	GLN	3.8
3	E	8	VAL	3.8
2	D	365	ALA	3.8
2	D	66	VAL	3.7
3	E	139	LEU	3.7
4	F	163	SER	3.7
4	F	237	THR	3.7
1	A	58	ALA	3.7
2	D	93	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	104	GLY	3.7
2	D	14	ASN	3.7
4	F	190	LEU	3.7
2	D	11	GLN	3.7
4	F	147	TRP	3.7
4	F	228	TYR	3.7
2	D	364	SER	3.7
4	F	306	HIS	3.7
2	D	408	PHE	3.7
4	F	199	PHE	3.7
2	D	144	GLY	3.7
2	D	289	LEU	3.7
4	F	135	TYR	3.7
2	D	353	VAL	3.7
4	F	380	HIS	3.7
2	D	139	LEU	3.7
2	D	182	PRO	3.7
2	B	245	GLN	3.6
2	D	292	GLN	3.6
2	D	143	THR	3.6
2	D	221	THR	3.6
4	F	191	LEU	3.6
2	D	37	HIS	3.6
2	D	149	THR	3.6
4	F	331	GLU	3.6
2	D	228	LEU	3.6
3	E	9	ILE	3.6
1	A	94	THR	3.6
2	D	119	VAL	3.6
2	D	219	THR	3.6
2	D	232	THR	3.6
2	D	126	SER	3.6
2	D	18	ALA	3.6
2	D	318	ARG	3.6
3	E	115	HIS	3.5
2	D	272	PRO	3.5
2	D	9	ALA	3.5
2	B	80	PRO	3.5
2	D	202	ILE	3.5
2	D	27	GLU	3.5
1	A	358	GLN	3.5
2	D	101	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	164	LYS	3.5
2	D	19	LYS	3.5
1	C	282	TYR	3.5
3	E	46	SER	3.5
4	F	164	SER	3.5
2	D	204	ASN	3.4
4	F	136	ASN	3.4
2	D	238	THR	3.4
1	A	368	LEU	3.4
2	D	135	LEU	3.4
2	D	240	LEU	3.4
1	A	81	GLY	3.4
2	D	4	ILE	3.4
2	D	398	TYR	3.4
4	F	256	TYR	3.4
2	D	389	PHE	3.4
4	F	96	GLU	3.4
2	D	21	TRP	3.4
2	D	79	GLY	3.4
3	E	130	ALA	3.4
2	B	278	SER	3.4
2	D	50	TYR	3.4
4	F	230	SER	3.4
2	B	323	MET	3.4
2	D	291	GLN	3.4
2	B	54	ALA	3.4
2	D	393	ALA	3.4
2	D	25	SER	3.4
2	D	354	CYS	3.4
3	E	28	SER	3.4
2	D	106	TYR	3.4
2	D	123	GLU	3.4
4	F	320	MET	3.4
1	A	47	ASP	3.4
2	D	379	LYS	3.4
2	D	33	THR	3.4
2	D	109	GLY	3.4
1	A	122	ILE	3.4
4	F	232	ASN	3.3
2	D	218	THR	3.3
2	D	285	THR	3.3
4	F	227	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	396	HIS	3.3
2	D	45	GLU	3.3
2	D	159	TYR	3.3
1	A	120	ASP	3.3
1	A	32	PRO	3.3
2	D	76	VAL	3.3
4	F	187	GLU	3.3
2	D	35	SER	3.3
2	D	95	SER	3.3
2	D	230	SER	3.3
1	A	49	PHE	3.3
2	D	99	ASN	3.3
2	D	136	THR	3.3
2	D	77	ARG	3.3
4	F	192	LEU	3.3
4	F	275	LEU	3.3
2	D	363	MET	3.3
2	D	381	ILE	3.3
1	C	245	ASP	3.2
2	D	207	LEU	3.2
2	D	38	GLY	3.2
2	D	174	LYS	3.2
4	F	90	SER	3.2
4	F	341	LYS	3.2
2	B	316	ILE	3.2
1	A	126	ALA	3.2
2	D	15	GLN	3.2
2	D	168	SER	3.2
2	D	67	ASP	3.2
2	D	150	LEU	3.2
2	D	416	ASN	3.2
1	C	357	TYR	3.2
2	D	411	ALA	3.2
2	D	8	GLN	3.2
2	D	134	GLN	3.2
1	C	283	HIS	3.2
4	F	229	ASN	3.2
1	A	363	VAL	3.2
4	F	179	VAL	3.2
4	F	92	THR	3.2
4	F	224	SER	3.1
2	D	224	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.1
2	D	415	MET	3.1
4	F	254	GLY	3.1
2	D	53	GLU	3.1
2	D	270	PHE	3.1
1	A	88	HIS	3.1
1	A	119	LEU	3.1
2	D	130	LEU	3.1
2	D	187	LEU	3.1
4	F	242	ASN	3.1
2	D	10	GLY	3.1
1	A	56	THR	3.1
1	A	91	GLN	3.1
4	F	234	GLN	3.1
4	F	89	GLU	3.1
4	F	1	MET	3.1
2	D	225	LEU	3.1
4	F	167	SER	3.1
1	A	221	ARG	3.1
1	A	55	GLU	3.1
1	A	251	ASP	3.1
3	E	17	GLY	3.1
4	F	334	GLY	3.1
2	D	169	VAL	3.1
1	C	302	MET	3.0
1	A	87	PHE	3.0
1	A	248	LEU	3.0
4	F	361	LEU	3.0
2	D	40	SER	3.0
4	F	246	GLN	3.0
2	D	147	MET	3.0
4	F	323	GLU	3.0
2	D	385	PHE	3.0
1	A	18	ASN	3.0
4	F	236	LYS	3.0
4	F	252	ASN	3.0
2	D	34	GLY	3.0
4	F	141	GLY	3.0
1	A	33	ASP	3.0
4	F	13	VAL	3.0
1	A	130	THR	3.0
3	E	141	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	129	GLU	3.0
1	A	360	PRO	3.0
2	D	41	ASP	3.0
2	D	209	ASP	3.0
3	E	16	SER	3.0
2	B	71	GLY	3.0
1	A	78	VAL	2.9
3	E	7	GLU	2.9
4	F	241	THR	2.9
2	B	283	ALA	2.9
2	D	2	ARG	2.9
2	D	86	ARG	2.9
4	F	194	PRO	2.9
2	D	392	LYS	2.9
3	E	135	LYS	2.9
4	F	188	LYS	2.9
2	D	302	ALA	2.9
2	D	357	PRO	2.9
1	A	48	SER	2.9
3	E	124	GLN	2.9
1	A	59	GLY	2.9
2	D	48	ASN	2.9
2	D	335	ASN	2.9
1	A	250	VAL	2.9
2	D	386	THR	2.9
2	D	358	PRO	2.9
4	F	189	PRO	2.9
4	F	46	ARG	2.9
4	F	243	HIS	2.9
2	D	57	ASN	2.8
4	F	142	ARG	2.8
4	F	145	ASN	2.8
1	A	112	LYS	2.8
2	D	58	LYS	2.8
2	D	113	VAL	2.8
3	E	133	VAL	2.8
2	D	39	ASP	2.8
2	D	177	ASP	2.8
2	D	133	PHE	2.8
1	A	57	GLY	2.8
4	F	225	SER	2.8
3	E	45	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	125	GLU	2.8
2	D	404	ASP	2.8
3	E	59	GLU	2.8
1	A	163	LYS	2.8
1	A	346	TRP	2.8
1	A	430	LYS	2.8
2	D	297	LYS	2.8
4	F	184	LYS	2.8
2	D	402	GLY	2.8
4	F	379	HIS	2.8
2	D	214	THR	2.8
1	C	163	LYS	2.8
3	E	126	LYS	2.8
1	A	277	SER	2.8
2	D	78	SER	2.8
2	B	33	THR	2.8
2	D	405	GLU	2.8
3	E	21	GLU	2.8
1	A	345	ASP	2.8
3	E	50	ILE	2.7
3	E	12	ASN	2.7
2	D	290	THR	2.7
2	D	406	MET	2.7
2	D	336	LYS	2.7
2	D	383	GLU	2.7
2	B	129	CYS	2.7
2	D	235	GLY	2.7
2	B	95	SER	2.7
2	D	246	LEU	2.7
1	A	73	THR	2.7
2	D	167	PHE	2.7
2	D	173	PRO	2.7
2	B	40	SER	2.7
4	F	216	TYR	2.7
1	A	278	ALA	2.7
2	D	320	ARG	2.7
1	A	176	GLN	2.7
1	C	46	ASP	2.7
2	D	163	ILE	2.7
3	E	23	ILE	2.7
4	F	283	ILE	2.7
3	E	136	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	296	SER	2.7
2	D	333	VAL	2.7
2	D	183	TYR	2.7
1	A	361	THR	2.7
3	E	10	GLU	2.7
4	F	344	ALA	2.7
2	B	37	HIS	2.7
2	D	26	ASP	2.6
2	B	75	SER	2.6
2	D	148	GLY	2.6
3	E	128	LYS	2.6
2	D	210	ILE	2.6
2	D	316	ILE	2.6
3	E	26	PRO	2.6
3	E	134	ARG	2.6
4	F	19	ARG	2.6
2	B	48	ASN	2.6
2	D	176	SER	2.6
1	A	40	LYS	2.6
2	D	31	ASP	2.6
2	D	308	GLY	2.6
4	F	177	GLY	2.6
1	A	364	PRO	2.6
2	D	62	ARG	2.6
2	D	306	ARG	2.6
4	F	100	ILE	2.6
1	C	340	SER	2.6
3	E	129	HIS	2.6
4	F	28	LYS	2.6
1	C	218	ASP	2.6
1	C	284	GLU	2.6
2	D	193	VAL	2.6
2	D	349	VAL	2.6
1	A	232	SER	2.6
2	D	172	SER	2.6
2	D	237	THR	2.6
4	F	339	ALA	2.6
1	A	84	ARG	2.5
2	B	320	ARG	2.5
2	D	355	ASP	2.5
4	F	9	GLU	2.5
3	E	54	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	35	GLN	2.5
1	A	50	ASN	2.5
1	A	315	CYS	2.5
3	E	97	ALA	2.5
2	D	196	THR	2.5
2	D	299	MET	2.5
2	D	388	MET	2.5
3	E	24	LEU	2.5
2	D	100	ASN	2.5
2	D	105	HIS	2.5
4	F	260	ASN	2.5
2	B	214	THR	2.5
4	F	338	CYS	2.5
2	D	233	MET	2.5
2	D	118	ASP	2.5
2	B	47	ILE	2.5
2	B	69	GLU	2.5
2	D	158	GLU	2.5
4	F	176	GLN	2.5
2	B	60	VAL	2.5
1	A	123	ARG	2.5
2	D	409	THR	2.5
4	F	238	CYS	2.5
2	D	189	VAL	2.5
4	F	222	ARG	2.5
1	A	347	CYS	2.4
1	A	97	GLU	2.4
1	A	113	GLU	2.4
2	D	205	GLU	2.4
3	E	121	GLU	2.4
2	D	103	LYS	2.4
4	F	174	ASP	2.4
3	E	122	ARG	2.4
1	A	371	VAL	2.4
3	E	22	VAL	2.4
2	B	237	THR	2.4
4	F	373	SER	2.4
1	A	144	GLY	2.4
2	D	114	ASP	2.4
4	F	200	ASP	2.4
2	B	59	TYR	2.4
2	D	329	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	270	TYR	2.4
2	B	92	PHE	2.4
1	A	226	ASN	2.4
4	F	276	ASN	2.4
4	F	257	GLU	2.4
2	D	152	ILE	2.4
3	E	44	ASP	2.4
4	F	91	CYS	2.4
2	B	43	GLN	2.4
1	A	61	HIS	2.4
2	D	352	ALA	2.4
4	F	335	ALA	2.4
1	A	223	THR	2.4
1	A	337	THR	2.4
2	B	238	THR	2.4
4	F	85	PRO	2.4
2	D	124	SER	2.4
1	A	246	GLY	2.4
2	D	13	GLY	2.4
1	A	46	ASP	2.4
1	A	256	GLN	2.4
4	F	178	GLN	2.4
4	F	196	HIS	2.4
4	F	221	LEU	2.4
2	D	181	GLU	2.4
2	D	421	GLU	2.4
4	F	223	THR	2.3
2	D	75	SER	2.3
2	D	319	GLY	2.3
2	B	291	GLN	2.3
2	D	74	ASP	2.3
4	F	21	LEU	2.3
3	E	96	MET	2.3
4	F	343	TYR	2.3
1	A	96	LYS	2.3
2	B	336	LYS	2.3
2	D	108	GLU	2.3
1	A	34	GLY	2.3
2	D	56	GLY	2.3
4	F	138	ARG	2.3
2	B	426	GLN	2.3
4	F	33	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	280	LYS	2.3
4	F	175	GLU	2.3
3	E	71	HIS	2.3
1	A	117	LEU	2.3
2	D	88	ASP	2.3
1	C	77	GLU	2.3
2	D	303	CYS	2.3
2	D	412	GLU	2.3
4	F	193	GLU	2.3
2	D	110	ALA	2.3
1	A	39	ASP	2.3
2	B	41	ASP	2.3
2	B	362	LYS	2.3
3	E	53	LYS	2.3
2	D	3	GLU	2.3
2	D	111	GLU	2.3
4	F	267	PHE	2.3
1	A	356	ASN	2.2
3	E	80	ARG	2.3
3	E	102	ALA	2.2
1	C	95	GLY	2.2
2	D	317	PHE	2.2
1	A	66	VAL	2.2
2	B	359	ARG	2.2
2	B	57	ASN	2.2
2	B	94	GLN	2.2
4	F	24	THR	2.2
1	C	96	LYS	2.2
2	B	246	LEU	2.2
2	B	406	MET	2.2
2	D	146	GLY	2.2
3	E	137	LYS	2.2
1	A	38	SER	2.2
1	A	75	ILE	2.2
2	D	328	GLU	2.2
2	D	294	PHE	2.2
2	D	137	HIS	2.2
4	F	70	LYS	2.2
1	A	80	THR	2.2
2	D	403	MET	2.2
3	E	120	LEU	2.2
4	F	22	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	144	GLY	2.2
4	F	171	ASP	2.2
4	F	235	ASP	2.2
2	D	122	LYS	2.2
1	A	128	GLN	2.2
2	B	73	MET	2.2
2	D	267	MET	2.2
1	A	132	LEU	2.2
1	A	153	LEU	2.2
1	A	316	CYS	2.2
1	A	433	GLU	2.2
4	F	165	GLU	2.2
4	F	202	ARG	2.2
3	E	27	PRO	2.2
1	A	370	LYS	2.2
3	E	25	LYS	2.2
2	D	248	ALA	2.1
1	A	29	GLY	2.1
2	B	93	GLY	2.1
1	C	341	ILE	2.1
2	D	198	GLU	2.1
4	F	168	GLU	2.1
1	C	178	SER	2.1
2	B	78	SER	2.1
2	B	427	ASP	2.1
4	F	88	SER	2.1
4	F	82	LYS	2.1
1	C	362	VAL	2.1
1	C	285	GLN	2.1
2	D	184	ASN	2.1
2	D	17	GLY	2.1
4	F	81	ILE	2.1
1	C	215	ARG	2.1
4	F	139	ARG	2.1
2	D	188	SER	2.1
2	D	322	SER	2.1
3	E	127	ASP	2.1
3	E	140	LYS	2.1
1	A	294	ALA	2.1
4	F	274	ALA	2.1
1	A	92	LEU	2.1
2	D	366	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	ARG	2.1
1	A	4	CYS	2.1
2	B	275	SER	2.1
2	D	420	SER	2.1
4	F	336	PRO	2.1
1	A	351	PHE	2.1
2	D	151	LEU	2.1
4	F	128	ARG	2.1
1	A	51	THR	2.1
1	A	434	GLU	2.1
2	D	288	GLU	2.1
4	F	83	THR	2.1
2	D	368	ILE	2.1
1	C	425	MET	2.1
3	E	20	PHE	2.0
2	D	390	ARG	2.0
2	D	89	ASN	2.0
2	D	400	GLY	2.0
1	A	124	LYS	2.0
2	D	399	THR	2.0
1	C	232	SER	2.0
1	A	135	PHE	2.0
2	B	276	ARG	2.0
3	E	47	LEU	2.0
1	A	95	GLY	2.0
1	A	216	ASN	2.0
1	C	41	THR	2.0
1	C	337	THR	2.0
1	A	1	MET	2.0
1	A	76	ASP	2.0
1	A	348	PRO	2.0
2	D	295	ASP	2.0
1	A	262	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

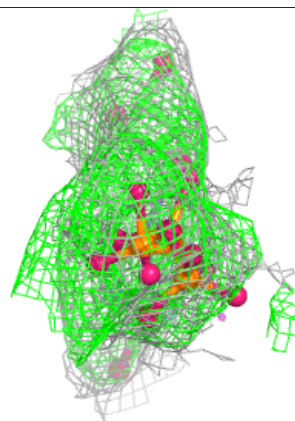
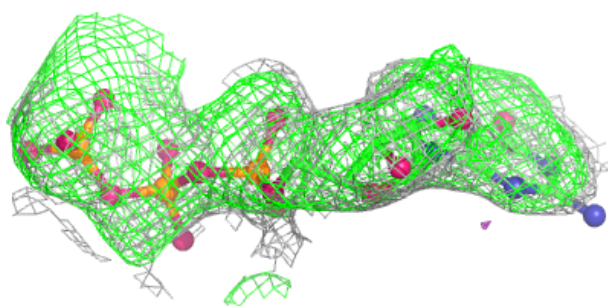
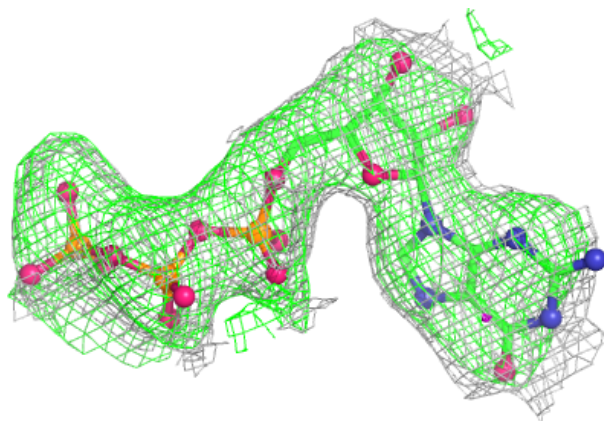
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	46,48,50,50	32
5	GTP	C	501	32/32	-	-	39,43,46,47	32
6	CA	A	502	1/1	-	-	85,85,85,85	1
6	CA	C	502	1/1	-	-	61,61,61,61	1
7	MG	A	503	1/1	-	-	50,50,50,50	1
7	MG	B	504	1/1	-	-	56,56,56,56	1
7	MG	C	503	1/1	-	-	44,44,44,44	1
8	GDP	B	501	28/28	-	-	45,49,51,52	28
8	GDP	D	501	28/28	-	-	83,91,98,99	28
9	MES	B	502	12/12	-	-	47,48,51,51	12
9	MES	B	503	12/12	-	-	64,66,68,70	12
10	A1EU1	D	502	22/22	0.76	0.20	56,69,77,87	0
10	A1EU1	B	505	22/22	0.87	0.18	42,57,70,185	0
11	ACP	F	401	31/31	-	-	107,118,142,146	45

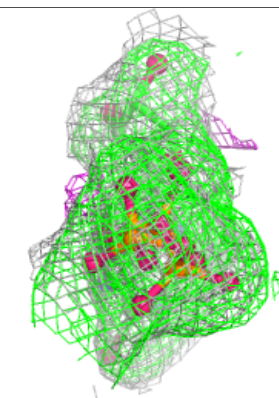
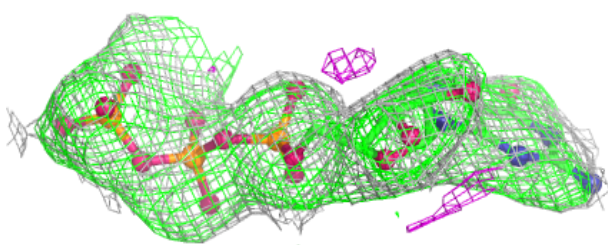
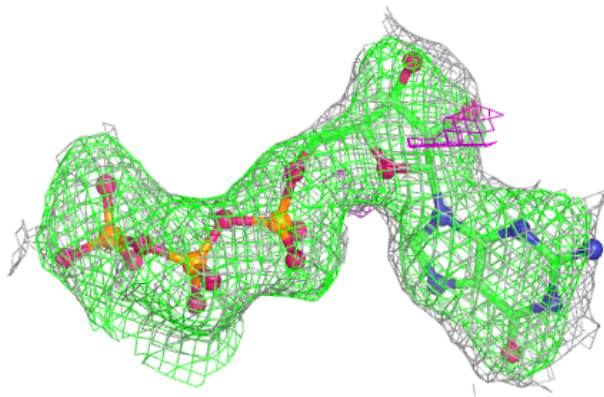
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

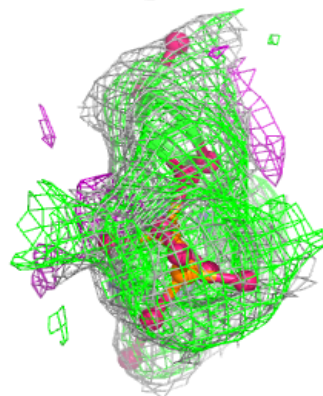
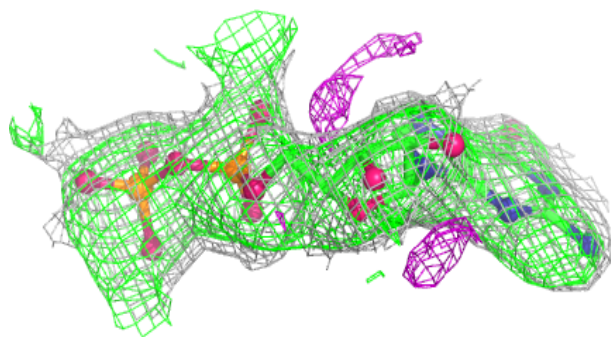
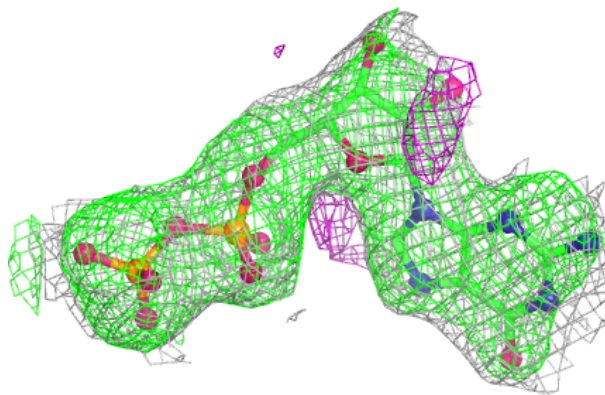
**Electron density around GTP C 501:**

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



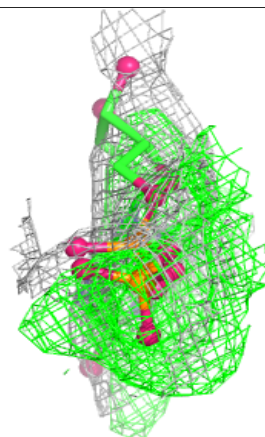
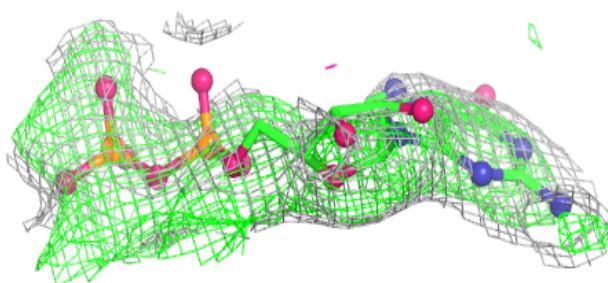
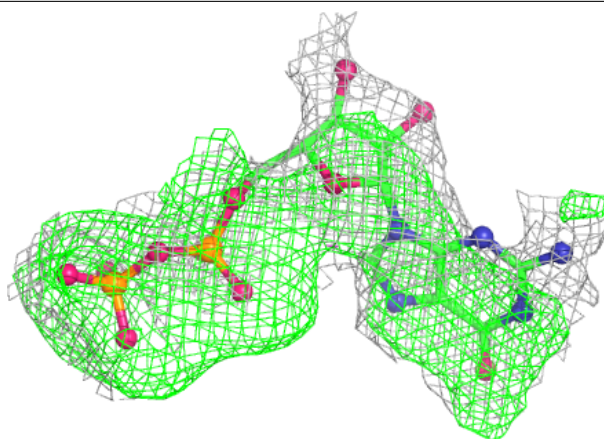
Electron density around GDP B 501:

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

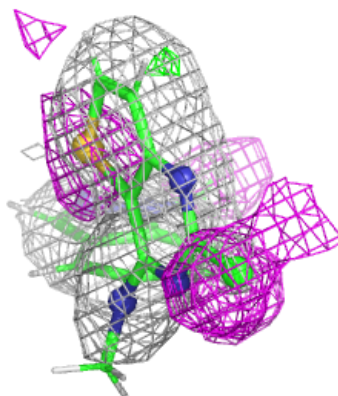
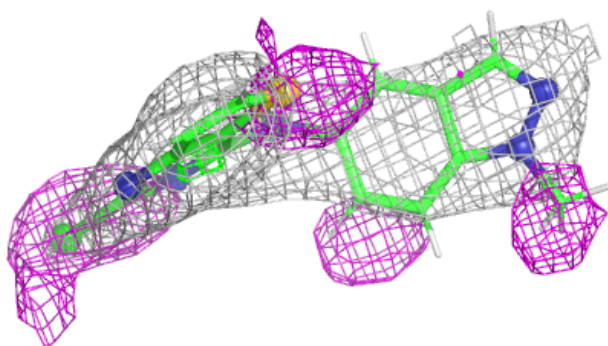
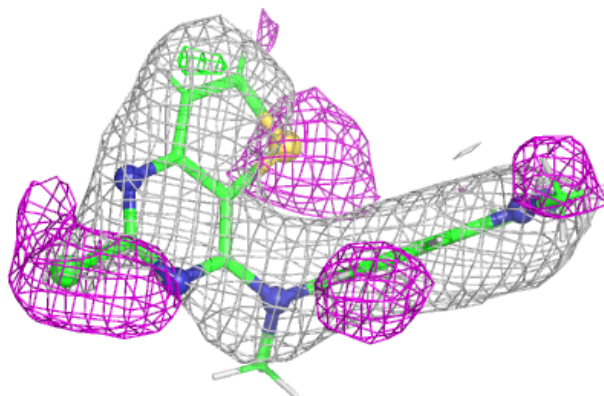


Electron density around GDP D 501:

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

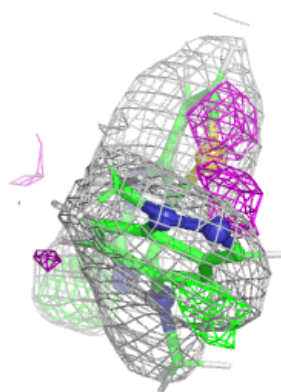
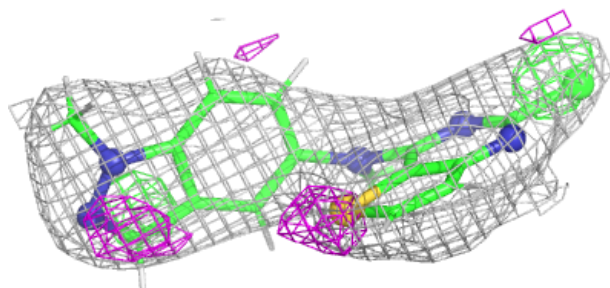
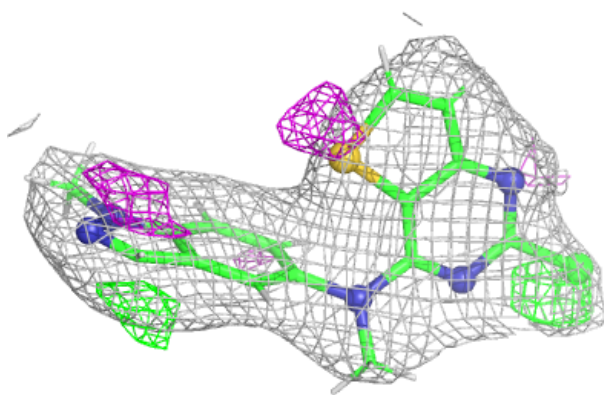
**Electron density around A1EU1 D 502:**

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

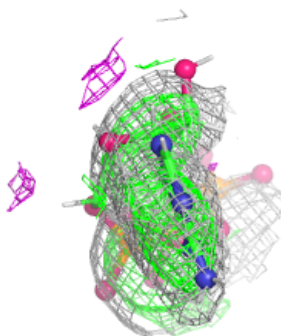
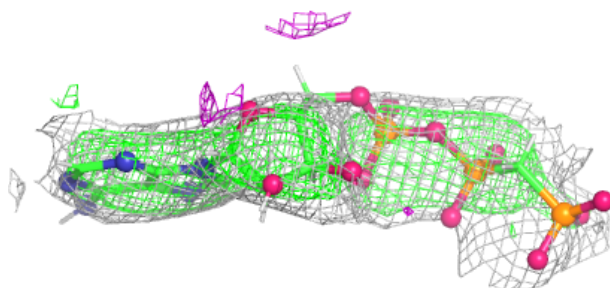
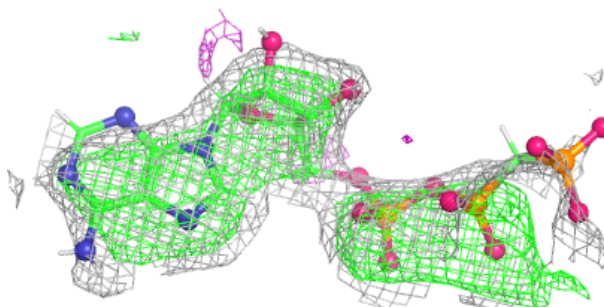


Electron density around A1EU1 B 505:

$2mF_o-DF_c$ (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.