



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:37 AM UTC

PDB ID : 9HXC / pdb_00009hxc
EMDB ID : EMD-52463
Title : CryoEM structure of Asgard AtubA/B2 microtubule
Authors : Wollweber, F.; Xu, J.; Ponce-Toledo, R.I.; Rodrigues-Oliveira, T.; Malit, J.J.L.; Kokhanovska, A.; Wiczorek, M.; Schleper, C.; Pilhofer, M.
Deposited on : 2025-01-07
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

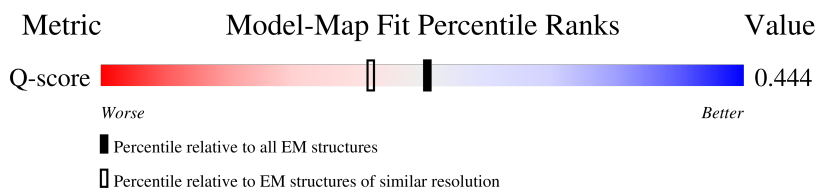
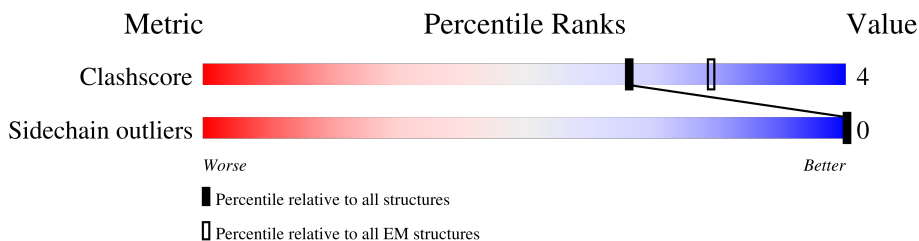
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	22% 91% 9%
1	B	428	18% 91% 9%
1	E	428	16% 91% 9%
1	G	428	15% 91% 8%
1	I	428	16% 91% 8%

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Mol	Chain	Length	Quality of chain
1	K	428	14% 91% 8%
1	M	428	14% 91% 9%
1	O	428	15% 89% 10%
1	Q	428	15% 89% 10%
1	S	428	16% 90% 9%
1	U	428	17% 90% 10%
1	W	428	18% 90% 9%
1	Y	428	19% 90% 10%
1	a	428	21% 89% 10%
2	C	423	14% 91% 9%
2	D	423	16% 91% 9%
2	F	423	15% 91% 8%
2	H	423	15% 91% 9%
2	J	423	14% 90% 9%
2	L	423	15% 91% 9%
2	N	423	15% 90% 9%
2	P	423	16% 92% 7%
2	R	423	17% 92% 8%
2	T	423	20% 92% 7%
2	V	423	21% 92% 7%
2	X	423	24% 92% 7%
2	Z	423	28% 92% 7%
2	b	423	35% 92% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 93142 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

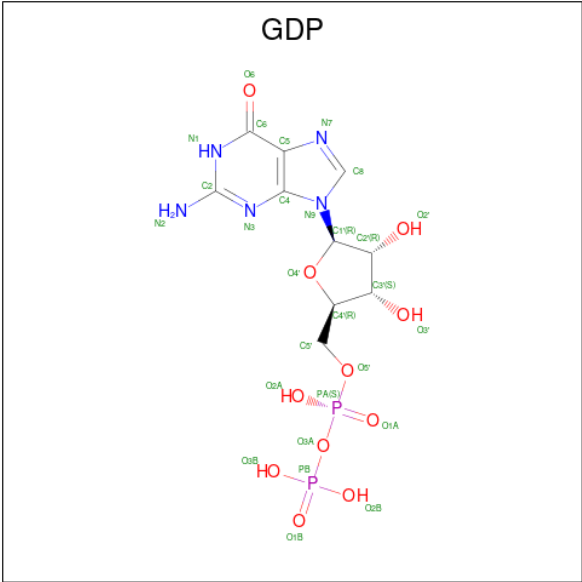
- Molecule 1 is a protein called Asgard tubulin AtubA with residues from TEV protease cleavage site.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	B	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	E	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	G	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	I	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	K	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	M	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	O	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	Q	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	S	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	U	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	W	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	Y	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		
1	a	427	Total	C	N	O	S	0	0
			3277	2091	540	634	12		

- Molecule 2 is a protein called Asgard tubulin AtubB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	C	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	F	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	H	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	J	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	L	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	N	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	P	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	R	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	T	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	V	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	X	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	Z	422	Total 3348	C 2138	N 554	O 634	S 22	0	0
2	b	422	Total 3348	C 2138	N 554	O 634	S 22	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).

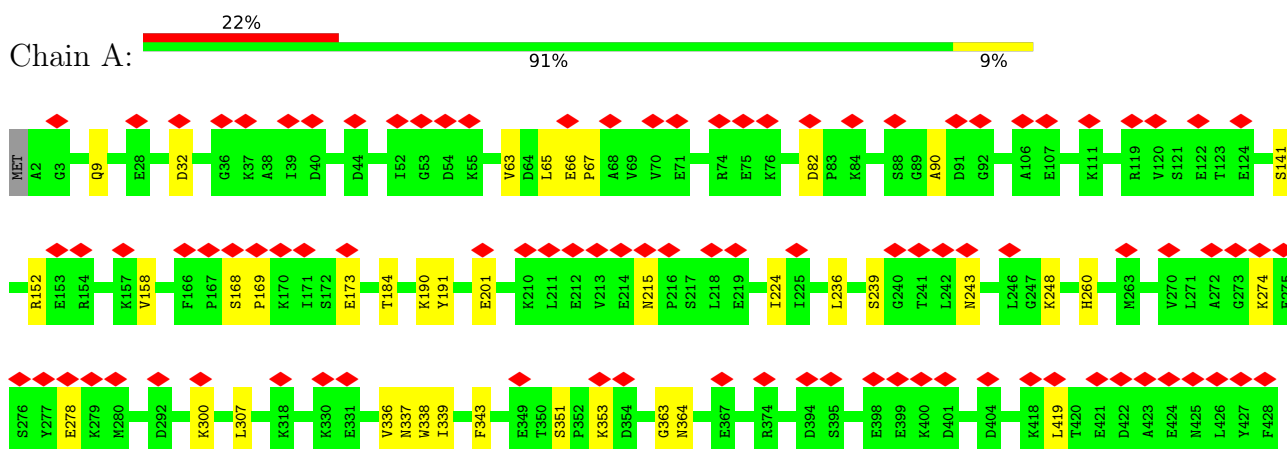


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	E	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	G	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	I	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	K	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	M	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	O	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	S	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	U	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	W	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	a	1	Total	C	N	O	P	0
			28	10	5	11	2	

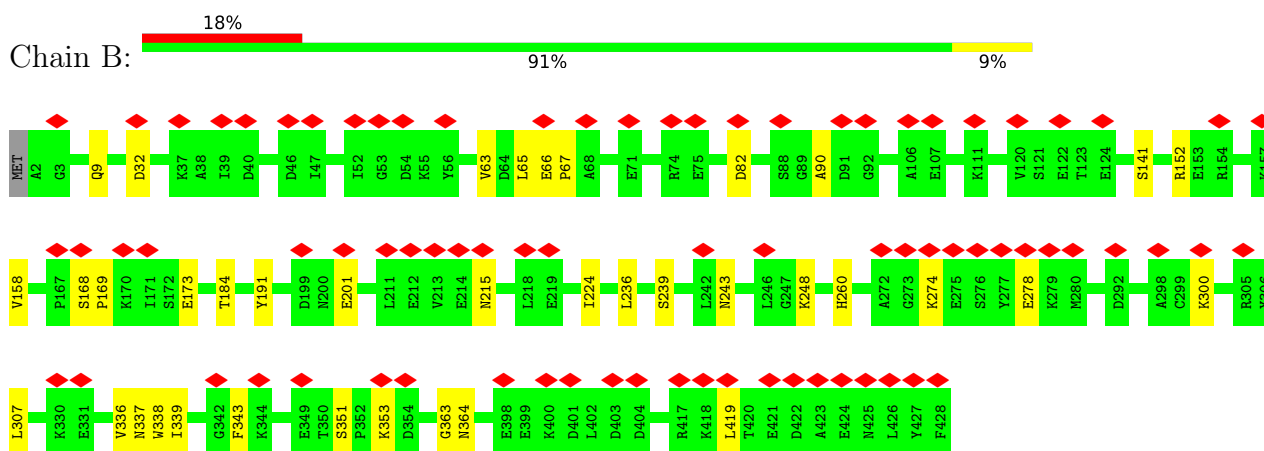
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

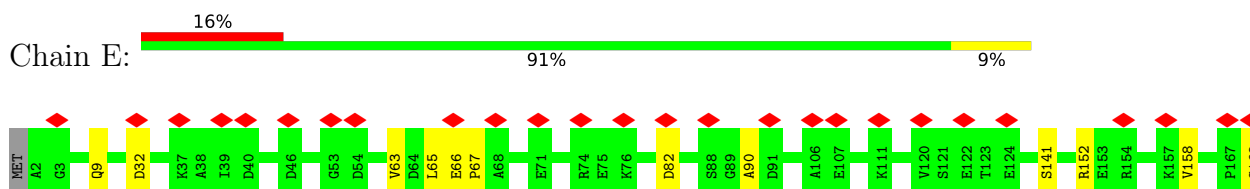
- Molecule 1: Asgard tubulin AtubA with residues from TEV protease cleavage site

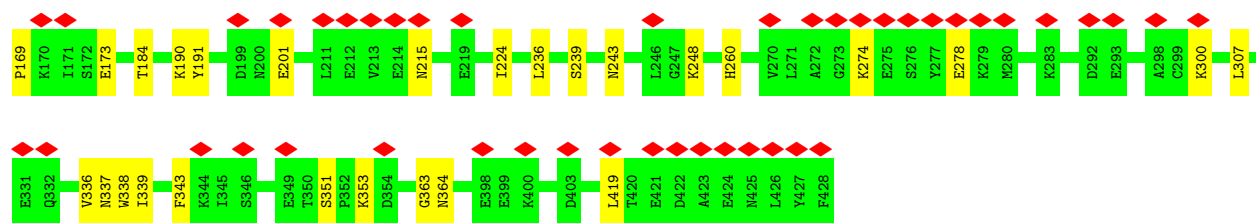


- Molecule 1: Asgard tubulin AtubA with residues from TEV protease cleavage site

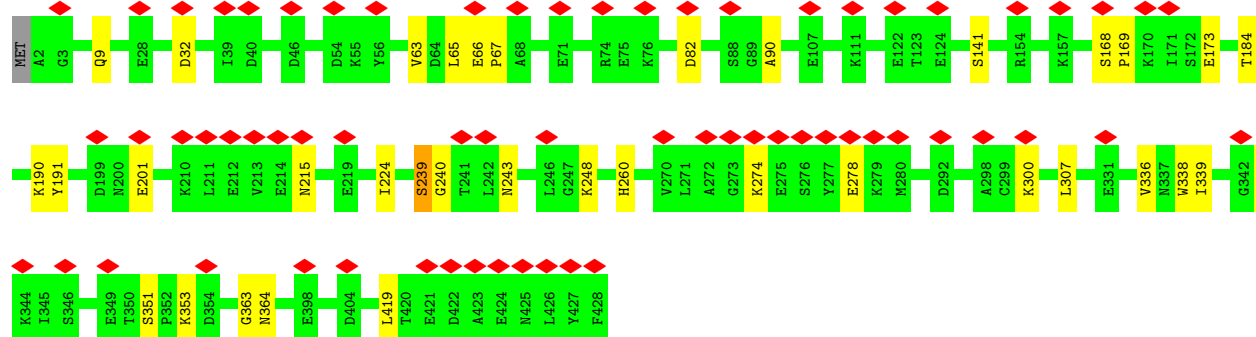
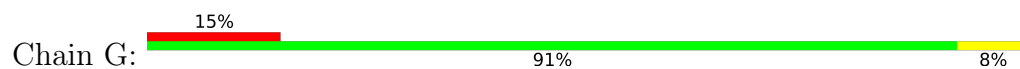


- Molecule 1: Asgard tubulin AtubA with residues from TEV protease cleavage site

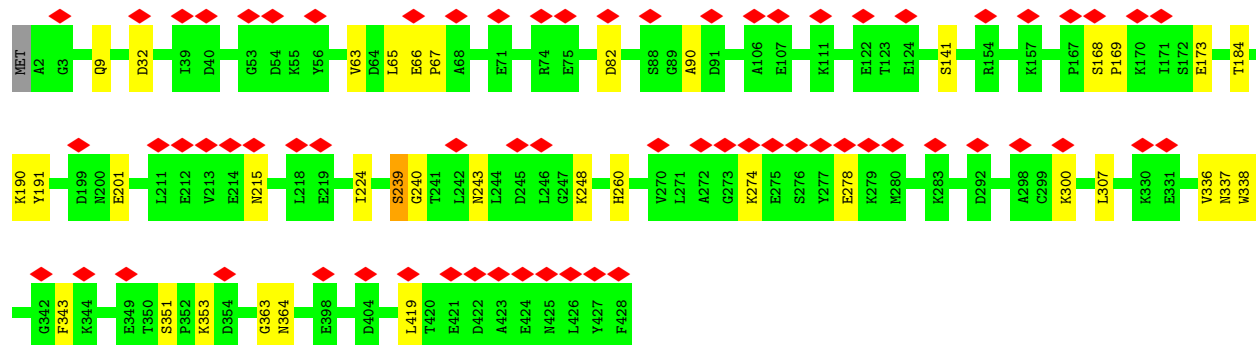
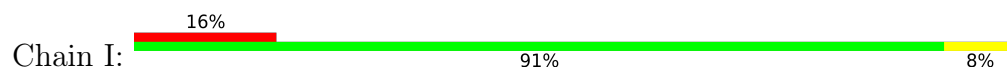




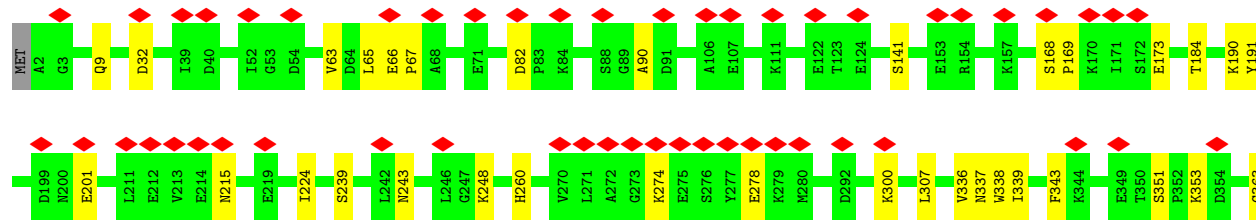
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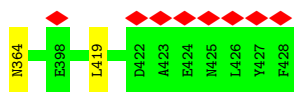


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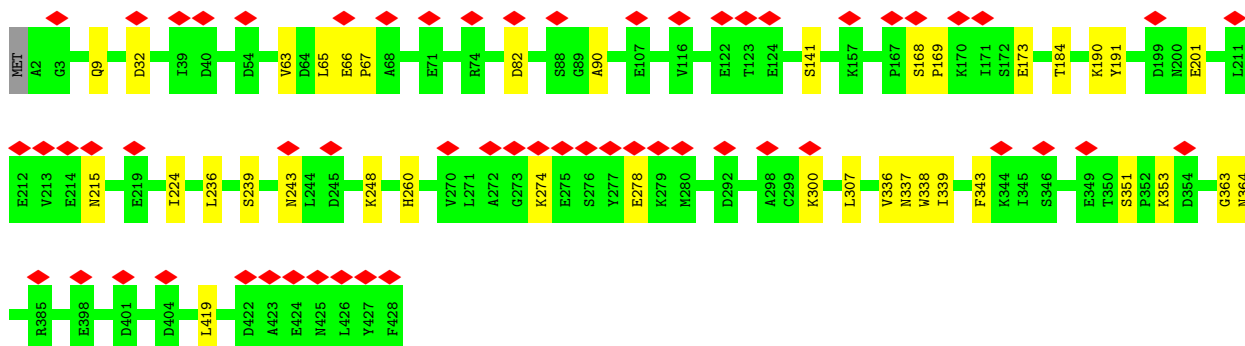
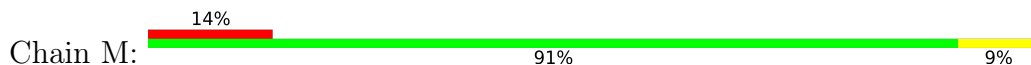


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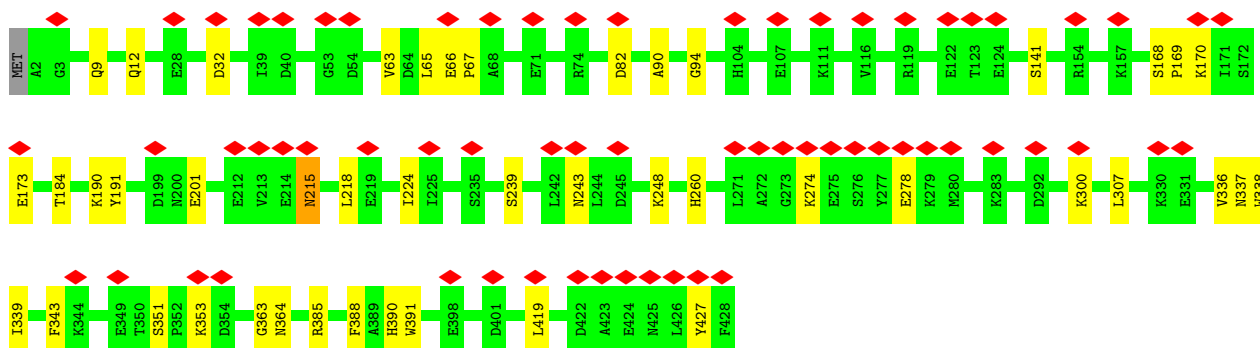
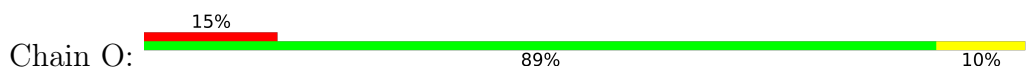




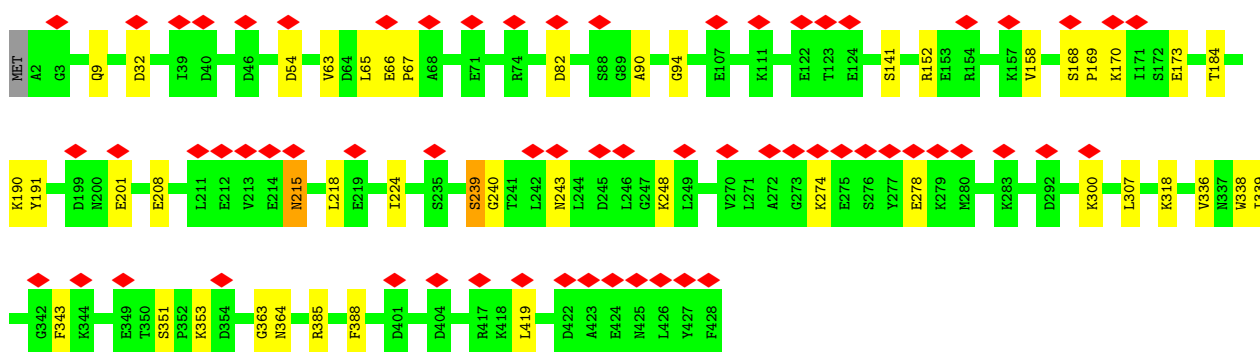
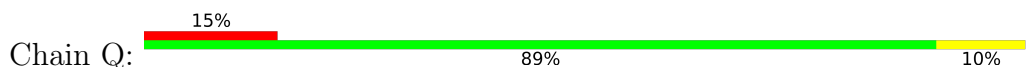
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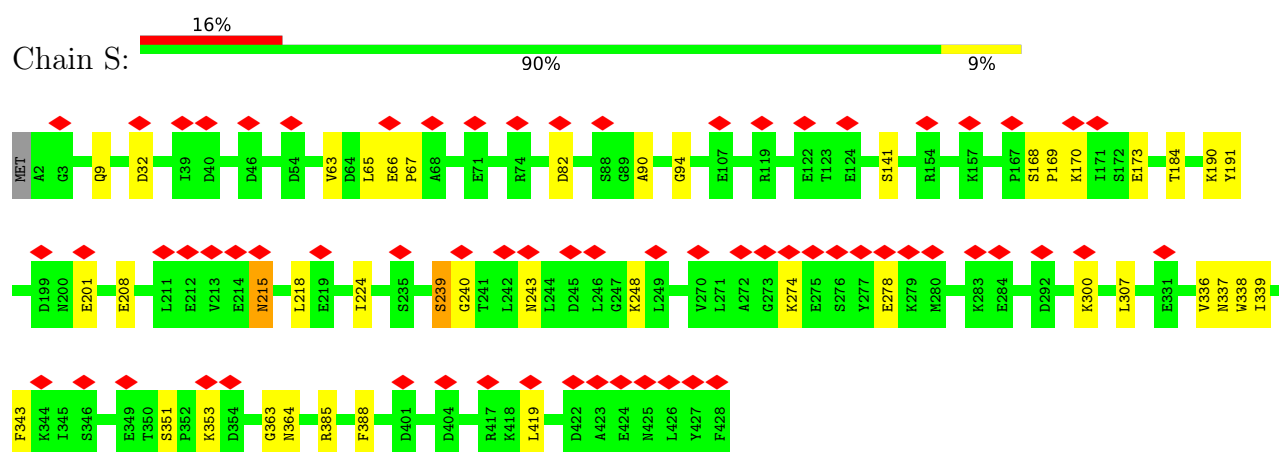
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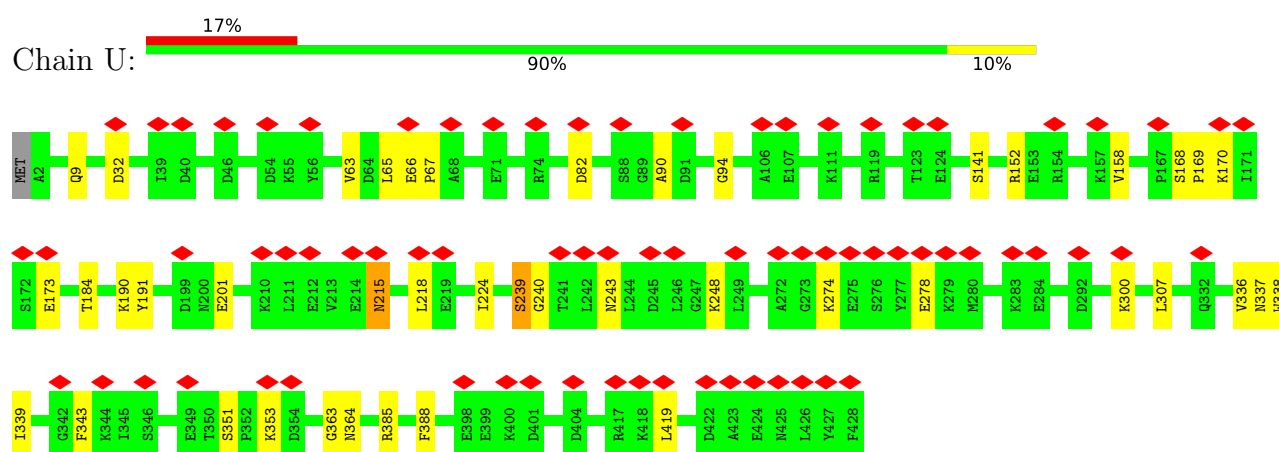
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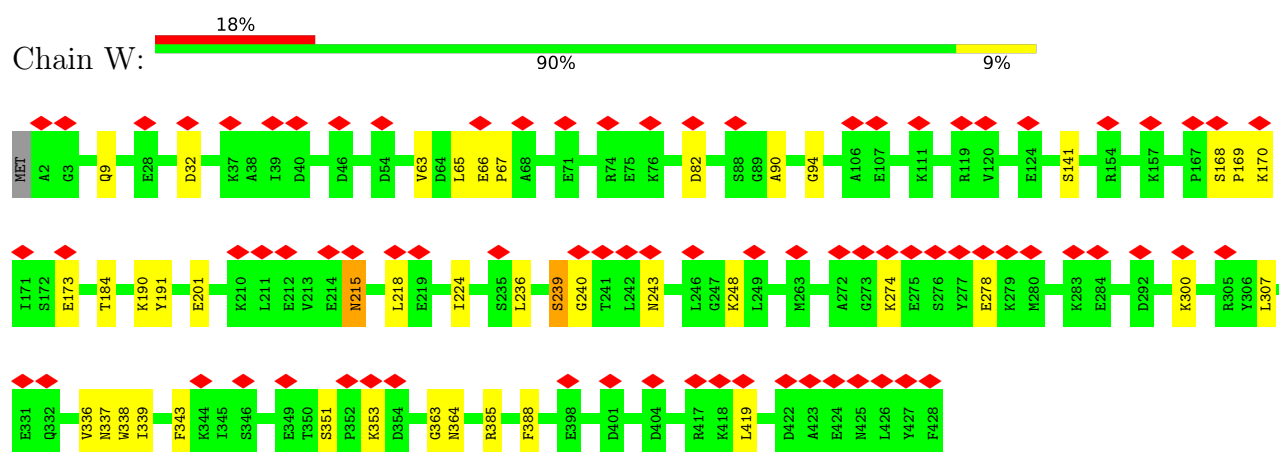
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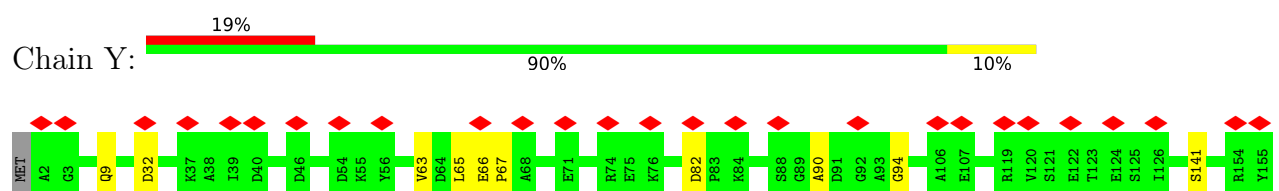
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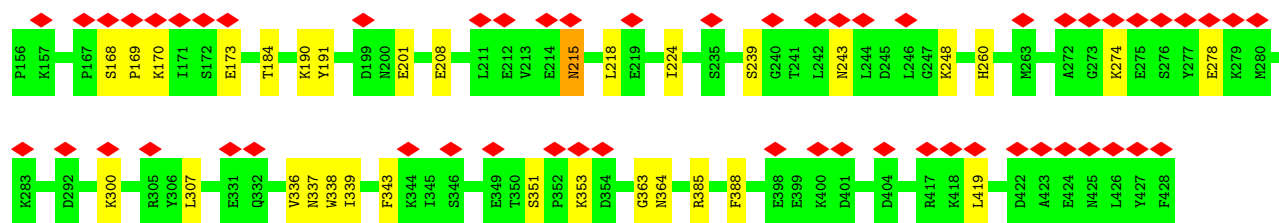


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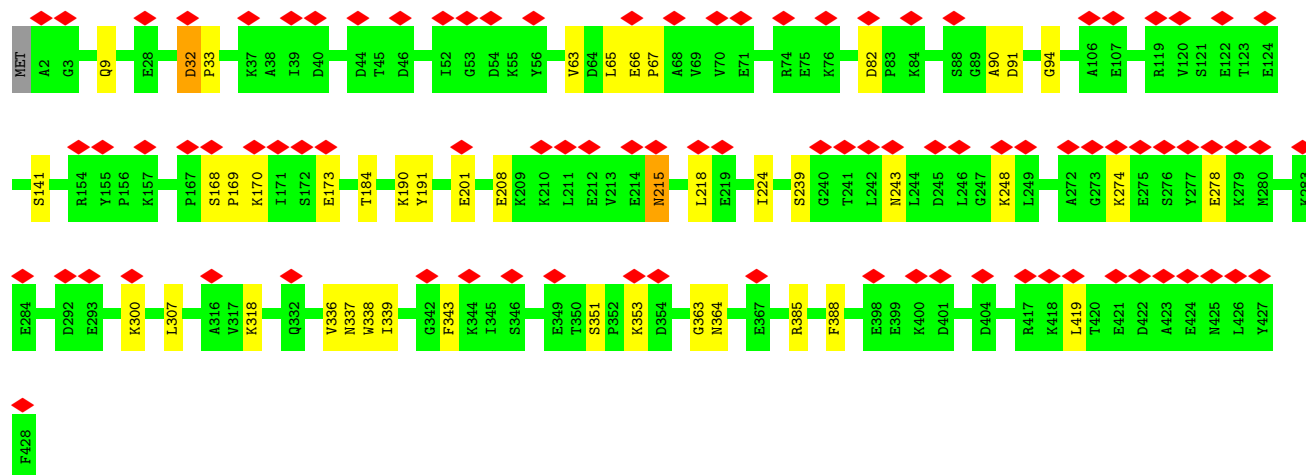
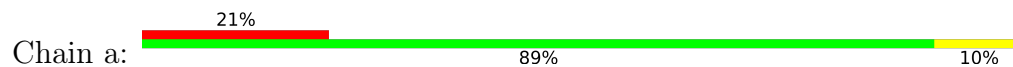


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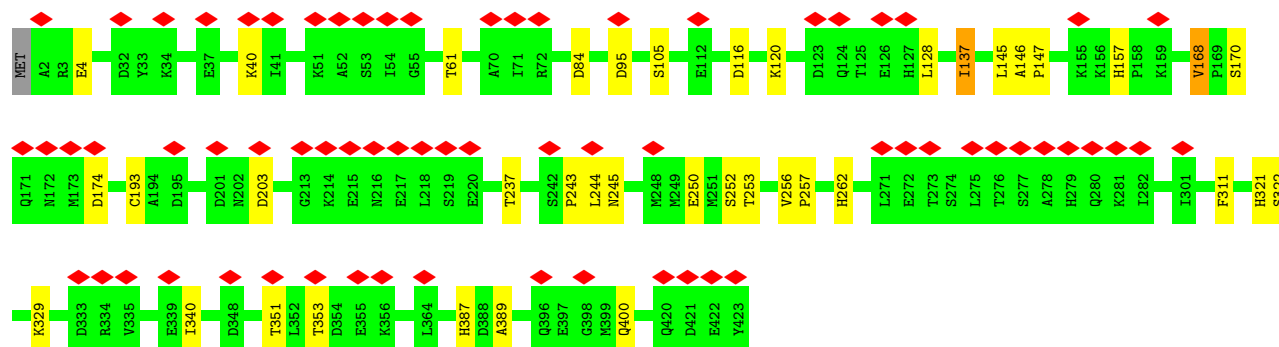




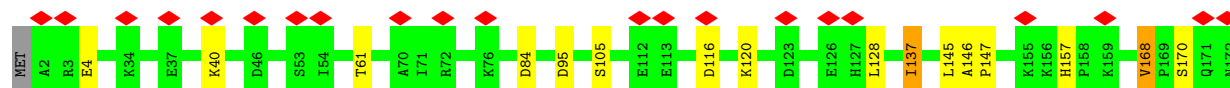
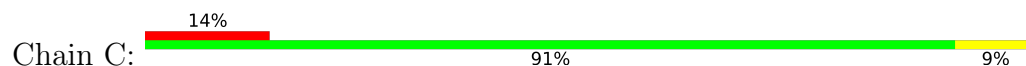
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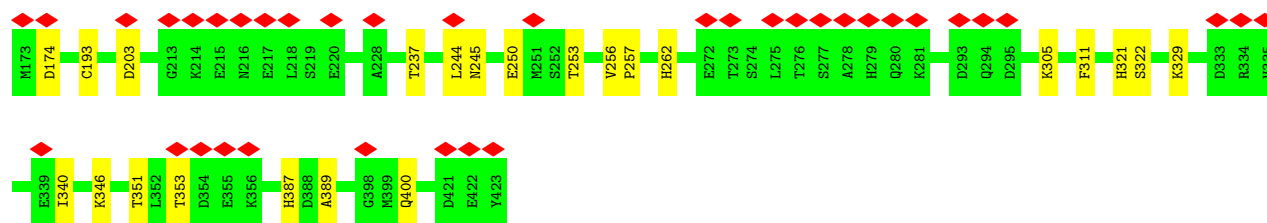


- Molecule 2: Asgard tubulin AtubB2

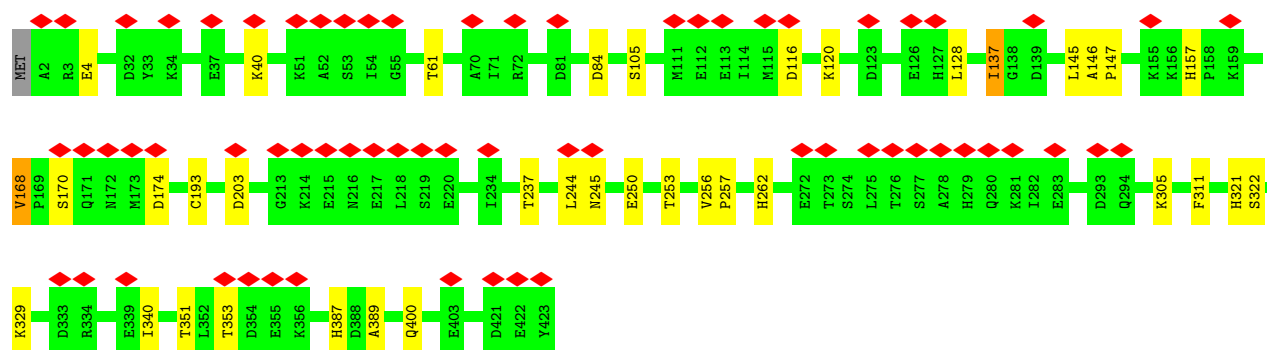
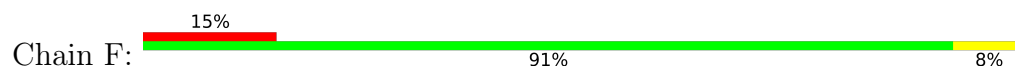


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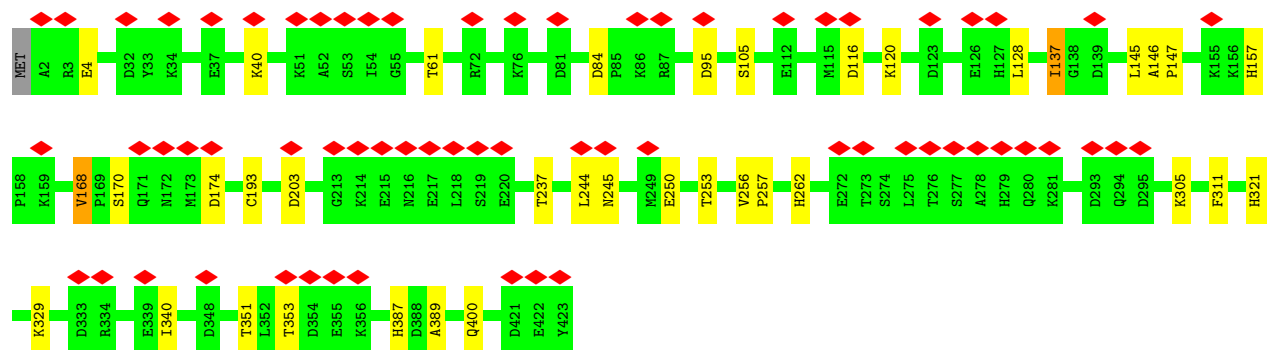
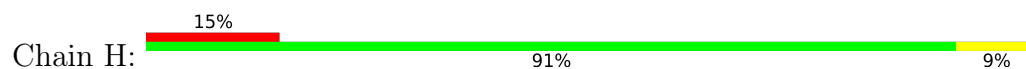




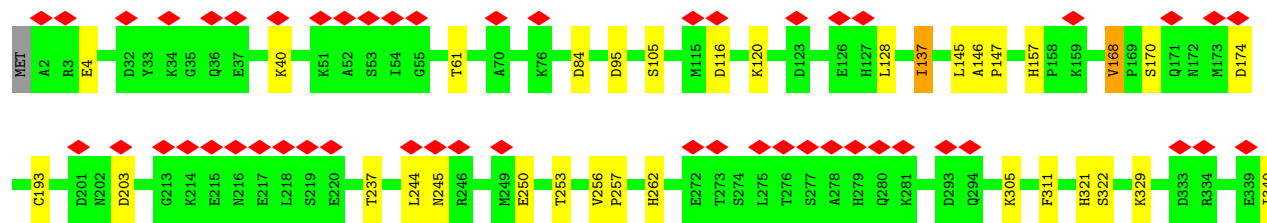
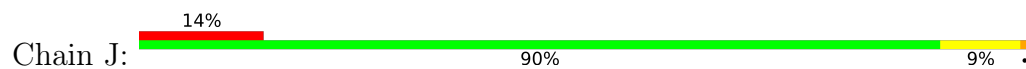
• Molecule 2: Asgard tubulin AtubB2

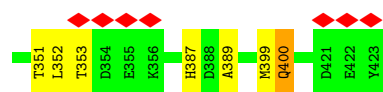


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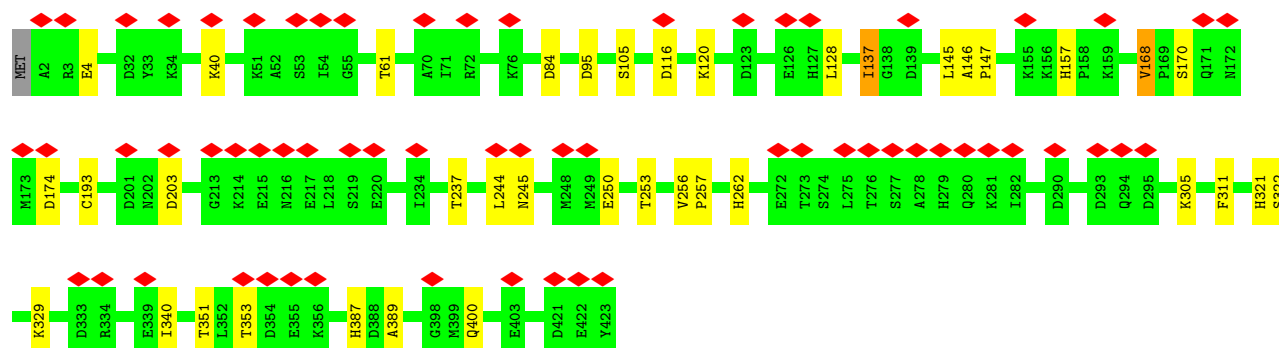


• Molecule 2: Asgard tubulin AtubB2

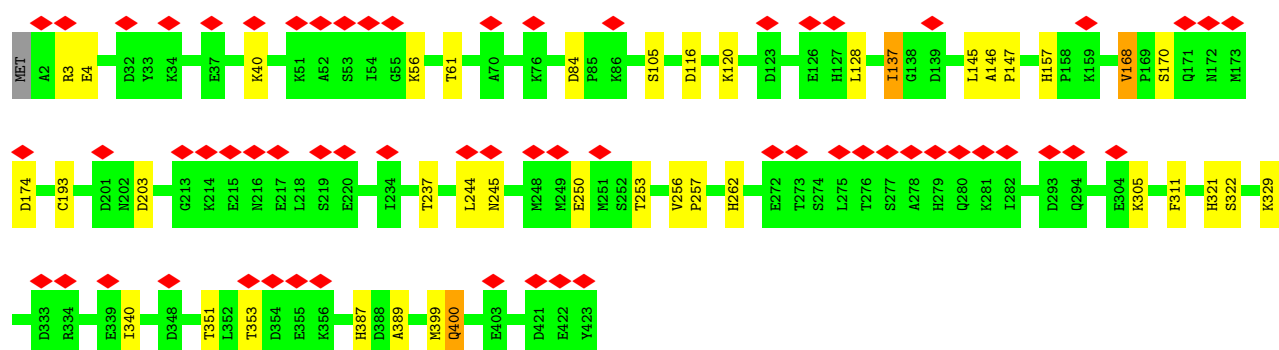
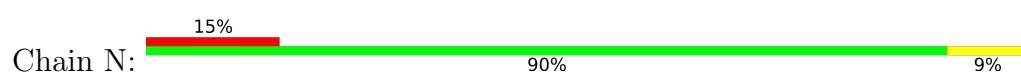




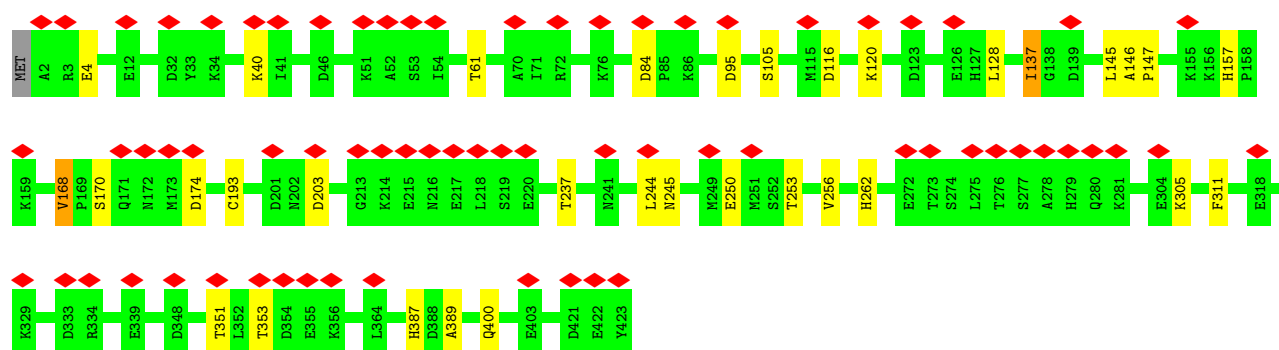
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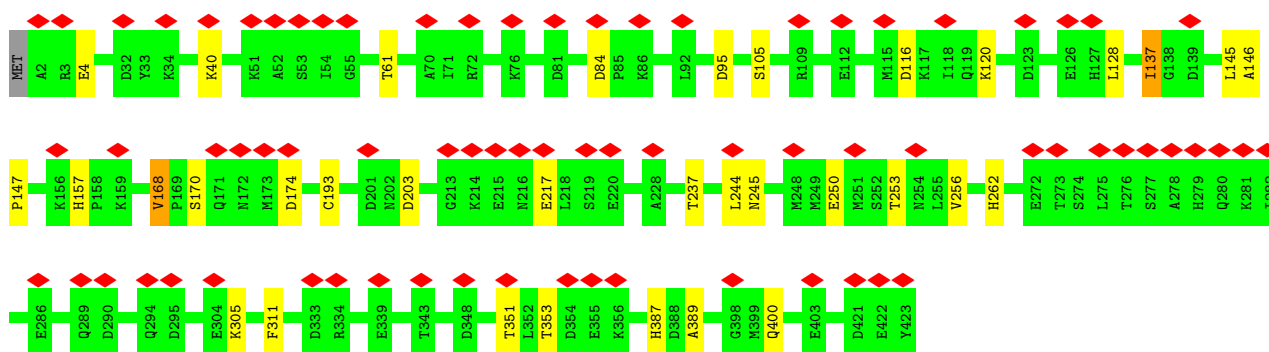
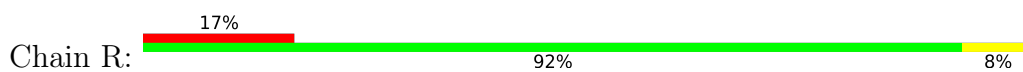
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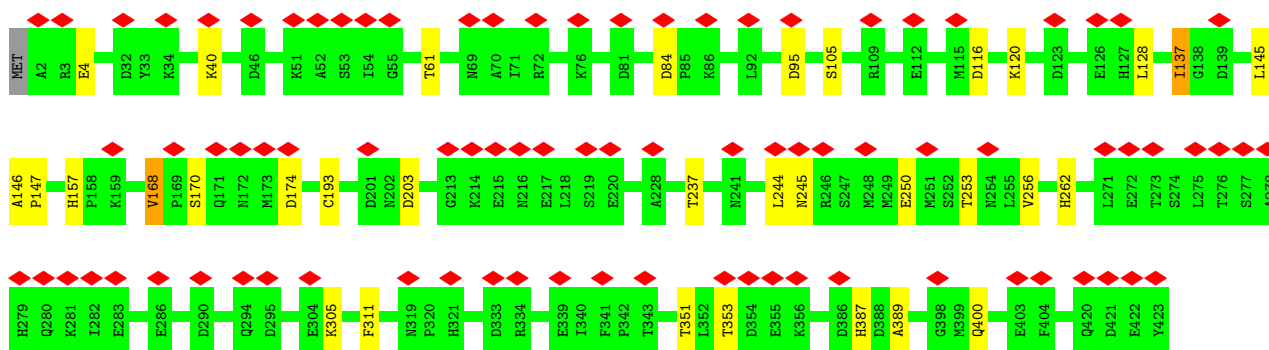
• Molecule 2: Asgard tubulin AtubB2



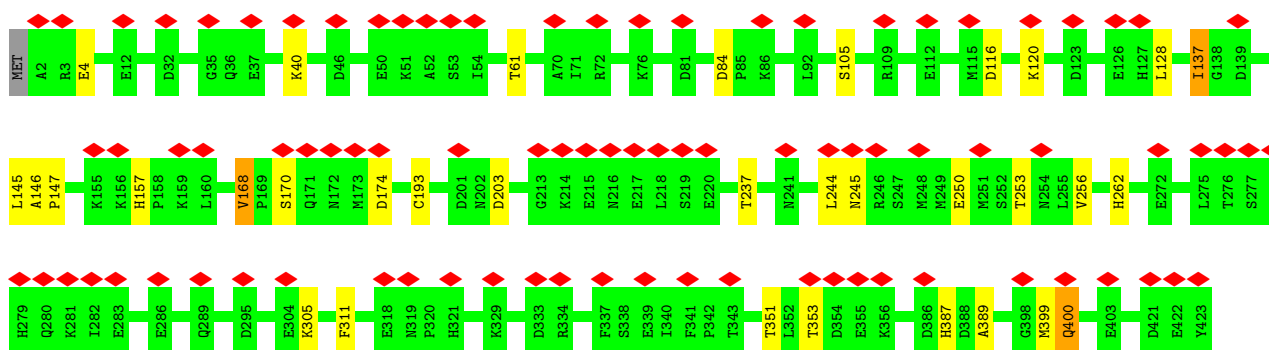
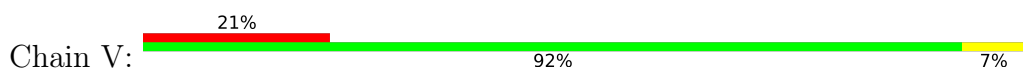
• Molecule 2: Asgard tubulin AtubB2



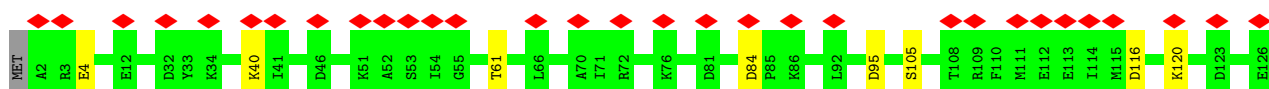
• Molecule 2: Asgard tubulin AtubB2

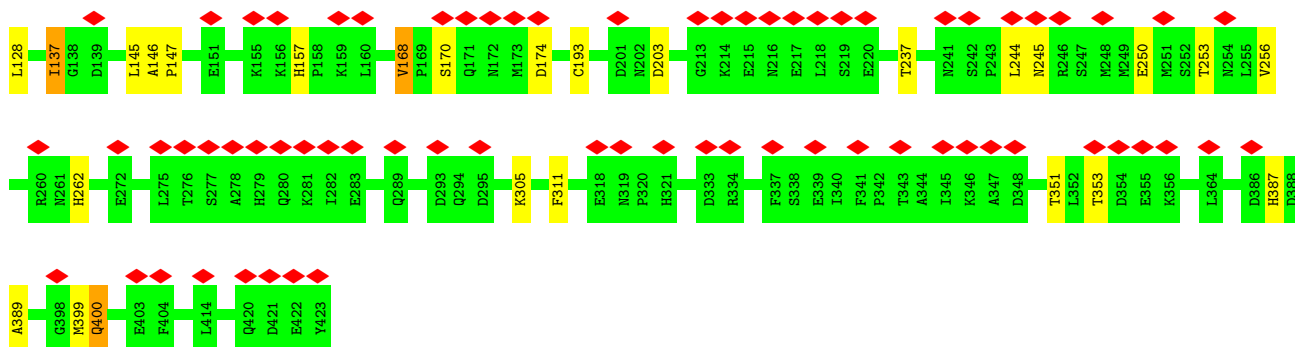


• Molecule 2: Asgard tubulin AtubB2

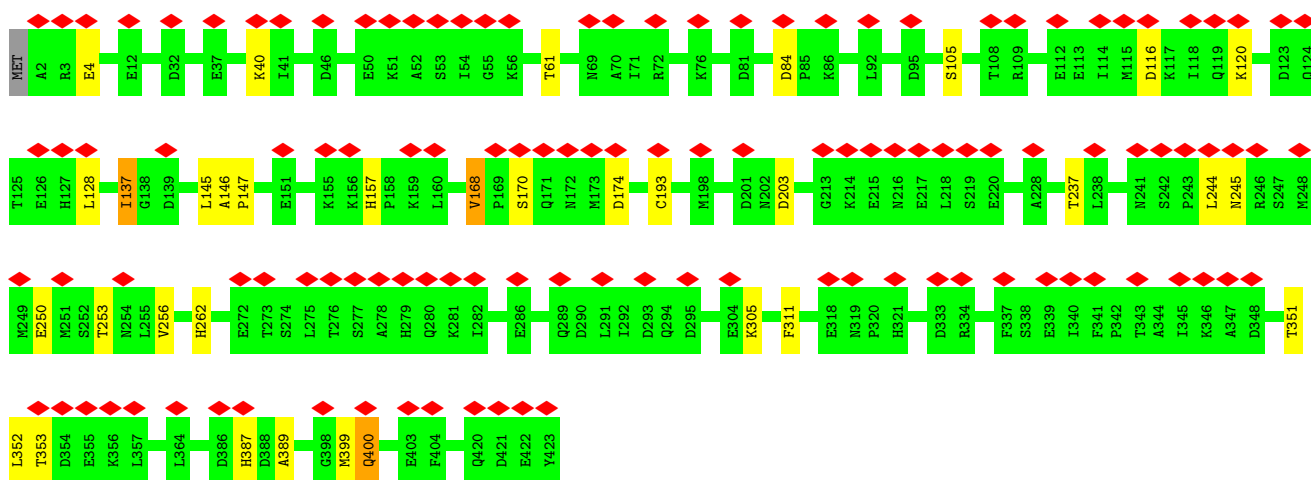


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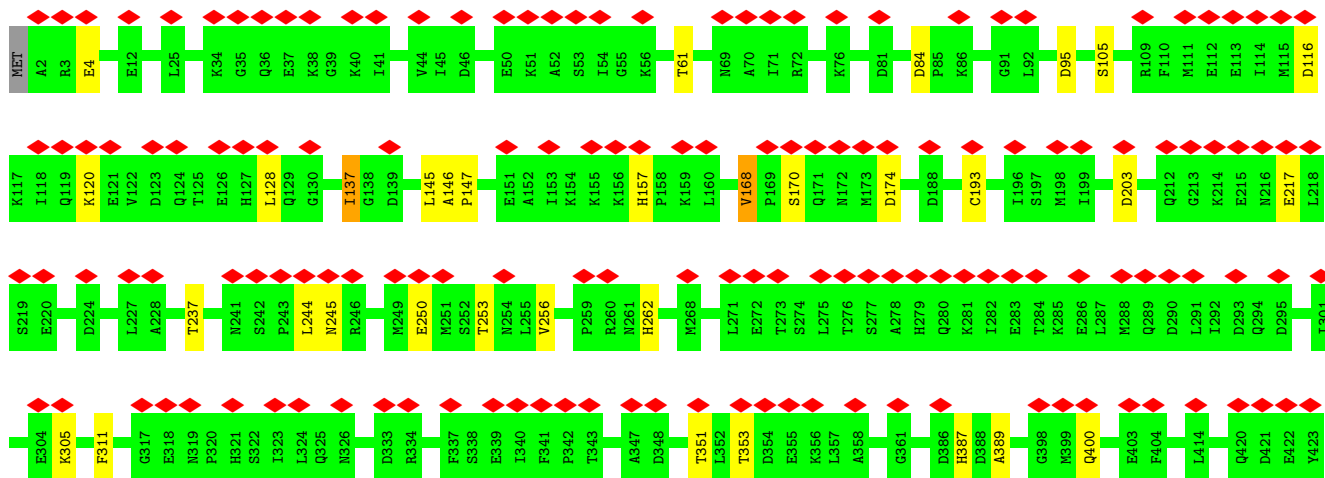




• Molecule 2: Asgard tubulin AtubB2



• Molecule 2: Asgard tubulin AtubB2



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=52.49°, rise=11.73 Å, axial sym=C1	Depositor
Number of segments used	39838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

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: GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	B	1.01	1/3339 (0.0%)	1.22	24/4524 (0.5%)
1	E	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	G	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	I	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	K	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	M	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	O	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	Q	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	S	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	U	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	W	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	Y	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
1	a	1.01	1/3339 (0.0%)	1.22	25/4524 (0.6%)
2	C	1.04	1/3415 (0.0%)	1.25	21/4611 (0.5%)
2	D	1.04	1/3415 (0.0%)	1.25	19/4611 (0.4%)
2	F	1.04	1/3415 (0.0%)	1.25	19/4611 (0.4%)
2	H	1.04	1/3415 (0.0%)	1.25	19/4611 (0.4%)
2	J	1.04	1/3415 (0.0%)	1.25	19/4611 (0.4%)
2	L	1.04	1/3415 (0.0%)	1.25	21/4611 (0.5%)
2	N	1.04	1/3415 (0.0%)	1.25	21/4611 (0.5%)
2	P	1.04	1/3415 (0.0%)	1.25	21/4611 (0.5%)
2	R	1.04	1/3415 (0.0%)	1.25	21/4611 (0.5%)
2	T	1.04	1/3415 (0.0%)	1.25	19/4611 (0.4%)
2	V	1.04	1/3415 (0.0%)	1.25	19/4611 (0.4%)
2	X	1.04	1/3415 (0.0%)	1.25	21/4611 (0.5%)
2	Z	1.04	1/3415 (0.0%)	1.25	21/4611 (0.5%)
2	b	1.04	1/3415 (0.0%)	1.25	19/4611 (0.4%)
All	All	1.02	28/94556 (0.0%)	1.24	629/127890 (0.5%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	364	ASN	CB-CG	-5.63	1.38	1.52
1	O	364	ASN	CB-CG	-5.63	1.38	1.52
1	K	364	ASN	CB-CG	-5.63	1.38	1.52
1	S	364	ASN	CB-CG	-5.63	1.38	1.52
1	Y	364	ASN	CB-CG	-5.63	1.38	1.52
1	B	364	ASN	CB-CG	-5.62	1.38	1.52
1	A	364	ASN	CB-CG	-5.62	1.38	1.52
1	W	364	ASN	CB-CG	-5.61	1.38	1.52
1	M	364	ASN	CB-CG	-5.61	1.38	1.52
1	E	364	ASN	CB-CG	-5.61	1.38	1.52
1	G	364	ASN	CB-CG	-5.61	1.38	1.52
1	Q	364	ASN	CB-CG	-5.60	1.38	1.52
1	U	364	ASN	CB-CG	-5.60	1.38	1.52
1	a	364	ASN	CB-CG	-5.59	1.38	1.52
2	b	262	HIS	CB-CG	-5.22	1.42	1.50
2	P	262	HIS	CB-CG	-5.21	1.42	1.50
2	T	262	HIS	CB-CG	-5.19	1.42	1.50
2	R	262	HIS	CB-CG	-5.18	1.42	1.50
2	H	262	HIS	CB-CG	-5.17	1.43	1.50
2	L	262	HIS	CB-CG	-5.17	1.43	1.50
2	Z	262	HIS	CB-CG	-5.17	1.43	1.50
2	D	262	HIS	CB-CG	-5.16	1.43	1.50
2	C	262	HIS	CB-CG	-5.15	1.43	1.50
2	J	262	HIS	CB-CG	-5.14	1.43	1.50
2	F	262	HIS	CB-CG	-5.14	1.43	1.50
2	X	262	HIS	CB-CG	-5.14	1.43	1.50
2	N	262	HIS	CB-CG	-5.13	1.43	1.50
2	V	262	HIS	CB-CG	-5.12	1.43	1.50

All (629) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	224	ILE	N-CA-C	-7.67	103.45	111.58
1	Y	224	ILE	N-CA-C	-7.67	103.45	111.58
1	U	224	ILE	N-CA-C	-7.65	103.47	111.58
1	K	224	ILE	N-CA-C	-7.65	103.47	111.58
1	G	224	ILE	N-CA-C	-7.64	103.48	111.58
1	B	224	ILE	N-CA-C	-7.63	103.49	111.58
1	A	224	ILE	N-CA-C	-7.63	103.49	111.58
1	I	224	ILE	N-CA-C	-7.63	103.50	111.58
1	Q	224	ILE	N-CA-C	-7.62	103.50	111.58
1	O	224	ILE	N-CA-C	-7.62	103.50	111.58
1	S	224	ILE	N-CA-C	-7.62	103.51	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	224	ILE	N-CA-C	-7.61	103.52	111.58
1	W	224	ILE	N-CA-C	-7.60	103.52	111.58
1	E	224	ILE	N-CA-C	-7.59	103.53	111.58
1	Q	300	LYS	CA-C-N	7.25	127.88	119.47
1	Q	300	LYS	C-N-CA	7.25	127.88	119.47
1	B	300	LYS	CA-C-N	7.24	127.87	119.47
1	B	300	LYS	C-N-CA	7.24	127.87	119.47
1	E	66	GLU	CA-C-N	7.24	126.94	119.56
1	E	66	GLU	C-N-CA	7.24	126.94	119.56
1	S	300	LYS	CA-C-N	7.23	127.85	119.47
1	S	300	LYS	C-N-CA	7.23	127.85	119.47
1	W	300	LYS	CA-C-N	7.23	127.85	119.47
1	W	300	LYS	C-N-CA	7.23	127.85	119.47
1	a	300	LYS	CA-C-N	7.22	127.85	119.47
1	a	300	LYS	C-N-CA	7.22	127.85	119.47
1	a	66	GLU	CA-C-N	7.22	126.92	119.56
1	a	66	GLU	C-N-CA	7.22	126.92	119.56
1	E	300	LYS	CA-C-N	7.21	127.83	119.47
1	E	300	LYS	C-N-CA	7.21	127.83	119.47
1	G	300	LYS	CA-C-N	7.21	127.83	119.47
1	G	300	LYS	C-N-CA	7.21	127.83	119.47
1	M	300	LYS	CA-C-N	7.20	127.83	119.47
1	M	300	LYS	C-N-CA	7.20	127.83	119.47
1	A	300	LYS	CA-C-N	7.20	127.83	119.47
1	A	300	LYS	C-N-CA	7.20	127.83	119.47
1	K	300	LYS	CA-C-N	7.20	127.82	119.47
1	K	300	LYS	C-N-CA	7.20	127.82	119.47
1	I	66	GLU	CA-C-N	7.19	126.89	119.56
1	I	66	GLU	C-N-CA	7.19	126.89	119.56
1	Y	300	LYS	CA-C-N	7.19	127.81	119.47
1	Y	300	LYS	C-N-CA	7.19	127.81	119.47
1	M	66	GLU	CA-C-N	7.18	126.89	119.56
1	M	66	GLU	C-N-CA	7.18	126.89	119.56
1	I	300	LYS	CA-C-N	7.18	127.80	119.47
1	I	300	LYS	C-N-CA	7.18	127.80	119.47
1	U	300	LYS	CA-C-N	7.18	127.80	119.47
1	U	300	LYS	C-N-CA	7.18	127.80	119.47
1	U	66	GLU	CA-C-N	7.18	126.88	119.56
1	U	66	GLU	C-N-CA	7.18	126.88	119.56
1	W	66	GLU	CA-C-N	7.18	126.88	119.56
1	W	66	GLU	C-N-CA	7.18	126.88	119.56
1	A	66	GLU	CA-C-N	7.17	126.88	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GLU	C-N-CA	7.17	126.88	119.56
1	O	66	GLU	CA-C-N	7.16	126.86	119.56
1	O	66	GLU	C-N-CA	7.16	126.86	119.56
1	S	66	GLU	CA-C-N	7.16	126.86	119.56
1	S	66	GLU	C-N-CA	7.16	126.86	119.56
1	G	66	GLU	CA-C-N	7.16	126.86	119.56
1	G	66	GLU	C-N-CA	7.16	126.86	119.56
1	K	66	GLU	CA-C-N	7.16	126.86	119.56
1	K	66	GLU	C-N-CA	7.16	126.86	119.56
1	O	300	LYS	CA-C-N	7.16	127.77	119.47
1	O	300	LYS	C-N-CA	7.16	127.77	119.47
1	Y	66	GLU	CA-C-N	7.15	126.86	119.56
1	Y	66	GLU	C-N-CA	7.15	126.86	119.56
1	Q	66	GLU	CA-C-N	7.13	126.83	119.56
1	Q	66	GLU	C-N-CA	7.13	126.83	119.56
1	B	66	GLU	CA-C-N	7.12	126.83	119.56
1	B	66	GLU	C-N-CA	7.12	126.83	119.56
2	F	256	VAL	N-CA-C	7.06	115.14	108.15
2	b	256	VAL	N-CA-C	7.05	115.14	108.15
2	L	157	HIS	CA-C-N	7.05	126.68	119.56
2	L	157	HIS	C-N-CA	7.05	126.68	119.56
1	O	343	PHE	N-CA-C	7.05	121.07	110.14
1	U	343	PHE	N-CA-C	7.05	121.07	110.14
1	B	343	PHE	N-CA-C	7.05	121.06	110.14
1	K	343	PHE	N-CA-C	7.05	121.06	110.14
2	R	157	HIS	CA-C-N	7.05	126.68	119.56
2	R	157	HIS	C-N-CA	7.05	126.68	119.56
2	X	256	VAL	N-CA-C	7.05	115.13	108.15
1	E	343	PHE	N-CA-C	7.04	121.06	110.14
1	A	343	PHE	N-CA-C	7.03	121.04	110.14
2	D	256	VAL	N-CA-C	7.03	115.11	108.15
1	I	343	PHE	N-CA-C	7.03	121.04	110.14
2	J	256	VAL	N-CA-C	7.03	115.11	108.15
2	N	256	VAL	N-CA-C	7.03	115.11	108.15
2	P	256	VAL	N-CA-C	7.03	115.11	108.15
1	Q	343	PHE	N-CA-C	7.03	121.03	110.14
2	H	256	VAL	N-CA-C	7.03	115.11	108.15
2	L	256	VAL	N-CA-C	7.03	115.11	108.15
1	Y	343	PHE	N-CA-C	7.03	121.03	110.14
1	G	343	PHE	N-CA-C	7.03	121.03	110.14
2	R	256	VAL	N-CA-C	7.03	115.11	108.15
1	M	343	PHE	N-CA-C	7.02	121.03	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	343	PHE	N-CA-C	7.02	121.02	110.14
2	C	256	VAL	N-CA-C	7.02	115.10	108.15
1	W	343	PHE	N-CA-C	7.02	121.02	110.14
2	J	157	HIS	CA-C-N	7.01	126.64	119.56
2	J	157	HIS	C-N-CA	7.01	126.64	119.56
2	Z	157	HIS	CA-C-N	7.01	126.64	119.56
2	Z	157	HIS	C-N-CA	7.01	126.64	119.56
1	a	343	PHE	N-CA-C	7.01	121.01	110.14
2	F	157	HIS	CA-C-N	7.01	126.64	119.56
2	F	157	HIS	C-N-CA	7.01	126.64	119.56
2	V	256	VAL	N-CA-C	7.01	115.09	108.15
2	Z	256	VAL	N-CA-C	7.01	115.09	108.15
2	X	157	HIS	CA-C-N	7.00	126.63	119.56
2	X	157	HIS	C-N-CA	7.00	126.63	119.56
2	D	157	HIS	CA-C-N	6.99	126.62	119.56
2	D	157	HIS	C-N-CA	6.99	126.62	119.56
2	T	256	VAL	N-CA-C	6.99	115.07	108.15
2	H	157	HIS	CA-C-N	6.99	126.62	119.56
2	H	157	HIS	C-N-CA	6.99	126.62	119.56
2	N	157	HIS	CA-C-N	6.99	126.62	119.56
2	N	157	HIS	C-N-CA	6.99	126.62	119.56
2	T	157	HIS	CA-C-N	6.98	126.61	119.56
2	T	157	HIS	C-N-CA	6.98	126.61	119.56
2	b	157	HIS	CA-C-N	6.98	126.61	119.56
2	b	157	HIS	C-N-CA	6.98	126.61	119.56
2	P	157	HIS	CA-C-N	6.98	126.61	119.56
2	P	157	HIS	C-N-CA	6.98	126.61	119.56
2	V	157	HIS	CA-C-N	6.95	126.58	119.56
2	V	157	HIS	C-N-CA	6.95	126.58	119.56
2	C	157	HIS	CA-C-N	6.94	126.57	119.56
2	C	157	HIS	C-N-CA	6.94	126.57	119.56
1	W	239	SER	CB-CA-C	-6.84	108.67	116.54
1	a	239	SER	CB-CA-C	-6.84	108.68	116.54
1	U	239	SER	CB-CA-C	-6.83	108.68	116.54
1	G	239	SER	CB-CA-C	-6.83	108.69	116.54
1	K	239	SER	CB-CA-C	-6.83	108.69	116.54
1	Y	239	SER	CB-CA-C	-6.82	108.69	116.54
1	A	239	SER	CB-CA-C	-6.82	108.70	116.54
1	M	239	SER	CB-CA-C	-6.81	108.70	116.54
1	B	239	SER	CB-CA-C	-6.81	108.71	116.54
1	S	239	SER	CB-CA-C	-6.81	108.71	116.54
1	E	239	SER	CB-CA-C	-6.81	108.71	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	239	SER	CB-CA-C	-6.80	108.72	116.54
1	Q	239	SER	CB-CA-C	-6.80	108.72	116.54
1	O	239	SER	CB-CA-C	-6.78	108.75	116.54
1	E	32	ASP	CA-C-N	6.42	126.11	119.56
1	E	32	ASP	C-N-CA	6.42	126.11	119.56
1	K	32	ASP	CA-C-N	6.41	126.10	119.56
1	K	32	ASP	C-N-CA	6.41	126.10	119.56
1	W	32	ASP	CA-C-N	6.40	126.09	119.56
1	W	32	ASP	C-N-CA	6.40	126.09	119.56
1	Q	32	ASP	CA-C-N	6.39	126.08	119.56
1	Q	32	ASP	C-N-CA	6.39	126.08	119.56
1	A	32	ASP	CA-C-N	6.39	126.07	119.56
1	A	32	ASP	C-N-CA	6.39	126.07	119.56
1	B	32	ASP	CA-C-N	6.39	126.07	119.56
1	B	32	ASP	C-N-CA	6.39	126.07	119.56
1	M	32	ASP	CA-C-N	6.38	126.07	119.56
1	M	32	ASP	C-N-CA	6.38	126.07	119.56
1	Y	32	ASP	CA-C-N	6.38	126.06	119.56
1	Y	32	ASP	C-N-CA	6.38	126.06	119.56
1	G	32	ASP	CA-C-N	6.37	126.06	119.56
1	G	32	ASP	C-N-CA	6.37	126.06	119.56
1	a	32	ASP	CA-C-N	6.37	126.06	119.56
1	a	32	ASP	C-N-CA	6.37	126.06	119.56
1	O	32	ASP	CA-C-N	6.36	126.05	119.56
1	O	32	ASP	C-N-CA	6.36	126.05	119.56
1	U	32	ASP	CA-C-N	6.36	126.04	119.56
1	U	32	ASP	C-N-CA	6.36	126.04	119.56
1	S	32	ASP	CA-C-N	6.35	126.04	119.56
1	S	32	ASP	C-N-CA	6.35	126.04	119.56
1	I	32	ASP	CA-C-N	6.35	126.04	119.56
1	I	32	ASP	C-N-CA	6.35	126.04	119.56
1	K	63	VAL	N-CA-C	6.30	116.93	108.11
1	O	63	VAL	N-CA-C	6.30	116.93	108.11
1	I	63	VAL	N-CA-C	6.29	116.92	108.11
1	B	65	LEU	N-CA-C	-6.29	105.37	114.12
2	F	137	ILE	N-CA-C	-6.29	106.19	112.17
1	S	63	VAL	N-CA-C	6.28	116.91	108.11
1	E	65	LEU	N-CA-C	-6.28	105.39	114.12
1	G	63	VAL	N-CA-C	6.28	116.90	108.11
1	M	63	VAL	N-CA-C	6.28	116.90	108.11
1	M	65	LEU	N-CA-C	-6.28	105.40	114.12
1	Y	63	VAL	N-CA-C	6.28	116.89	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	65	LEU	N-CA-C	-6.27	105.40	114.12
1	A	63	VAL	N-CA-C	6.27	116.89	108.11
1	Q	63	VAL	N-CA-C	6.27	116.89	108.11
1	O	65	LEU	N-CA-C	-6.27	105.40	114.12
2	J	137	ILE	N-CA-C	-6.27	106.21	112.17
1	U	63	VAL	N-CA-C	6.27	116.88	108.11
1	a	63	VAL	N-CA-C	6.27	116.89	108.11
2	P	137	ILE	N-CA-C	-6.26	106.22	112.17
1	A	65	LEU	N-CA-C	-6.26	105.42	114.12
1	E	63	VAL	N-CA-C	6.26	116.88	108.11
1	K	65	LEU	N-CA-C	-6.26	105.42	114.12
1	Y	65	LEU	N-CA-C	-6.26	105.42	114.12
1	B	63	VAL	N-CA-C	6.26	116.87	108.11
1	W	63	VAL	N-CA-C	6.25	116.86	108.11
1	W	65	LEU	N-CA-C	-6.25	105.43	114.12
2	Z	137	ILE	N-CA-C	-6.25	106.23	112.17
2	C	137	ILE	N-CA-C	-6.25	106.23	112.17
1	G	65	LEU	N-CA-C	-6.25	105.44	114.12
1	Q	65	LEU	N-CA-C	-6.25	105.43	114.12
1	S	65	LEU	N-CA-C	-6.25	105.44	114.12
2	L	137	ILE	N-CA-C	-6.25	106.23	112.17
2	V	137	ILE	N-CA-C	-6.25	106.23	112.17
1	a	65	LEU	N-CA-C	-6.25	105.44	114.12
1	I	65	LEU	N-CA-C	-6.24	105.45	114.12
2	D	137	ILE	N-CA-C	-6.24	106.25	112.17
2	N	137	ILE	N-CA-C	-6.23	106.25	112.17
2	R	137	ILE	N-CA-C	-6.22	106.26	112.17
2	b	137	ILE	N-CA-C	-6.22	106.26	112.17
2	T	137	ILE	N-CA-C	-6.21	106.27	112.17
2	H	137	ILE	N-CA-C	-6.19	106.29	112.17
2	Z	174	ASP	CA-CB-CG	6.18	118.78	112.60
2	X	137	ILE	N-CA-C	-6.18	106.30	112.17
2	V	174	ASP	CA-CB-CG	6.18	118.78	112.60
1	W	353	LYS	N-CA-C	6.18	118.81	111.71
1	B	353	LYS	N-CA-C	6.17	118.81	111.71
2	J	174	ASP	CA-CB-CG	6.17	118.77	112.60
1	I	353	LYS	N-CA-C	6.16	118.79	111.71
1	K	353	LYS	N-CA-C	6.15	118.79	111.71
1	O	353	LYS	N-CA-C	6.15	118.78	111.71
2	P	174	ASP	CA-CB-CG	6.15	118.75	112.60
1	E	353	LYS	N-CA-C	6.14	118.77	111.71
1	G	353	LYS	N-CA-C	6.14	118.78	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	353	LYS	N-CA-C	6.14	118.77	111.71
1	A	353	LYS	N-CA-C	6.14	118.77	111.71
2	R	174	ASP	CA-CB-CG	6.14	118.74	112.60
2	D	174	ASP	CA-CB-CG	6.14	118.74	112.60
1	S	353	LYS	N-CA-C	6.13	118.76	111.71
2	T	174	ASP	CA-CB-CG	6.13	118.73	112.60
2	X	174	ASP	CA-CB-CG	6.13	118.73	112.60
1	M	353	LYS	N-CA-C	6.13	118.76	111.71
2	F	168	VAL	CA-C-N	6.12	126.09	119.78
2	F	168	VAL	C-N-CA	6.12	126.09	119.78
2	L	174	ASP	CA-CB-CG	6.12	118.72	112.60
2	N	174	ASP	CA-CB-CG	6.12	118.72	112.60
1	Y	353	LYS	N-CA-C	6.12	118.75	111.71
2	b	174	ASP	CA-CB-CG	6.12	118.72	112.60
2	H	174	ASP	CA-CB-CG	6.11	118.71	112.60
2	R	168	VAL	CA-C-N	6.11	126.07	119.78
2	R	168	VAL	C-N-CA	6.11	126.07	119.78
1	a	353	LYS	N-CA-C	6.11	118.73	111.71
2	X	168	VAL	CA-C-N	6.10	126.07	119.78
2	X	168	VAL	C-N-CA	6.10	126.07	119.78
1	Q	353	LYS	N-CA-C	6.10	118.73	111.71
2	b	168	VAL	CA-C-N	6.10	126.06	119.78
2	b	168	VAL	C-N-CA	6.10	126.06	119.78
2	H	168	VAL	CA-C-N	6.10	126.06	119.78
2	H	168	VAL	C-N-CA	6.10	126.06	119.78
2	C	168	VAL	CA-C-N	6.10	126.06	119.78
2	C	168	VAL	C-N-CA	6.10	126.06	119.78
2	C	174	ASP	CA-CB-CG	6.10	118.70	112.60
2	Z	168	VAL	CA-C-N	6.09	126.05	119.78
2	Z	168	VAL	C-N-CA	6.09	126.05	119.78
2	D	168	VAL	CA-C-N	6.08	126.05	119.78
2	D	168	VAL	C-N-CA	6.08	126.05	119.78
2	F	174	ASP	CA-CB-CG	6.07	118.67	112.60
2	N	168	VAL	CA-C-N	6.06	126.02	119.78
2	N	168	VAL	C-N-CA	6.06	126.02	119.78
2	V	168	VAL	CA-C-N	6.06	126.02	119.78
2	V	168	VAL	C-N-CA	6.06	126.02	119.78
2	T	168	VAL	CA-C-N	6.06	126.02	119.78
2	T	168	VAL	C-N-CA	6.06	126.02	119.78
2	P	168	VAL	CA-C-N	6.05	126.01	119.78
2	P	168	VAL	C-N-CA	6.05	126.01	119.78
2	L	168	VAL	CA-C-N	6.05	126.01	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	168	VAL	C-N-CA	6.05	126.01	119.78
2	J	168	VAL	CA-C-N	6.04	126.00	119.78
2	J	168	VAL	C-N-CA	6.04	126.00	119.78
2	J	61	THR	N-CA-C	5.94	118.31	108.99
2	X	61	THR	N-CA-C	5.93	118.30	108.99
2	F	61	THR	N-CA-C	5.93	118.29	108.99
2	Z	61	THR	N-CA-C	5.92	118.28	108.99
2	H	61	THR	N-CA-C	5.92	118.28	108.99
2	C	61	THR	N-CA-C	5.91	118.28	108.99
2	V	61	THR	N-CA-C	5.91	118.28	108.99
2	b	61	THR	N-CA-C	5.91	118.27	108.99
2	D	61	THR	N-CA-C	5.91	118.27	108.99
2	L	61	THR	N-CA-C	5.91	118.26	108.99
2	R	61	THR	N-CA-C	5.91	118.26	108.99
2	P	61	THR	N-CA-C	5.90	118.25	108.99
2	N	61	THR	N-CA-C	5.89	118.24	108.99
2	T	61	THR	N-CA-C	5.88	118.22	108.99
2	Z	84	ASP	CA-C-N	5.70	125.37	119.56
2	Z	84	ASP	C-N-CA	5.70	125.37	119.56
2	J	84	ASP	CA-C-N	5.67	125.35	119.56
2	J	84	ASP	C-N-CA	5.67	125.35	119.56
2	X	84	ASP	CA-C-N	5.67	125.34	119.56
2	X	84	ASP	C-N-CA	5.67	125.34	119.56
2	R	84	ASP	CA-C-N	5.67	125.34	119.56
2	R	84	ASP	C-N-CA	5.67	125.34	119.56
2	T	84	ASP	CA-C-N	5.67	125.34	119.56
2	T	84	ASP	C-N-CA	5.67	125.34	119.56
2	V	84	ASP	CA-C-N	5.66	125.33	119.56
2	V	84	ASP	C-N-CA	5.66	125.33	119.56
2	N	84	ASP	CA-C-N	5.66	125.33	119.56
2	N	84	ASP	C-N-CA	5.66	125.33	119.56
2	D	84	ASP	CA-C-N	5.65	125.33	119.56
2	D	84	ASP	C-N-CA	5.65	125.33	119.56
2	F	84	ASP	CA-C-N	5.65	125.32	119.56
2	F	84	ASP	C-N-CA	5.65	125.32	119.56
2	b	84	ASP	CA-C-N	5.65	125.32	119.56
2	b	84	ASP	C-N-CA	5.65	125.32	119.56
2	C	84	ASP	CA-C-N	5.64	125.32	119.56
2	C	84	ASP	C-N-CA	5.64	125.32	119.56
1	S	248	LYS	N-CA-C	-5.64	104.75	111.69
2	L	84	ASP	CA-C-N	5.64	125.31	119.56
2	L	84	ASP	C-N-CA	5.64	125.31	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	84	ASP	CA-C-N	5.64	125.31	119.56
2	H	84	ASP	C-N-CA	5.64	125.31	119.56
1	I	248	LYS	N-CA-C	-5.63	104.76	111.69
1	Y	248	LYS	N-CA-C	-5.63	104.76	111.69
1	O	248	LYS	N-CA-C	-5.63	104.77	111.69
1	W	248	LYS	N-CA-C	-5.63	104.77	111.69
2	P	84	ASP	CA-C-N	5.63	125.30	119.56
2	P	84	ASP	C-N-CA	5.63	125.30	119.56
1	a	248	LYS	N-CA-C	-5.63	104.77	111.69
1	Q	248	LYS	N-CA-C	-5.63	104.77	111.69
1	A	248	LYS	N-CA-C	-5.62	104.77	111.69
1	G	248	LYS	N-CA-C	-5.62	104.78	111.69
1	K	248	LYS	N-CA-C	-5.61	104.79	111.69
1	U	248	LYS	N-CA-C	-5.61	104.79	111.69
1	B	248	LYS	N-CA-C	-5.61	104.79	111.69
1	M	248	LYS	N-CA-C	-5.60	104.80	111.69
1	E	248	LYS	N-CA-C	-5.60	104.81	111.69
2	b	311	PHE	CA-CB-CG	5.57	119.37	113.80
2	R	311	PHE	CA-CB-CG	5.55	119.35	113.80
2	X	311	PHE	CA-CB-CG	5.55	119.35	113.80
2	b	400	GLN	CA-C-N	5.54	125.90	119.47
2	b	400	GLN	C-N-CA	5.54	125.90	119.47
2	F	311	PHE	CA-CB-CG	5.54	119.34	113.80
2	V	311	PHE	CA-CB-CG	5.54	119.34	113.80
2	T	311	PHE	CA-CB-CG	5.53	119.33	113.80
2	N	400	GLN	CA-C-N	5.53	125.88	119.47
2	N	400	GLN	C-N-CA	5.53	125.88	119.47
2	F	400	GLN	CA-C-N	5.53	125.88	119.47
2	F	400	GLN	C-N-CA	5.53	125.88	119.47
2	Z	400	GLN	CA-C-N	5.53	125.88	119.47
2	Z	400	GLN	C-N-CA	5.53	125.88	119.47
2	T	400	GLN	CA-C-N	5.53	125.88	119.47
2	T	400	GLN	C-N-CA	5.53	125.88	119.47
2	D	311	PHE	CA-CB-CG	5.52	119.32	113.80
2	R	400	GLN	CA-C-N	5.52	125.88	119.47
2	R	400	GLN	C-N-CA	5.52	125.88	119.47
2	Z	311	PHE	CA-CB-CG	5.52	119.32	113.80
2	D	400	GLN	CA-C-N	5.51	125.87	119.47
2	D	400	GLN	C-N-CA	5.51	125.87	119.47
2	P	311	PHE	CA-CB-CG	5.51	119.31	113.80
2	V	400	GLN	CA-C-N	5.51	125.86	119.47
2	V	400	GLN	C-N-CA	5.51	125.86	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	311	PHE	CA-CB-CG	5.51	119.31	113.80
2	L	311	PHE	CA-CB-CG	5.51	119.31	113.80
2	C	311	PHE	CA-CB-CG	5.50	119.30	113.80
2	J	311	PHE	CA-CB-CG	5.50	119.30	113.80
2	F	351	THR	N-CA-C	5.50	118.21	109.96
2	H	400	GLN	CA-C-N	5.50	125.85	119.47
2	H	400	GLN	C-N-CA	5.50	125.85	119.47
2	R	105	SER	N-CA-C	5.49	120.11	113.41
2	C	351	THR	N-CA-C	5.49	118.19	109.96
2	N	311	PHE	CA-CB-CG	5.49	119.29	113.80
2	P	400	GLN	CA-C-N	5.49	125.84	119.47
2	P	400	GLN	C-N-CA	5.49	125.84	119.47
2	L	400	GLN	CA-C-N	5.49	125.84	119.47
2	L	400	GLN	C-N-CA	5.49	125.84	119.47
2	P	351	THR	N-CA-C	5.49	118.19	109.96
2	J	400	GLN	CA-C-N	5.49	125.83	119.47
2	J	400	GLN	C-N-CA	5.49	125.83	119.47
2	N	351	THR	N-CA-C	5.48	118.18	109.96
2	C	400	GLN	CA-C-N	5.48	125.83	119.47
2	C	400	GLN	C-N-CA	5.48	125.83	119.47
2	D	351	THR	N-CA-C	5.48	118.18	109.96
2	V	351	THR	N-CA-C	5.48	118.17	109.96
2	b	351	THR	N-CA-C	5.48	118.18	109.96
2	L	105	SER	N-CA-C	5.48	120.09	113.41
2	P	105	SER	N-CA-C	5.48	120.09	113.41
2	L	351	THR	N-CA-C	5.47	118.17	109.96
2	R	351	THR	N-CA-C	5.47	118.17	109.96
2	H	105	SER	N-CA-C	5.47	120.09	113.41
2	V	105	SER	N-CA-C	5.47	120.09	113.41
2	X	400	GLN	CA-C-N	5.47	125.82	119.47
2	X	400	GLN	C-N-CA	5.47	125.82	119.47
2	C	105	SER	N-CA-C	5.47	120.08	113.41
2	X	351	THR	N-CA-C	5.47	118.16	109.96
2	H	351	THR	N-CA-C	5.47	118.16	109.96
2	X	105	SER	N-CA-C	5.47	120.08	113.41
2	Z	351	THR	N-CA-C	5.47	118.16	109.96
2	N	105	SER	N-CA-C	5.47	120.08	113.41
2	J	105	SER	N-CA-C	5.46	120.08	113.41
2	b	105	SER	N-CA-C	5.46	120.08	113.41
2	D	105	SER	N-CA-C	5.46	120.07	113.41
2	T	105	SER	N-CA-C	5.46	120.07	113.41
2	T	351	THR	N-CA-C	5.45	118.14	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	351	THR	N-CA-C	5.45	118.14	109.96
1	O	351	SER	CA-C-N	5.45	125.35	119.85
1	O	351	SER	C-N-CA	5.45	125.35	119.85
2	F	105	SER	N-CA-C	5.43	120.04	113.41
1	W	82	ASP	CA-C-N	5.43	126.62	119.84
1	W	82	ASP	C-N-CA	5.43	126.62	119.84
1	G	351	SER	CA-C-N	5.42	125.33	119.85
1	G	351	SER	C-N-CA	5.42	125.33	119.85
2	Z	105	SER	N-CA-C	5.42	120.03	113.41
1	a	351	SER	CA-C-N	5.42	125.33	119.85
1	a	351	SER	C-N-CA	5.42	125.33	119.85
1	a	82	ASP	CA-C-N	5.42	126.62	119.84
1	a	82	ASP	C-N-CA	5.42	126.62	119.84
1	B	351	SER	CA-C-N	5.41	125.31	119.85
1	B	351	SER	C-N-CA	5.41	125.31	119.85
1	S	351	SER	CA-C-N	5.41	125.31	119.85
1	S	351	SER	C-N-CA	5.41	125.31	119.85
1	I	351	SER	CA-C-N	5.41	125.31	119.85
1	I	351	SER	C-N-CA	5.41	125.31	119.85
1	M	82	ASP	CA-C-N	5.41	126.60	119.84
1	M	82	ASP	C-N-CA	5.41	126.60	119.84
1	Y	82	ASP	CA-C-N	5.40	126.59	119.84
1	Y	82	ASP	C-N-CA	5.40	126.59	119.84
1	Y	351	SER	CA-C-N	5.40	125.31	119.85
1	Y	351	SER	C-N-CA	5.40	125.31	119.85
1	A	351	SER	CA-C-N	5.40	125.30	119.85
1	A	351	SER	C-N-CA	5.40	125.30	119.85
1	Q	82	ASP	CA-C-N	5.40	126.59	119.84
1	Q	82	ASP	C-N-CA	5.40	126.59	119.84
1	I	82	ASP	CA-C-N	5.40	126.59	119.84
1	I	82	ASP	C-N-CA	5.40	126.59	119.84
1	B	82	ASP	CA-C-N	5.39	126.58	119.84
1	B	82	ASP	C-N-CA	5.39	126.58	119.84
1	G	82	ASP	CA-C-N	5.39	126.58	119.84
1	G	82	ASP	C-N-CA	5.39	126.58	119.84
1	A	82	ASP	CA-C-N	5.39	126.58	119.84
1	A	82	ASP	C-N-CA	5.39	126.58	119.84
1	K	351	SER	CA-C-N	5.39	125.29	119.85
1	K	351	SER	C-N-CA	5.39	125.29	119.85
1	E	82	ASP	CA-C-N	5.38	126.57	119.84
1	E	82	ASP	C-N-CA	5.38	126.57	119.84
1	K	82	ASP	CA-C-N	5.38	126.57	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	82	ASP	C-N-CA	5.38	126.57	119.84
1	S	82	ASP	CA-C-N	5.38	126.57	119.84
1	S	82	ASP	C-N-CA	5.38	126.57	119.84
1	E	351	SER	CA-C-N	5.38	125.28	119.85
1	E	351	SER	C-N-CA	5.38	125.28	119.85
1	E	191	TYR	N-CA-C	5.37	120.85	113.97
1	Q	351	SER	CA-C-N	5.37	125.28	119.85
1	Q	351	SER	C-N-CA	5.37	125.28	119.85
1	M	351	SER	CA-C-N	5.37	125.27	119.85
1	M	351	SER	C-N-CA	5.37	125.27	119.85
1	U	351	SER	CA-C-N	5.37	125.27	119.85
1	U	351	SER	C-N-CA	5.37	125.27	119.85
1	O	191	TYR	N-CA-C	5.36	120.83	113.97
1	W	351	SER	CA-C-N	5.36	125.27	119.85
1	W	351	SER	C-N-CA	5.36	125.27	119.85
1	O	82	ASP	CA-C-N	5.36	126.54	119.84
1	O	82	ASP	C-N-CA	5.36	126.54	119.84
1	U	82	ASP	CA-C-N	5.35	126.53	119.84
1	U	82	ASP	C-N-CA	5.35	126.53	119.84
1	M	191	TYR	N-CA-C	5.35	120.82	113.97
2	N	174	ASP	CB-CA-C	-5.35	101.68	110.72
1	a	191	TYR	N-CA-C	5.34	120.81	113.97
1	A	191	TYR	N-CA-C	5.34	120.81	113.97
1	G	191	TYR	N-CA-C	5.34	120.80	113.97
1	B	191	TYR	N-CA-C	5.34	120.80	113.97
1	Q	191	TYR	N-CA-C	5.33	120.80	113.97
1	U	191	TYR	N-CA-C	5.33	120.80	113.97
1	K	191	TYR	N-CA-C	5.33	120.79	113.97
1	Y	191	TYR	N-CA-C	5.33	120.79	113.97
2	b	174	ASP	CB-CA-C	-5.33	101.72	110.72
2	H	174	ASP	CB-CA-C	-5.32	101.72	110.72
2	R	174	ASP	CB-CA-C	-5.32	101.72	110.72
1	S	191	TYR	N-CA-C	5.32	120.78	113.97
2	T	174	ASP	CB-CA-C	-5.32	101.72	110.72
2	L	174	ASP	CB-CA-C	-5.32	101.72	110.72
2	D	174	ASP	CB-CA-C	-5.32	101.73	110.72
2	C	174	ASP	CB-CA-C	-5.32	101.73	110.72
2	F	174	ASP	CB-CA-C	-5.32	101.73	110.72
1	I	191	TYR	N-CA-C	5.32	120.78	113.97
2	X	174	ASP	CB-CA-C	-5.32	101.73	110.72
2	J	174	ASP	CB-CA-C	-5.32	101.73	110.72
1	W	191	TYR	N-CA-C	5.32	120.77	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	174	ASP	CB-CA-C	-5.31	101.74	110.72
2	V	174	ASP	CB-CA-C	-5.31	101.75	110.72
1	M	243	ASN	N-CA-C	5.31	115.54	108.38
2	Z	174	ASP	CB-CA-C	-5.30	101.76	110.72
2	C	193	CYS	N-CA-C	5.30	117.87	111.40
1	O	243	ASN	N-CA-C	5.30	115.53	108.38
1	W	243	ASN	N-CA-C	5.30	115.53	108.38
1	G	243	ASN	N-CA-C	5.29	115.52	108.38
1	K	243	ASN	N-CA-C	5.29	115.52	108.38
1	Y	243	ASN	N-CA-C	5.29	115.52	108.38
2	Z	387	HIS	CA-CB-CG	5.29	119.09	113.80
2	b	193	CYS	N-CA-C	5.29	117.85	111.40
2	R	387	HIS	CA-CB-CG	5.28	119.08	113.80
2	Z	193	CYS	N-CA-C	5.28	117.84	111.40
1	A	243	ASN	N-CA-C	5.28	115.51	108.38
1	Q	243	ASN	N-CA-C	5.28	115.51	108.38
1	U	243	ASN	N-CA-C	5.28	115.51	108.38
1	a	243	ASN	N-CA-C	5.28	115.50	108.38
1	B	243	ASN	N-CA-C	5.27	115.50	108.38
1	U	215	ASN	CA-C-N	5.27	125.18	119.85
1	U	215	ASN	C-N-CA	5.27	125.18	119.85
1	B	215	ASN	CA-C-N	5.27	125.18	119.85
1	B	215	ASN	C-N-CA	5.27	125.18	119.85
2	F	387	HIS	CA-CB-CG	5.27	119.07	113.80
1	W	215	ASN	CA-C-N	5.27	125.18	119.85
1	W	215	ASN	C-N-CA	5.27	125.18	119.85
2	L	193	CYS	N-CA-C	5.27	117.83	111.40
1	I	243	ASN	N-CA-C	5.27	115.50	108.38
1	S	243	ASN	N-CA-C	5.27	115.49	108.38
2	T	193	CYS	N-CA-C	5.27	117.83	111.40
2	J	387	HIS	CA-CB-CG	5.27	119.07	113.80
2	N	387	HIS	CA-CB-CG	5.27	119.07	113.80
1	Y	215	ASN	CA-C-N	5.27	125.17	119.85
1	Y	215	ASN	C-N-CA	5.27	125.17	119.85
1	E	243	ASN	N-CA-C	5.26	115.49	108.38
1	G	215	ASN	CA-C-N	5.26	125.17	119.85
1	G	215	ASN	C-N-CA	5.26	125.17	119.85
2	P	193	CYS	N-CA-C	5.26	117.82	111.40
2	V	387	HIS	CA-CB-CG	5.26	119.06	113.80
2	D	193	CYS	N-CA-C	5.26	117.82	111.40
2	X	387	HIS	CA-CB-CG	5.25	119.06	113.80
2	D	387	HIS	CA-CB-CG	5.25	119.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	215	ASN	CA-C-N	5.25	125.16	119.85
1	E	215	ASN	C-N-CA	5.25	125.16	119.85
2	J	193	CYS	N-CA-C	5.25	117.81	111.40
2	N	193	CYS	N-CA-C	5.25	117.81	111.40
1	S	215	ASN	CA-C-N	5.25	125.15	119.85
1	S	215	ASN	C-N-CA	5.25	125.15	119.85
2	V	193	CYS	N-CA-C	5.25	117.81	111.40
1	W	9	GLN	CA-C-N	-5.25	116.11	123.10
1	W	9	GLN	C-N-CA	-5.25	116.11	123.10
2	C	387	HIS	CA-CB-CG	5.25	119.05	113.80
1	Q	9	GLN	CA-C-N	-5.25	116.12	123.10
1	Q	9	GLN	C-N-CA	-5.25	116.12	123.10
2	H	387	HIS	CA-CB-CG	5.25	119.05	113.80
2	L	387	HIS	CA-CB-CG	5.25	119.05	113.80
2	X	193	CYS	N-CA-C	5.24	117.80	111.40
1	A	215	ASN	CA-C-N	5.24	125.14	119.85
1	A	215	ASN	C-N-CA	5.24	125.14	119.85
2	F	193	CYS	N-CA-C	5.24	117.80	111.40
2	P	387	HIS	CA-CB-CG	5.24	119.04	113.80
1	M	215	ASN	CA-C-N	5.24	125.14	119.85
1	M	215	ASN	C-N-CA	5.24	125.14	119.85
2	R	193	CYS	N-CA-C	5.24	117.79	111.40
2	b	387	HIS	CA-CB-CG	5.23	119.03	113.80
1	A	9	GLN	CA-C-N	-5.23	116.14	123.10
1	A	9	GLN	C-N-CA	-5.23	116.14	123.10
1	E	9	GLN	CA-C-N	-5.23	116.14	123.10
1	E	9	GLN	C-N-CA	-5.23	116.14	123.10
1	G	9	GLN	CA-C-N	-5.23	116.14	123.10
1	G	9	GLN	C-N-CA	-5.23	116.14	123.10
1	M	9	GLN	CA-C-N	-5.23	116.14	123.10
1	M	9	GLN	C-N-CA	-5.23	116.14	123.10
1	I	215	ASN	CA-C-N	5.23	125.13	119.85
1	I	215	ASN	C-N-CA	5.23	125.13	119.85
1	O	9	GLN	CA-C-N	-5.23	116.15	123.10
1	O	9	GLN	C-N-CA	-5.23	116.15	123.10
1	K	9	GLN	CA-C-N	-5.22	116.15	123.10
1	K	9	GLN	C-N-CA	-5.22	116.15	123.10
1	Q	215	ASN	CA-C-N	5.22	125.13	119.85
1	Q	215	ASN	C-N-CA	5.22	125.13	119.85
1	U	9	GLN	CA-C-N	-5.22	116.15	123.10
1	U	9	GLN	C-N-CA	-5.22	116.15	123.10
1	I	9	GLN	CA-C-N	-5.22	116.15	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	9	GLN	C-N-CA	-5.22	116.15	123.10
1	B	9	GLN	CA-C-N	-5.22	116.16	123.10
1	B	9	GLN	C-N-CA	-5.22	116.16	123.10
1	a	215	ASN	CA-C-N	5.22	125.12	119.85
1	a	215	ASN	C-N-CA	5.22	125.12	119.85
2	T	387	HIS	CA-CB-CG	5.22	119.02	113.80
1	Y	9	GLN	CA-C-N	-5.22	116.16	123.10
1	Y	9	GLN	C-N-CA	-5.22	116.16	123.10
2	H	193	CYS	N-CA-C	5.21	117.76	111.40
2	Z	353	THR	N-CA-CB	-5.21	103.42	110.67
1	S	9	GLN	CA-C-N	-5.21	116.17	123.10
1	S	9	GLN	C-N-CA	-5.21	116.17	123.10
2	V	353	THR	N-CA-CB	-5.21	103.43	110.67
2	R	353	THR	N-CA-CB	-5.20	103.44	110.67
2	D	353	THR	N-CA-CB	-5.20	103.44	110.67
2	T	353	THR	N-CA-CB	-5.20	103.45	110.67
2	J	353	THR	N-CA-CB	-5.20	103.45	110.67
1	O	215	ASN	CA-C-N	5.20	125.10	119.85
1	O	215	ASN	C-N-CA	5.20	125.10	119.85
2	P	353	THR	N-CA-CB	-5.19	103.45	110.67
2	F	353	THR	N-CA-CB	-5.19	103.45	110.67
2	H	353	THR	N-CA-CB	-5.19	103.46	110.67
1	K	215	ASN	CA-C-N	5.19	125.09	119.85
1	K	215	ASN	C-N-CA	5.19	125.09	119.85
2	N	353	THR	N-CA-CB	-5.19	103.45	110.67
2	X	353	THR	N-CA-CB	-5.19	103.46	110.67
1	a	9	GLN	CA-C-N	-5.19	116.20	123.10
1	a	9	GLN	C-N-CA	-5.19	116.20	123.10
2	C	353	THR	N-CA-CB	-5.18	103.47	110.67
2	L	353	THR	N-CA-CB	-5.18	103.47	110.67
2	b	353	THR	N-CA-CB	-5.18	103.47	110.67
1	K	363	GLY	N-CA-C	5.11	118.15	110.18
1	I	363	GLY	N-CA-C	5.11	118.15	110.18
1	M	363	GLY	N-CA-C	5.11	118.15	110.18
1	G	363	GLY	N-CA-C	5.11	118.15	110.18
1	W	363	GLY	N-CA-C	5.11	118.14	110.18
1	E	190	LYS	N-CA-C	5.10	116.92	111.36
1	U	363	GLY	N-CA-C	5.09	118.12	110.18
1	Y	363	GLY	N-CA-C	5.09	118.12	110.18
1	A	363	GLY	N-CA-C	5.09	118.12	110.18
1	E	363	GLY	N-CA-C	5.09	118.12	110.18
1	O	363	GLY	N-CA-C	5.08	118.11	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	GLY	N-CA-C	5.08	118.10	110.18
1	Q	190	LYS	N-CA-C	5.07	116.89	111.36
1	U	190	LYS	N-CA-C	5.07	116.89	111.36
1	a	190	LYS	N-CA-C	5.07	116.89	111.36
1	M	190	LYS	N-CA-C	5.06	116.88	111.36
1	S	363	GLY	N-CA-C	5.06	118.08	110.18
1	Q	363	GLY	N-CA-C	5.06	118.08	110.18
1	W	190	LYS	N-CA-C	5.06	116.88	111.36
2	N	256	VAL	CA-C-N	5.05	124.66	119.56
2	N	256	VAL	C-N-CA	5.05	124.66	119.56
1	A	190	LYS	N-CA-C	5.05	116.86	111.36
1	O	190	LYS	N-CA-C	5.05	116.86	111.36
1	Y	190	LYS	N-CA-C	5.04	116.86	111.36
1	K	190	LYS	N-CA-C	5.04	116.86	111.36
2	L	256	VAL	CA-C-N	5.04	124.65	119.56
2	L	256	VAL	C-N-CA	5.04	124.65	119.56
1	a	363	GLY	N-CA-C	5.04	118.04	110.18
2	C	256	VAL	CA-C-N	5.03	124.64	119.56
2	C	256	VAL	C-N-CA	5.03	124.64	119.56
2	P	256	VAL	CA-C-N	5.03	124.64	119.56
2	P	256	VAL	C-N-CA	5.03	124.64	119.56
2	R	256	VAL	CA-C-N	5.02	124.64	119.56
2	R	256	VAL	C-N-CA	5.02	124.64	119.56
2	Z	256	VAL	CA-C-N	5.02	124.63	119.56
2	Z	256	VAL	C-N-CA	5.02	124.63	119.56
2	X	256	VAL	CA-C-N	5.02	124.63	119.56
2	X	256	VAL	C-N-CA	5.02	124.63	119.56
1	G	190	LYS	N-CA-C	5.02	116.83	111.36
1	I	190	LYS	N-CA-C	5.02	116.83	111.36
1	S	190	LYS	N-CA-C	5.00	116.81	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3277	0	3265	17	0
1	B	3277	0	3265	17	0
1	E	3277	0	3265	17	0
1	G	3277	0	3265	15	0
1	I	3277	0	3265	16	0
1	K	3277	0	3265	15	0
1	M	3277	0	3265	16	0
1	O	3277	0	3265	66	0
1	Q	3277	0	3265	59	0
1	S	3277	0	3265	54	0
1	U	3277	0	3265	57	0
1	W	3277	0	3265	57	0
1	Y	3277	0	3265	55	0
1	a	3277	0	3265	59	0
2	C	3348	0	3353	68	0
2	D	3348	0	3353	71	0
2	F	3348	0	3353	59	0
2	H	3348	0	3353	63	0
2	J	3348	0	3353	65	0
2	L	3348	0	3353	62	0
2	N	3348	0	3353	64	0
2	P	3348	0	3353	24	0
2	R	3348	0	3353	27	0
2	T	3348	0	3353	21	0
2	V	3348	0	3353	22	0
2	X	3348	0	3353	23	0
2	Z	3348	0	3353	23	0
2	b	3348	0	3353	18	0
3	A	28	0	12	1	0
3	B	28	0	12	1	0
3	E	28	0	12	1	0
3	G	28	0	12	1	0
3	I	28	0	12	1	0
3	K	28	0	12	1	0
3	M	28	0	12	1	0
3	O	28	0	12	1	0
3	Q	28	0	12	1	0
3	S	28	0	12	1	0
3	U	28	0	12	1	0
3	W	28	0	12	1	0
3	Y	28	0	12	1	0
3	a	28	0	12	1	0
All	All	93142	0	92820	733	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (733) 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:L:257:PRO:HB3	1:Y:388:PHE:CE1	1.39	1.55
2:N:257:PRO:HB3	1:a:388:PHE:CE1	1.39	1.54
2:J:257:PRO:HB3	1:W:388:PHE:CE1	1.41	1.53
2:C:257:PRO:HB3	1:Q:388:PHE:CE1	1.44	1.51
2:H:257:PRO:HB3	1:U:388:PHE:CE1	1.40	1.50
2:F:257:PRO:HB3	1:S:388:PHE:CE1	1.45	1.50
2:N:340:ILE:HD11	1:a:385:ARG:NH1	1.19	1.46
2:C:340:ILE:HD11	1:Q:385:ARG:NH1	1.21	1.43
2:D:257:PRO:HB3	1:O:388:PHE:CE1	1.54	1.42
2:F:340:ILE:HD11	1:S:385:ARG:NH1	1.16	1.42
2:L:340:ILE:HD11	1:Y:385:ARG:NH1	1.13	1.41
2:H:340:ILE:HD11	1:U:385:ARG:NH1	1.09	1.36
2:J:340:ILE:HD11	1:W:385:ARG:NH1	1.07	1.35
2:D:257:PRO:HB3	1:O:388:PHE:CD1	1.62	1.34
2:D:340:ILE:CD1	1:O:385:ARG:HD2	1.58	1.33
2:D:340:ILE:HD11	1:O:385:ARG:NH1	1.06	1.33
2:N:329:LYS:NZ	1:a:170:LYS:HZ1	1.31	1.28
2:D:340:ILE:CD1	1:O:385:ARG:HH11	1.46	1.27
2:J:340:ILE:CD1	1:W:385:ARG:NH1	1.99	1.26
2:D:340:ILE:HD12	1:O:385:ARG:CD	1.65	1.25
2:H:340:ILE:CD1	1:U:385:ARG:NH1	2.01	1.23
2:C:329:LYS:NZ	1:Q:170:LYS:HZ1	1.36	1.22
2:F:329:LYS:NZ	1:S:170:LYS:HZ1	1.39	1.20
2:L:329:LYS:NZ	1:Y:170:LYS:HZ1	1.40	1.19
2:N:257:PRO:HB3	1:a:388:PHE:CD1	1.75	1.19
2:L:340:ILE:CD1	1:Y:385:ARG:NH1	2.05	1.18
2:D:321:HIS:ND1	1:O:218:LEU:HG	1.57	1.18
2:D:253:THR:HG21	1:O:94:GLY:O	1.42	1.18
2:C:257:PRO:HB3	1:Q:388:PHE:CD1	1.79	1.18
2:D:340:ILE:CD1	1:O:385:ARG:CD	2.18	1.18
2:L:257:PRO:HB3	1:Y:388:PHE:CD1	1.78	1.17
2:N:257:PRO:CB	1:a:388:PHE:CE1	2.27	1.17
2:H:340:ILE:CD1	1:U:385:ARG:HH11	1.56	1.16
2:J:340:ILE:CD1	1:W:385:ARG:HH11	1.54	1.16
2:J:329:LYS:NZ	1:W:170:LYS:HZ1	1.44	1.15
2:D:340:ILE:CD1	1:O:385:ARG:NH1	2.03	1.15
2:F:340:ILE:CD1	1:S:385:ARG:NH1	2.08	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:257:PRO:CB	1:Y:388:PHE:CE1	2.28	1.15
2:H:257:PRO:CB	1:U:388:PHE:CE1	2.30	1.15
2:D:250:GLU:HG2	1:O:94:GLY:CA	1.76	1.14
2:J:257:PRO:HB3	1:W:388:PHE:CD1	1.81	1.13
2:N:340:ILE:CD1	1:a:385:ARG:NH1	2.12	1.13
2:J:257:PRO:CB	1:W:388:PHE:CE1	2.31	1.13
2:C:257:PRO:CB	1:Q:388:PHE:CE1	2.31	1.12
2:L:340:ILE:CD1	1:Y:385:ARG:HH11	1.59	1.12
2:F:257:PRO:HB3	1:S:388:PHE:CD1	1.84	1.12
2:C:340:ILE:HD12	1:Q:385:ARG:HD2	1.32	1.11
2:F:257:PRO:CB	1:S:388:PHE:CE1	2.33	1.11
2:H:329:LYS:NZ	1:U:170:LYS:HZ1	1.49	1.10
2:H:257:PRO:HB3	1:U:388:PHE:CD1	1.84	1.10
2:C:340:ILE:CD1	1:Q:385:ARG:NH1	2.14	1.10
2:F:340:ILE:HD12	1:S:385:ARG:HD2	1.33	1.08
2:J:340:ILE:HD12	1:W:385:ARG:HD2	1.34	1.08
2:D:40:LYS:HE3	2:C:305:LYS:HE3	1.35	1.08
2:D:250:GLU:HG2	1:O:94:GLY:HA2	1.11	1.07
2:L:340:ILE:HD12	1:Y:385:ARG:HD2	1.35	1.07
2:P:40:LYS:HE3	2:R:305:LYS:HE3	1.35	1.07
2:F:340:ILE:CD1	1:S:385:ARG:HH11	1.65	1.06
2:N:340:ILE:CD1	1:a:385:ARG:HH11	1.65	1.06
2:C:340:ILE:CD1	1:Q:385:ARG:HH11	1.69	1.05
2:N:340:ILE:HD12	1:a:385:ARG:HD2	1.35	1.05
2:C:329:LYS:NZ	1:Q:170:LYS:NZ	2.03	1.04
2:N:250:GLU:HG2	1:a:94:GLY:HA2	1.35	1.04
2:H:340:ILE:HD12	1:U:385:ARG:HD2	1.38	1.03
2:N:329:LYS:NZ	1:a:170:LYS:NZ	2.07	1.02
2:D:340:ILE:HD11	1:O:385:ARG:CZ	1.88	1.02
2:L:250:GLU:HG2	1:Y:94:GLY:HA2	1.39	1.02
2:D:340:ILE:HD12	1:O:385:ARG:HD2	1.17	1.02
2:C:250:GLU:HG2	1:Q:94:GLY:HA2	1.38	1.02
2:D:257:PRO:CB	1:O:388:PHE:CE1	2.43	1.01
2:F:329:LYS:NZ	1:S:170:LYS:NZ	2.06	1.00
2:L:257:PRO:HB3	1:Y:388:PHE:HE1	1.23	1.00
2:H:137:ILE:HD11	2:H:168:VAL:HG22	1.44	1.00
2:J:137:ILE:HD11	2:J:168:VAL:HG22	1.44	0.99
2:C:257:PRO:HB3	1:Q:388:PHE:HE1	1.24	0.99
2:F:137:ILE:HD11	2:F:168:VAL:HG22	1.44	0.99
2:L:329:LYS:NZ	1:Y:170:LYS:NZ	2.11	0.99
2:J:340:ILE:HD12	1:W:385:ARG:CD	1.93	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:257:PRO:HB3	1:a:388:PHE:HE1	1.22	0.98
2:F:250:GLU:HG2	1:S:94:GLY:HA2	1.44	0.98
2:X:137:ILE:HD11	2:X:168:VAL:HG22	1.44	0.98
2:L:137:ILE:HD11	2:L:168:VAL:HG22	1.44	0.98
2:Z:137:ILE:HD11	2:Z:168:VAL:HG22	1.44	0.98
2:J:250:GLU:HG2	1:W:94:GLY:HA2	1.41	0.97
2:C:340:ILE:CD1	1:Q:385:ARG:HD2	1.93	0.97
2:C:137:ILE:HD11	2:C:168:VAL:HG22	1.44	0.97
2:N:340:ILE:CD1	1:a:385:ARG:HD2	1.94	0.97
2:V:137:ILE:HD11	2:V:168:VAL:HG22	1.44	0.97
2:P:40:LYS:CE	2:R:305:LYS:HE3	1.95	0.97
2:T:137:ILE:HD11	2:T:168:VAL:HG22	1.44	0.96
2:b:137:ILE:HD11	2:b:168:VAL:HG22	1.44	0.96
2:D:340:ILE:HD13	1:O:385:ARG:HD2	1.48	0.96
2:D:40:LYS:CE	2:C:305:LYS:HE3	1.95	0.96
2:R:137:ILE:HD11	2:R:168:VAL:HG22	1.44	0.96
2:D:137:ILE:HD11	2:D:168:VAL:HG22	1.44	0.96
2:L:340:ILE:CD1	1:Y:385:ARG:HD2	1.95	0.96
2:J:329:LYS:NZ	1:W:170:LYS:NZ	2.14	0.95
2:H:329:LYS:HZ1	1:U:170:LYS:HZ1	1.07	0.95
2:N:137:ILE:HD11	2:N:168:VAL:HG22	1.44	0.95
2:P:137:ILE:HD11	2:P:168:VAL:HG22	1.44	0.95
2:J:340:ILE:CD1	1:W:385:ARG:HD2	1.94	0.95
2:F:257:PRO:HB3	1:S:388:PHE:HE1	1.23	0.95
2:L:340:ILE:HD12	1:Y:385:ARG:CD	1.96	0.94
2:C:340:ILE:HD12	1:Q:385:ARG:CD	1.98	0.94
2:F:340:ILE:HD12	1:S:385:ARG:CD	1.98	0.94
2:H:329:LYS:NZ	1:U:170:LYS:NZ	2.15	0.94
2:L:329:LYS:HZ1	1:Y:170:LYS:NZ	1.63	0.93
2:H:250:GLU:HG2	1:U:94:GLY:HA2	1.47	0.93
2:F:340:ILE:CD1	1:S:385:ARG:HD2	1.96	0.93
2:J:340:ILE:HD11	1:W:385:ARG:CZ	1.99	0.93
2:C:329:LYS:HZ1	1:Q:170:LYS:HZ1	1.00	0.93
2:H:340:ILE:HD12	1:U:385:ARG:CD	1.99	0.93
2:N:340:ILE:HD12	1:a:385:ARG:CD	1.99	0.92
2:N:253:THR:HG21	1:a:94:GLY:O	1.70	0.92
2:D:250:GLU:CG	1:O:94:GLY:HA2	1.97	0.92
2:D:257:PRO:CB	1:O:388:PHE:CD1	2.51	0.91
2:J:257:PRO:HB3	1:W:388:PHE:HE1	1.25	0.91
2:D:340:ILE:HD12	1:O:385:ARG:HD3	1.50	0.91
2:H:257:PRO:HB3	1:U:388:PHE:HE1	1.20	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:253:THR:HG21	1:Y:94:GLY:O	1.71	0.91
2:N:329:LYS:HZ1	1:a:170:LYS:HZ1	1.02	0.91
2:D:329:LYS:NZ	1:O:170:LYS:NZ	2.18	0.90
2:N:250:GLU:HG2	1:a:94:GLY:CA	2.01	0.90
2:C:250:GLU:HG2	1:Q:94:GLY:CA	2.01	0.90
2:H:340:ILE:CD1	1:U:385:ARG:HD2	2.00	0.89
2:J:329:LYS:HZ1	1:W:170:LYS:HZ1	0.93	0.89
2:J:253:THR:HG21	1:W:94:GLY:O	1.72	0.88
2:N:321:HIS:ND1	1:a:218:LEU:HG	1.87	0.88
2:H:340:ILE:HD11	1:U:385:ARG:CZ	2.03	0.88
2:F:340:ILE:HD11	1:S:385:ARG:CZ	2.04	0.88
2:N:321:HIS:CE1	1:a:218:LEU:HG	2.09	0.88
2:L:250:GLU:HG2	1:Y:94:GLY:CA	2.04	0.88
2:L:321:HIS:ND1	1:Y:218:LEU:HG	1.88	0.87
2:J:321:HIS:ND1	1:W:218:LEU:HG	1.89	0.87
2:C:321:HIS:ND1	1:Q:218:LEU:HG	1.90	0.87
2:D:321:HIS:CE1	1:O:218:LEU:HG	2.09	0.86
2:F:329:LYS:HZ1	1:S:170:LYS:HZ1	0.89	0.86
2:L:340:ILE:HD11	1:Y:385:ARG:CZ	2.04	0.86
2:C:321:HIS:CE1	1:Q:218:LEU:HG	2.11	0.86
2:J:250:GLU:HG2	1:W:94:GLY:CA	2.06	0.85
2:F:250:GLU:HG2	1:S:94:GLY:CA	2.06	0.85
2:C:257:PRO:CB	1:Q:388:PHE:CD1	2.57	0.85
2:D:321:HIS:HE1	1:O:218:LEU:CD1	1.88	0.85
2:C:253:THR:HG21	1:Q:94:GLY:O	1.75	0.85
2:N:329:LYS:HZ3	1:a:170:LYS:HZ1	1.25	0.85
2:L:321:HIS:CE1	1:Y:218:LEU:HG	2.12	0.84
2:N:257:PRO:CB	1:a:388:PHE:CD1	2.53	0.84
2:N:340:ILE:HD11	1:a:385:ARG:CZ	2.08	0.84
2:H:253:THR:HG21	1:U:94:GLY:O	1.77	0.84
2:F:321:HIS:ND1	1:S:218:LEU:HG	1.94	0.83
2:C:340:ILE:HD11	1:Q:385:ARG:CZ	2.07	0.83
2:D:321:HIS:HE1	1:O:218:LEU:HD12	1.41	0.83
2:F:253:THR:HG21	1:S:94:GLY:O	1.79	0.83
2:D:321:HIS:CE1	1:O:218:LEU:CD1	2.62	0.83
2:F:329:LYS:HZ1	1:S:170:LYS:NZ	1.70	0.83
2:H:321:HIS:ND1	1:U:218:LEU:HG	1.94	0.82
2:L:257:PRO:CB	1:Y:388:PHE:CD1	2.57	0.82
2:F:40:LYS:HE3	2:H:305:LYS:HE3	1.61	0.82
2:C:340:ILE:HD11	1:Q:385:ARG:HH11	1.00	0.82
2:J:40:LYS:HE3	2:L:305:LYS:HE3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:40:LYS:HE3	2:V:305:LYS:HE3	1.61	0.81
2:L:40:LYS:HE3	2:N:305:LYS:HE3	1.62	0.81
2:Z:40:LYS:HE3	2:b:305:LYS:HE3	1.63	0.81
2:F:321:HIS:CE1	1:S:218:LEU:HG	2.16	0.81
2:D:329:LYS:HZ3	1:O:170:LYS:NZ	1.79	0.81
2:J:321:HIS:CE1	1:W:218:LEU:HG	2.16	0.81
2:D:329:LYS:CE	1:O:170:LYS:HZ1	1.94	0.80
2:J:329:LYS:HZ1	1:W:170:LYS:NZ	1.74	0.80
2:H:257:PRO:CB	1:U:388:PHE:CD1	2.62	0.80
2:X:40:LYS:HE3	2:Z:305:LYS:HE3	1.62	0.80
2:J:257:PRO:CB	1:W:388:PHE:CD1	2.61	0.80
2:F:340:ILE:HD11	1:S:385:ARG:HH11	0.98	0.79
2:H:250:GLU:HG2	1:U:94:GLY:CA	2.12	0.79
2:L:329:LYS:HZ1	1:Y:170:LYS:HZ1	0.79	0.79
2:C:40:LYS:HE3	2:F:305:LYS:HE3	1.65	0.78
2:C:329:LYS:HZ3	1:Q:170:LYS:NZ	1.81	0.78
2:H:321:HIS:CE1	1:U:218:LEU:HG	2.19	0.78
2:V:40:LYS:HE3	2:X:305:LYS:HE3	1.65	0.77
1:Q:338:TRP:HZ2	1:Q:419:LEU:HD11	1.50	0.77
2:N:329:LYS:HZ3	1:a:170:LYS:NZ	1.81	0.77
2:J:340:ILE:CD1	1:W:385:ARG:CD	2.58	0.77
2:R:40:LYS:HE3	2:T:305:LYS:HE3	1.65	0.77
1:I:338:TRP:HZ2	1:I:419:LEU:HD11	1.50	0.76
2:C:329:LYS:CE	1:Q:170:LYS:NZ	2.48	0.76
1:K:338:TRP:HZ2	1:K:419:LEU:HD11	1.50	0.76
1:E:338:TRP:HZ2	1:E:419:LEU:HD11	1.50	0.76
1:Y:338:TRP:HZ2	1:Y:419:LEU:HD11	1.50	0.76
1:A:338:TRP:HZ2	1:A:419:LEU:HD11	1.50	0.76
2:F:257:PRO:CB	1:S:388:PHE:CD1	2.62	0.76
1:M:338:TRP:HZ2	1:M:419:LEU:HD11	1.50	0.76
1:G:338:TRP:HZ2	1:G:419:LEU:HD11	1.50	0.76
2:H:40:LYS:HE3	2:J:305:LYS:HE3	1.65	0.76
1:O:338:TRP:HZ2	1:O:419:LEU:HD11	1.50	0.75
1:a:338:TRP:HZ2	1:a:419:LEU:HD11	1.50	0.75
1:B:338:TRP:HZ2	1:B:419:LEU:HD11	1.50	0.75
2:L:340:ILE:CD1	1:Y:385:ARG:CD	2.60	0.75
1:U:338:TRP:HZ2	1:U:419:LEU:HD11	1.50	0.75
2:N:340:ILE:HD11	1:a:385:ARG:HH11	0.95	0.75
1:W:338:TRP:HZ2	1:W:419:LEU:HD11	1.50	0.75
2:N:340:ILE:CD1	1:a:385:ARG:CD	2.61	0.74
2:D:40:LYS:NZ	2:C:305:LYS:HE2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:338:TRP:HZ2	1:S:419:LEU:HD11	1.50	0.74
2:D:329:LYS:NZ	1:O:170:LYS:HZ1	1.82	0.74
2:H:340:ILE:HD11	1:U:385:ARG:HH11	0.92	0.74
2:P:40:LYS:NZ	2:R:305:LYS:HE2	2.02	0.74
2:N:329:LYS:CE	1:a:170:LYS:NZ	2.51	0.74
1:Q:338:TRP:CZ2	1:Q:419:LEU:HD11	2.23	0.73
1:A:338:TRP:CZ2	1:A:419:LEU:HD11	2.24	0.73
2:H:340:ILE:CD1	1:U:385:ARG:CD	2.64	0.73
2:L:340:ILE:HD11	1:Y:385:ARG:HH11	0.91	0.73
1:a:338:TRP:CZ2	1:a:419:LEU:HD11	2.24	0.73
2:C:329:LYS:CE	1:Q:170:LYS:HZ2	2.02	0.73
1:B:338:TRP:CZ2	1:B:419:LEU:HD11	2.23	0.73
2:C:329:LYS:HZ3	1:Q:170:LYS:HZ1	1.30	0.73
1:M:338:TRP:CZ2	1:M:419:LEU:HD11	2.24	0.73
1:K:338:TRP:CZ2	1:K:419:LEU:HD11	2.24	0.73
1:O:338:TRP:CZ2	1:O:419:LEU:HD11	2.24	0.73
1:E:338:TRP:CZ2	1:E:419:LEU:HD11	2.24	0.73
1:G:338:TRP:CZ2	1:G:419:LEU:HD11	2.24	0.73
1:Y:338:TRP:CZ2	1:Y:419:LEU:HD11	2.24	0.73
1:I:338:TRP:CZ2	1:I:419:LEU:HD11	2.23	0.72
2:C:340:ILE:CD1	1:Q:385:ARG:CD	2.61	0.72
1:S:338:TRP:CZ2	1:S:419:LEU:HD11	2.24	0.72
2:F:340:ILE:CD1	1:S:385:ARG:CD	2.63	0.72
1:U:338:TRP:CZ2	1:U:419:LEU:HD11	2.23	0.72
1:W:338:TRP:CZ2	1:W:419:LEU:HD11	2.24	0.72
2:D:321:HIS:CE1	1:O:218:LEU:CG	2.72	0.72
2:F:329:LYS:CE	1:S:170:LYS:NZ	2.52	0.71
2:J:40:LYS:CE	2:L:305:LYS:HE3	2.21	0.71
2:N:250:GLU:CG	1:a:94:GLY:HA2	2.17	0.71
2:P:40:LYS:NZ	2:R:305:LYS:CE	2.54	0.71
2:D:329:LYS:NZ	1:O:170:LYS:HZ3	1.88	0.70
2:D:40:LYS:NZ	2:C:305:LYS:CE	2.54	0.70
2:X:40:LYS:CE	2:Z:305:LYS:HE3	2.21	0.70
2:J:340:ILE:HD11	1:W:385:ARG:HH11	0.87	0.70
2:F:40:LYS:CE	2:H:305:LYS:HE3	2.22	0.70
2:F:329:LYS:CE	1:S:170:LYS:HZ2	2.06	0.69
2:Z:40:LYS:CE	2:b:305:LYS:HE3	2.23	0.69
2:L:329:LYS:CE	1:Y:170:LYS:NZ	2.56	0.68
2:T:40:LYS:CE	2:V:305:LYS:HE3	2.22	0.68
2:L:40:LYS:CE	2:N:305:LYS:HE3	2.23	0.68
2:H:40:LYS:CE	2:J:305:LYS:HE3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:40:LYS:CE	2:X:305:LYS:HE3	2.24	0.66
2:C:250:GLU:CG	1:Q:94:GLY:HA2	2.19	0.66
2:C:40:LYS:CE	2:F:305:LYS:HE3	2.26	0.66
2:R:40:LYS:CE	2:T:305:LYS:HE3	2.26	0.66
2:D:340:ILE:CD1	1:O:385:ARG:CZ	2.62	0.65
2:H:322:SER:OG	1:U:215:ASN:HA	1.97	0.65
2:H:329:LYS:HZ3	1:U:170:LYS:NZ	1.94	0.65
2:H:329:LYS:CE	1:U:170:LYS:NZ	2.60	0.65
2:F:329:LYS:HZ3	1:S:170:LYS:NZ	1.95	0.65
2:J:329:LYS:CE	1:W:170:LYS:NZ	2.60	0.65
2:F:329:LYS:HZ3	1:S:170:LYS:HZ1	1.44	0.64
2:J:340:ILE:CD1	1:W:385:ARG:CZ	2.67	0.64
2:L:322:SER:OG	1:Y:215:ASN:HA	1.98	0.64
2:H:329:LYS:CE	1:U:170:LYS:HZ2	2.12	0.63
2:L:250:GLU:CG	1:Y:94:GLY:HA2	2.22	0.63
2:H:329:LYS:HZ1	1:U:170:LYS:NZ	1.86	0.62
2:N:322:SER:OG	1:a:215:ASN:HA	1.99	0.61
2:D:321:HIS:ND1	1:O:218:LEU:CG	2.49	0.61
2:C:329:LYS:HE2	1:Q:170:LYS:NZ	2.15	0.61
2:J:322:SER:OG	1:W:215:ASN:HA	1.99	0.61
2:H:340:ILE:CD1	1:U:385:ARG:CZ	2.70	0.61
2:N:321:HIS:HE1	1:a:218:LEU:CD1	2.14	0.61
2:D:250:GLU:HG2	1:O:94:GLY:HA3	1.75	0.60
2:C:329:LYS:HZ1	1:Q:170:LYS:NZ	1.80	0.60
2:N:329:LYS:HE2	1:a:170:LYS:NZ	2.16	0.60
2:F:322:SER:OG	1:S:215:ASN:HA	2.02	0.60
2:P:40:LYS:CE	2:R:305:LYS:CE	2.76	0.60
2:L:329:LYS:CE	1:Y:170:LYS:HZ2	2.15	0.59
2:D:257:PRO:O	1:O:390:HIS:CE1	2.55	0.59
2:D:40:LYS:CE	2:C:305:LYS:CE	2.76	0.59
2:C:321:HIS:HE1	1:Q:218:LEU:CD1	2.16	0.59
2:C:322:SER:OG	1:Q:215:ASN:HA	2.03	0.59
2:P:40:LYS:HZ1	2:R:305:LYS:HE2	1.67	0.58
2:J:250:GLU:CG	1:W:94:GLY:HA2	2.25	0.58
2:N:321:HIS:CE1	1:a:218:LEU:CG	2.85	0.58
2:F:250:GLU:CG	1:S:94:GLY:HA2	2.25	0.58
2:L:321:HIS:HE1	1:Y:218:LEU:CD1	2.17	0.58
2:J:329:LYS:HZ3	1:W:170:LYS:HZ1	1.49	0.57
2:L:340:ILE:CD1	1:Y:385:ARG:CZ	2.73	0.57
2:C:321:HIS:CE1	1:Q:218:LEU:CG	2.88	0.57
2:N:329:LYS:HZ1	1:a:170:LYS:NZ	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:257:PRO:CA	1:a:388:PHE:CD1	2.88	0.57
2:N:329:LYS:CE	1:a:170:LYS:HZ2	2.18	0.57
2:D:321:HIS:CE1	1:O:218:LEU:HD12	2.29	0.57
2:J:329:LYS:CE	1:W:170:LYS:HZ2	2.18	0.57
1:a:338:TRP:CE3	2:b:389:ALA:HB2	2.40	0.57
1:M:338:TRP:CE3	2:N:389:ALA:HB2	2.40	0.56
2:D:40:LYS:HZ2	2:C:305:LYS:HE2	1.69	0.56
2:C:329:LYS:HE2	1:Q:170:LYS:HZ2	1.67	0.56
2:F:329:LYS:HE2	1:S:170:LYS:NZ	2.19	0.56
2:F:340:ILE:CD1	1:S:385:ARG:CZ	2.74	0.56
1:O:338:TRP:CE3	2:P:389:ALA:HB2	2.40	0.56
1:Y:338:TRP:CE3	2:Z:389:ALA:HB2	2.40	0.56
1:I:338:TRP:CE3	2:J:389:ALA:HB2	2.40	0.56
1:E:338:TRP:CE3	2:F:389:ALA:HB2	2.40	0.56
1:K:338:TRP:CE3	2:L:389:ALA:HB2	2.40	0.56
2:L:321:HIS:CE1	1:Y:218:LEU:CG	2.88	0.56
1:B:338:TRP:CE3	2:C:389:ALA:HB2	2.40	0.56
1:S:338:TRP:CE3	2:T:389:ALA:HB2	2.40	0.56
1:A:338:TRP:CE3	2:D:389:ALA:HB2	2.40	0.56
2:D:340:ILE:CD1	1:O:385:ARG:NE	2.68	0.56
1:Q:338:TRP:CE3	2:R:389:ALA:HB2	2.40	0.56
1:G:338:TRP:CE3	2:H:389:ALA:HB2	2.40	0.55
2:J:340:ILE:HD12	1:W:385:ARG:HD3	1.86	0.55
1:U:338:TRP:CE3	2:V:389:ALA:HB2	2.40	0.55
2:F:329:LYS:HE2	1:S:170:LYS:HZ2	1.70	0.55
2:J:321:HIS:HE1	1:W:218:LEU:CD1	2.18	0.55
1:W:338:TRP:CE3	2:X:389:ALA:HB2	2.40	0.55
2:N:257:PRO:CA	1:a:388:PHE:CE1	2.90	0.55
2:C:340:ILE:CD1	1:Q:385:ARG:CZ	2.78	0.55
2:P:40:LYS:NZ	2:R:305:LYS:HE3	2.22	0.55
2:C:257:PRO:CA	1:Q:388:PHE:CD1	2.89	0.54
2:P:40:LYS:HZ1	2:R:305:LYS:CE	2.21	0.54
2:L:329:LYS:HE2	1:Y:170:LYS:NZ	2.21	0.54
2:D:252:SER:OG	1:O:391:TRP:CH2	2.61	0.54
2:F:321:HIS:HE1	1:S:218:LEU:CD1	2.20	0.54
2:L:250:GLU:HA	2:L:253:THR:HG22	1.90	0.53
2:J:250:GLU:HA	2:J:253:THR:HG22	1.90	0.53
2:X:250:GLU:HA	2:X:253:THR:HG22	1.90	0.53
2:T:4:GLU:O	2:T:128:LEU:HD12	2.09	0.53
2:Z:4:GLU:O	2:Z:128:LEU:HD12	2.09	0.53
2:Z:250:GLU:HA	2:Z:253:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:4:GLU:O	2:b:128:LEU:HD12	2.09	0.53
2:C:4:GLU:O	2:C:128:LEU:HD12	2.09	0.53
2:H:250:GLU:CG	1:U:94:GLY:HA2	2.30	0.53
2:P:4:GLU:O	2:P:128:LEU:HD12	2.09	0.53
2:H:4:GLU:O	2:H:128:LEU:HD12	2.09	0.53
2:N:4:GLU:O	2:N:128:LEU:HD12	2.09	0.53
2:b:250:GLU:HA	2:b:253:THR:HG22	1.90	0.53
2:J:4:GLU:O	2:J:128:LEU:HD12	2.09	0.53
2:D:4:GLU:O	2:D:128:LEU:HD12	2.09	0.53
2:N:250:GLU:HA	2:N:253:THR:HG22	1.90	0.53
2:D:329:LYS:HZ3	1:O:170:LYS:HZ3	1.46	0.52
2:R:4:GLU:O	2:R:128:LEU:HD12	2.09	0.52
2:R:250:GLU:HA	2:R:253:THR:HG22	1.90	0.52
2:H:250:GLU:HA	2:H:253:THR:HG22	1.90	0.52
2:H:329:LYS:HE2	1:U:170:LYS:HZ2	1.74	0.52
2:V:4:GLU:O	2:V:128:LEU:HD12	2.09	0.52
2:V:250:GLU:HA	2:V:253:THR:HG22	1.90	0.52
2:D:250:GLU:HA	2:D:253:THR:HG22	1.90	0.52
2:L:4:GLU:O	2:L:128:LEU:HD12	2.09	0.52
2:T:250:GLU:HA	2:T:253:THR:HG22	1.90	0.52
2:P:250:GLU:HA	2:P:253:THR:HG22	1.90	0.52
2:X:4:GLU:O	2:X:128:LEU:HD12	2.09	0.52
2:F:4:GLU:O	2:F:128:LEU:HD12	2.09	0.52
2:N:340:ILE:CD1	1:a:385:ARG:CZ	2.78	0.52
2:H:329:LYS:HE2	1:U:170:LYS:NZ	2.24	0.51
2:D:40:LYS:NZ	2:C:305:LYS:HE3	2.22	0.51
2:F:250:GLU:HA	2:F:253:THR:HG22	1.90	0.51
2:C:257:PRO:CA	1:Q:388:PHE:CE1	2.92	0.51
2:J:329:LYS:HE2	1:W:170:LYS:NZ	2.26	0.51
2:L:257:PRO:CA	1:Y:388:PHE:CD1	2.93	0.51
2:F:257:PRO:CA	1:S:388:PHE:CE1	2.93	0.51
2:C:250:GLU:HA	2:C:253:THR:HG22	1.90	0.51
2:H:321:HIS:HE1	1:U:218:LEU:CD1	2.24	0.50
2:J:340:ILE:HD12	1:W:385:ARG:HH11	1.66	0.50
2:F:257:PRO:CA	1:S:388:PHE:CD1	2.94	0.50
2:D:40:LYS:HZ1	2:C:305:LYS:HE2	1.76	0.50
2:J:40:LYS:NZ	2:L:305:LYS:CE	2.75	0.50
2:J:321:HIS:CE1	1:W:218:LEU:CG	2.91	0.50
2:N:40:LYS:HE3	2:P:305:LYS:HE3	1.93	0.50
2:X:40:LYS:NZ	2:Z:305:LYS:CE	2.75	0.50
2:H:257:PRO:CA	1:U:388:PHE:CE1	2.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:329:LYS:HZ3	1:W:170:LYS:NZ	2.04	0.50
2:H:340:ILE:HD12	1:U:385:ARG:HH11	1.65	0.49
1:I:169:PRO:HD2	1:I:201:GLU:CB	2.42	0.49
2:J:145:LEU:O	2:J:146:ALA:C	2.55	0.49
2:C:257:PRO:HA	1:Q:388:PHE:CD1	2.48	0.49
2:H:329:LYS:HZ3	1:U:170:LYS:HZ1	1.43	0.49
1:I:307:LEU:O	1:I:339:ILE:HD12	2.13	0.49
2:N:257:PRO:HA	1:a:388:PHE:CD1	2.47	0.49
1:A:169:PRO:HD2	1:A:201:GLU:CB	2.42	0.49
1:G:169:PRO:HD2	1:G:201:GLU:CB	2.42	0.49
1:G:307:LEU:O	1:G:339:ILE:HD12	2.13	0.49
2:H:340:ILE:HD11	1:U:385:ARG:HH12	1.51	0.49
1:Q:169:PRO:HD2	1:Q:201:GLU:CB	2.42	0.49
1:U:307:LEU:O	1:U:339:ILE:HD12	2.13	0.49
1:Y:169:PRO:HD2	1:Y:201:GLU:CB	2.42	0.49
1:G:274:LYS:NZ	1:G:278:GLU:OE2	2.46	0.49
1:K:169:PRO:HD2	1:K:201:GLU:CB	2.42	0.49
2:L:116:ASP:OD2	2:L:120:LYS:NZ	2.46	0.49
2:b:145:LEU:O	2:b:146:ALA:C	2.55	0.49
1:S:307:LEU:O	1:S:339:ILE:HD12	2.13	0.49
1:W:169:PRO:HD2	1:W:201:GLU:CB	2.42	0.49
1:W:307:LEU:O	1:W:339:ILE:HD12	2.13	0.49
1:B:169:PRO:HD2	1:B:201:GLU:CB	2.42	0.48
1:K:307:LEU:O	1:K:339:ILE:HD12	2.13	0.48
1:O:169:PRO:HD2	1:O:201:GLU:CB	2.42	0.48
1:a:169:PRO:HD2	1:a:201:GLU:CB	2.42	0.48
2:J:116:ASP:OD2	2:J:120:LYS:NZ	2.46	0.48
2:N:116:ASP:OD2	2:N:120:LYS:NZ	2.46	0.48
1:S:169:PRO:HD2	1:S:201:GLU:CB	2.42	0.48
2:L:257:PRO:CA	1:Y:388:PHE:CE1	2.93	0.48
1:U:169:PRO:HD2	1:U:201:GLU:CB	2.42	0.48
1:Y:307:LEU:O	1:Y:339:ILE:HD12	2.13	0.48
1:a:307:LEU:O	1:a:339:ILE:HD12	2.13	0.48
1:Q:307:LEU:O	1:Q:339:ILE:HD12	2.13	0.48
2:D:329:LYS:HZ1	1:O:170:LYS:NZ	2.06	0.48
2:H:257:PRO:CA	1:U:388:PHE:CD1	2.97	0.48
1:S:336:VAL:HG11	1:S:338:TRP:NE1	2.29	0.48
2:T:116:ASP:OD2	2:T:120:LYS:NZ	2.46	0.48
1:A:336:VAL:HG11	1:A:338:TRP:NE1	2.29	0.48
2:D:329:LYS:HZ3	1:O:170:LYS:HZ1	1.48	0.48
2:F:116:ASP:OD2	2:F:120:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:40:LYS:HE3	2:R:305:LYS:CE	2.25	0.48
1:U:336:VAL:HG11	1:U:338:TRP:NE1	2.29	0.48
1:W:336:VAL:HG11	1:W:338:TRP:NE1	2.29	0.48
1:A:307:LEU:O	1:A:339:ILE:HD12	2.13	0.48
2:P:116:ASP:OD2	2:P:120:LYS:NZ	2.46	0.48
1:Q:336:VAL:HG11	1:Q:338:TRP:NE1	2.29	0.48
2:X:116:ASP:OD2	2:X:120:LYS:NZ	2.46	0.48
2:Z:116:ASP:OD2	2:Z:120:LYS:NZ	2.46	0.48
1:B:336:VAL:HG11	1:B:338:TRP:NE1	2.29	0.48
1:E:307:LEU:O	1:E:339:ILE:HD12	2.13	0.48
2:H:340:ILE:HD12	1:U:385:ARG:HD3	1.93	0.48
1:O:307:LEU:O	1:O:339:ILE:HD12	2.13	0.48
1:Q:274:LYS:NZ	1:Q:278:GLU:OE2	2.46	0.48
1:B:307:LEU:O	1:B:339:ILE:HD12	2.13	0.48
1:E:169:PRO:HD2	1:E:201:GLU:CB	2.42	0.48
1:E:260:HIS:ND1	1:E:260:HIS:N	2.61	0.48
1:G:260:HIS:ND1	1:G:260:HIS:N	2.61	0.48
2:H:116:ASP:OD2	2:H:120:LYS:NZ	2.46	0.48
2:P:145:LEU:O	2:P:146:ALA:C	2.55	0.48
2:T:40:LYS:NZ	2:V:305:LYS:CE	2.77	0.48
2:Z:40:LYS:NZ	2:b:305:LYS:CE	2.77	0.48
1:O:336:VAL:HG11	1:O:338:TRP:NE1	2.29	0.48
1:Y:336:VAL:HG11	1:Y:338:TRP:NE1	2.29	0.48
2:F:321:HIS:CE1	1:S:218:LEU:CG	2.92	0.47
1:K:336:VAL:HG11	1:K:338:TRP:NE1	2.29	0.47
2:L:40:LYS:NZ	2:N:305:LYS:CE	2.77	0.47
1:U:274:LYS:NZ	1:U:278:GLU:OE2	2.46	0.47
2:Z:145:LEU:O	2:Z:146:ALA:C	2.55	0.47
1:I:336:VAL:HG11	1:I:338:TRP:NE1	2.29	0.47
1:M:336:VAL:HG11	1:M:338:TRP:NE1	2.29	0.47
1:S:274:LYS:NZ	1:S:278:GLU:OE2	2.46	0.47
2:b:116:ASP:OD2	2:b:120:LYS:NZ	2.46	0.47
2:D:116:ASP:OD2	2:D:120:LYS:NZ	2.46	0.47
2:D:257:PRO:CG	1:O:388:PHE:CE1	2.96	0.47
1:G:336:VAL:HG11	1:G:338:TRP:NE1	2.29	0.47
1:M:169:PRO:HD2	1:M:201:GLU:CB	2.42	0.47
1:a:336:VAL:HG11	1:a:338:TRP:NE1	2.29	0.47
2:D:329:LYS:CE	1:O:170:LYS:NZ	2.67	0.47
1:E:336:VAL:HG11	1:E:338:TRP:NE1	2.29	0.47
2:R:116:ASP:OD2	2:R:120:LYS:NZ	2.46	0.47
1:G:168:SER:OG	1:G:201:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:40:LYS:NZ	2:L:305:LYS:HE2	2.30	0.47
2:V:116:ASP:OD2	2:V:120:LYS:NZ	2.46	0.47
2:X:40:LYS:NZ	2:Z:305:LYS:HE2	2.30	0.47
1:Y:168:SER:OG	1:Y:201:GLU:HB2	2.15	0.47
1:I:260:HIS:ND1	1:I:260:HIS:N	2.61	0.47
1:M:274:LYS:NZ	1:M:278:GLU:OE2	2.46	0.47
1:S:168:SER:OG	1:S:201:GLU:HB2	2.15	0.47
2:V:40:LYS:NZ	2:X:305:LYS:CE	2.78	0.47
1:A:169:PRO:HD2	1:A:201:GLU:HB3	1.96	0.47
1:B:169:PRO:HD2	1:B:201:GLU:HB3	1.96	0.47
1:M:307:LEU:O	1:M:339:ILE:HD12	2.13	0.47
2:N:321:HIS:CE1	1:a:218:LEU:CD1	2.96	0.47
1:O:168:SER:OG	1:O:201:GLU:HB2	2.15	0.47
1:O:169:PRO:HD2	1:O:201:GLU:HB3	1.96	0.47
1:Q:168:SER:OG	1:Q:201:GLU:HB2	2.15	0.47
1:Q:169:PRO:HD2	1:Q:201:GLU:HB3	1.96	0.47
1:a:168:SER:OG	1:a:201:GLU:HB2	2.15	0.47
2:C:116:ASP:OD2	2:C:120:LYS:NZ	2.46	0.47
2:C:145:LEU:O	2:C:146:ALA:C	2.55	0.47
2:F:40:LYS:NZ	2:H:305:LYS:CE	2.77	0.47
1:M:168:SER:OG	1:M:201:GLU:HB2	2.15	0.47
1:a:169:PRO:HD2	1:a:201:GLU:HB3	1.96	0.47
2:H:145:LEU:O	2:H:146:ALA:C	2.55	0.47
1:I:168:SER:OG	1:I:201:GLU:HB2	2.15	0.47
2:P:40:LYS:HZ2	2:R:305:LYS:HE2	1.78	0.47
1:W:168:SER:OG	1:W:201:GLU:HB2	2.15	0.47
2:D:257:PRO:O	1:O:390:HIS:HE1	1.97	0.47
1:B:260:HIS:ND1	1:B:260:HIS:N	2.61	0.47
1:E:168:SER:OG	1:E:201:GLU:HB2	2.15	0.47
2:H:40:LYS:NZ	2:J:305:LYS:CE	2.78	0.47
1:M:169:PRO:HD2	1:M:201:GLU:HB3	1.96	0.47
1:B:168:SER:OG	1:B:201:GLU:HB2	2.15	0.46
1:E:169:PRO:HD2	1:E:201:GLU:HB3	1.96	0.46
1:U:169:PRO:HD2	1:U:201:GLU:HB3	1.96	0.46
2:F:145:LEU:O	2:F:146:ALA:C	2.55	0.46
2:N:321:HIS:HE1	1:a:218:LEU:HD12	1.80	0.46
1:W:169:PRO:HD2	1:W:201:GLU:HB3	1.96	0.46
1:G:169:PRO:HD2	1:G:201:GLU:HB3	1.96	0.46
2:H:237:THR:OG1	2:H:245:ASN:HB2	2.16	0.46
1:I:169:PRO:HD2	1:I:201:GLU:HB3	1.96	0.46
2:J:257:PRO:CA	1:W:388:PHE:CD1	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:168:SER:OG	1:U:201:GLU:HB2	2.15	0.46
2:F:257:PRO:HA	1:S:388:PHE:CD1	2.51	0.46
2:T:145:LEU:O	2:T:146:ALA:C	2.55	0.46
1:W:338:TRP:HE3	2:X:389:ALA:HB2	1.81	0.46
1:Y:169:PRO:HD2	1:Y:201:GLU:HB3	1.96	0.46
2:D:237:THR:OG1	2:D:245:ASN:HB2	2.16	0.46
1:K:168:SER:OG	1:K:201:GLU:HB2	2.15	0.46
2:X:237:THR:OG1	2:X:245:ASN:HB2	2.16	0.46
1:E:338:TRP:HE3	2:F:389:ALA:HB2	1.81	0.46
2:L:237:THR:OG1	2:L:245:ASN:HB2	2.16	0.46
1:S:169:PRO:HD2	1:S:201:GLU:HB3	1.96	0.46
1:Y:274:LYS:NZ	1:Y:278:GLU:OE2	2.46	0.46
2:J:237:THR:OG1	2:J:245:ASN:HB2	2.16	0.46
2:L:321:HIS:CE1	1:Y:218:LEU:CD1	2.98	0.46
2:T:237:THR:OG1	2:T:245:ASN:HB2	2.16	0.46
2:Z:237:THR:OG1	2:Z:245:ASN:HB2	2.16	0.46
2:b:237:THR:OG1	2:b:245:ASN:HB2	2.16	0.46
1:G:338:TRP:HE3	2:H:389:ALA:HB2	1.81	0.46
1:K:260:HIS:ND1	1:K:260:HIS:N	2.61	0.46
2:N:237:THR:OG1	2:N:245:ASN:HB2	2.16	0.46
1:U:338:TRP:HE3	2:V:389:ALA:HB2	1.81	0.46
1:A:168:SER:OG	1:A:201:GLU:HB2	2.15	0.46
1:B:338:TRP:HE3	2:C:389:ALA:HB2	1.81	0.46
2:H:321:HIS:CE1	1:U:218:LEU:CG	2.95	0.46
2:C:322:SER:HB2	1:Q:208:GLU:OE2	2.16	0.46
1:K:169:PRO:HD2	1:K:201:GLU:HB3	1.96	0.46
2:R:237:THR:OG1	2:R:245:ASN:HB2	2.16	0.46
1:W:274:LYS:NZ	1:W:278:GLU:OE2	2.46	0.46
2:X:145:LEU:O	2:X:146:ALA:C	2.55	0.46
1:O:260:HIS:ND1	1:O:260:HIS:N	2.61	0.45
1:O:338:TRP:HE3	2:P:389:ALA:HB2	1.81	0.45
2:T:40:LYS:NZ	2:V:305:LYS:HE2	2.32	0.45
2:N:145:LEU:O	2:N:146:ALA:C	2.55	0.45
2:R:145:LEU:O	2:R:146:ALA:C	2.55	0.45
1:Y:260:HIS:ND1	1:Y:260:HIS:N	2.61	0.45
2:F:237:THR:OG1	2:F:245:ASN:HB2	2.16	0.45
2:C:329:LYS:HE2	1:Q:170:LYS:CE	2.47	0.45
1:M:338:TRP:HE3	2:N:389:ALA:HB2	1.81	0.45
2:C:321:HIS:CE1	1:Q:218:LEU:CD1	2.98	0.45
1:I:274:LYS:NZ	1:I:278:GLU:OE2	2.46	0.45
2:L:321:HIS:HE1	1:Y:218:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:329:LYS:HE2	1:Y:170:LYS:HZ2	1.78	0.45
1:Y:338:TRP:HE3	2:Z:389:ALA:HB2	1.81	0.45
1:B:274:LYS:NZ	1:B:278:GLU:OE2	2.46	0.45
2:L:40:LYS:NZ	2:N:305:LYS:HE2	2.31	0.45
1:A:260:HIS:ND1	1:A:260:HIS:N	2.61	0.45
2:D:340:ILE:CD1	1:O:385:ARG:HD3	2.21	0.45
2:C:237:THR:OG1	2:C:245:ASN:HB2	2.16	0.45
2:V:237:THR:OG1	2:V:245:ASN:HB2	2.16	0.45
1:M:260:HIS:ND1	1:M:260:HIS:N	2.61	0.45
2:P:237:THR:OG1	2:P:245:ASN:HB2	2.16	0.45
1:Q:338:TRP:HE3	2:R:389:ALA:HB2	1.81	0.45
2:V:145:LEU:O	2:V:146:ALA:C	2.55	0.45
2:D:40:LYS:HE3	2:C:305:LYS:CE	2.25	0.45
1:I:338:TRP:HE3	2:J:389:ALA:HB2	1.81	0.45
2:J:321:HIS:HE1	1:W:218:LEU:HD12	1.80	0.45
1:K:338:TRP:HE3	2:L:389:ALA:HB2	1.81	0.45
2:X:40:LYS:NZ	2:Z:305:LYS:HE3	2.32	0.45
1:A:274:LYS:NZ	1:A:278:GLU:OE2	2.46	0.45
2:F:40:LYS:NZ	2:H:305:LYS:HE2	2.32	0.45
2:L:340:ILE:HD13	1:Y:385:ARG:HD2	1.95	0.44
2:Z:40:LYS:NZ	2:b:305:LYS:HE2	2.31	0.44
1:E:274:LYS:NZ	1:E:278:GLU:OE2	2.46	0.44
1:K:274:LYS:NZ	1:K:278:GLU:OE2	2.46	0.44
2:N:322:SER:HB2	1:a:208:GLU:OE2	2.17	0.44
2:N:56:LYS:NZ	1:O:427:TYR:HB3	2.33	0.44
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.89	0.44
1:A:338:TRP:HE3	2:D:389:ALA:HB2	1.81	0.44
2:J:40:LYS:NZ	2:L:305:LYS:HE3	2.32	0.44
2:J:257:PRO:CA	1:W:388:PHE:CE1	2.97	0.44
1:O:173:GLU:HG2	3:O:501:GDP:O3'	2.18	0.44
2:L:257:PRO:HA	1:Y:388:PHE:CD1	2.52	0.44
1:E:173:GLU:HG2	3:E:501:GDP:O3'	2.18	0.44
2:P:170:SER:HB2	2:P:203:ASP:OD1	2.18	0.44
1:Q:173:GLU:HG2	3:Q:501:GDP:O3'	2.18	0.44
1:G:173:GLU:HG2	3:G:501:GDP:O3'	2.18	0.44
2:H:40:LYS:NZ	2:J:305:LYS:HE2	2.33	0.44
2:L:145:LEU:O	2:L:146:ALA:C	2.55	0.44
1:M:173:GLU:HG2	3:M:501:GDP:O3'	2.18	0.44
2:V:40:LYS:NZ	2:X:305:LYS:HE2	2.33	0.44
2:Z:170:SER:HB2	2:Z:203:ASP:OD1	2.18	0.44
2:D:145:LEU:O	2:D:146:ALA:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:SER:HB2	2:C:203:ASP:OD1	2.18	0.43
1:K:173:GLU:HG2	3:K:501:GDP:O3'	2.18	0.43
1:S:173:GLU:HG2	3:S:501:GDP:O3'	2.18	0.43
2:D:322:SER:OG	1:O:215:ASN:HA	2.18	0.43
2:D:329:LYS:HE2	1:O:170:LYS:CE	2.48	0.43
2:N:329:LYS:HE2	1:a:170:LYS:CE	2.49	0.43
1:U:173:GLU:HG2	3:U:501:GDP:O3'	2.18	0.43
1:W:173:GLU:HG2	3:W:501:GDP:O3'	2.18	0.43
1:a:274:LYS:NZ	1:a:278:GLU:OE2	2.46	0.43
1:a:338:TRP:HE3	2:b:389:ALA:HB2	1.81	0.43
2:R:40:LYS:NZ	2:T:305:LYS:CE	2.81	0.43
1:S:338:TRP:HE3	2:T:389:ALA:HB2	1.81	0.43
2:T:170:SER:HB2	2:T:203:ASP:OD1	2.18	0.43
2:X:170:SER:HB2	2:X:203:ASP:OD1	2.18	0.43
2:b:170:SER:HB2	2:b:203:ASP:OD1	2.18	0.43
1:B:173:GLU:HG2	3:B:501:GDP:O3'	2.18	0.43
2:H:170:SER:HB2	2:H:203:ASP:OD1	2.18	0.43
1:I:173:GLU:HG2	3:I:501:GDP:O3'	2.18	0.43
2:J:170:SER:HB2	2:J:203:ASP:OD1	2.18	0.43
2:J:321:HIS:CE1	1:W:218:LEU:CD1	2.99	0.43
2:N:170:SER:HB2	2:N:203:ASP:OD1	2.18	0.43
2:J:95:ASP:C	2:J:95:ASP:OD1	2.61	0.43
2:D:329:LYS:HE2	1:O:170:LYS:HZ1	1.80	0.43
2:L:170:SER:HB2	2:L:203:ASP:OD1	2.18	0.43
1:O:274:LYS:NZ	1:O:278:GLU:OE2	2.46	0.43
2:R:170:SER:HB2	2:R:203:ASP:OD1	2.18	0.43
1:a:173:GLU:HG2	3:a:501:GDP:O3'	2.18	0.43
2:V:170:SER:HB2	2:V:203:ASP:OD1	2.18	0.43
1:Y:173:GLU:HG2	3:Y:501:GDP:O3'	2.18	0.43
2:F:170:SER:HB2	2:F:203:ASP:OD1	2.18	0.43
2:C:95:ASP:OD1	2:C:95:ASP:C	2.61	0.42
2:F:244:LEU:O	2:F:245:ASN:C	2.62	0.42
2:H:257:PRO:HA	1:U:388:PHE:CD1	2.54	0.42
2:J:244:LEU:O	2:J:245:ASN:C	2.62	0.42
1:A:173:GLU:HG2	3:A:501:GDP:O3'	2.18	0.42
2:F:322:SER:HB2	1:S:208:GLU:OE2	2.19	0.42
2:R:244:LEU:O	2:R:245:ASN:C	2.62	0.42
2:V:244:LEU:O	2:V:245:ASN:C	2.62	0.42
2:D:170:SER:HB2	2:D:203:ASP:OD1	2.18	0.42
2:J:340:ILE:HD13	1:W:385:ARG:HD2	1.93	0.42
2:R:40:LYS:NZ	2:T:305:LYS:HE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:244:LEU:O	2:X:245:ASN:C	2.62	0.42
2:C:40:LYS:NZ	2:F:305:LYS:CE	2.81	0.42
2:C:346:LYS:HB2	1:Q:173:GLU:O	2.20	0.42
2:H:40:LYS:NZ	2:J:305:LYS:HE3	2.35	0.42
2:H:95:ASP:OD1	2:H:95:ASP:C	2.61	0.42
2:H:146:ALA:HB3	2:H:147:PRO:HD3	2.02	0.42
2:L:244:LEU:O	2:L:245:ASN:C	2.62	0.42
2:b:244:LEU:O	2:b:245:ASN:C	2.62	0.42
2:D:244:LEU:O	2:D:245:ASN:C	2.62	0.42
2:C:321:HIS:HE1	1:Q:218:LEU:HD12	1.83	0.42
2:L:146:ALA:HB3	2:L:147:PRO:HD3	2.02	0.42
2:N:244:LEU:O	2:N:245:ASN:C	2.62	0.42
2:X:146:ALA:HB3	2:X:147:PRO:HD3	2.02	0.42
1:B:67:PRO:HG3	1:B:90:ALA:O	2.20	0.42
2:J:146:ALA:HB3	2:J:147:PRO:HD3	2.02	0.42
2:T:95:ASP:OD1	2:T:95:ASP:C	2.61	0.42
2:Z:146:ALA:HB3	2:Z:147:PRO:HD3	2.02	0.42
2:Z:244:LEU:O	2:Z:245:ASN:C	2.62	0.42
1:M:67:PRO:HG3	1:M:90:ALA:O	2.20	0.42
1:O:67:PRO:HG3	1:O:90:ALA:O	2.20	0.42
2:X:95:ASP:C	2:X:95:ASP:OD1	2.61	0.42
2:Z:40:LYS:NZ	2:b:305:LYS:HE3	2.35	0.42
2:Z:352:LEU:HD12	2:Z:352:LEU:HA	1.87	0.42
1:a:67:PRO:HG3	1:a:90:ALA:O	2.20	0.42
1:E:141:SER:HB2	1:E:184:THR:OG1	2.20	0.42
1:U:141:SER:HB2	1:U:184:THR:OG1	2.20	0.42
1:a:141:SER:HB2	1:a:184:THR:OG1	2.20	0.42
2:D:329:LYS:HE2	1:O:170:LYS:HE3	2.01	0.42
1:I:141:SER:HB2	1:I:184:THR:OG1	2.20	0.42
1:O:141:SER:HB2	1:O:184:THR:OG1	2.20	0.42
1:Q:67:PRO:HG3	1:Q:90:ALA:O	2.20	0.42
2:T:244:LEU:O	2:T:245:ASN:C	2.62	0.42
2:V:40:LYS:NZ	2:X:305:LYS:HE3	2.35	0.42
2:V:146:ALA:HB3	2:V:147:PRO:HD3	2.02	0.42
2:b:146:ALA:HB3	2:b:147:PRO:HD3	2.02	0.42
1:A:67:PRO:HG3	1:A:90:ALA:O	2.20	0.42
1:A:141:SER:HB2	1:A:184:THR:OG1	2.20	0.42
2:C:40:LYS:NZ	2:F:305:LYS:HE2	2.35	0.42
2:F:40:LYS:NZ	2:H:305:LYS:HE3	2.35	0.42
1:G:239:SER:OG	1:G:240:GLY:N	2.53	0.42
1:K:337:ASN:O	1:K:338:TRP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:239:SER:OG	1:S:240:GLY:N	2.53	0.42
1:A:337:ASN:O	1:A:338:TRP:C	2.63	0.41
2:D:243:PRO:HB3	1:O:12:GLN:HE22	1.85	0.41
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.89	0.41
1:K:67:PRO:HG3	1:K:90:ALA:O	2.20	0.41
2:T:146:ALA:HB3	2:T:147:PRO:HD3	2.02	0.41
1:W:337:ASN:O	1:W:338:TRP:C	2.63	0.41
1:B:141:SER:HB2	1:B:184:THR:OG1	2.20	0.41
1:E:67:PRO:HG3	1:E:90:ALA:O	2.20	0.41
2:P:244:LEU:O	2:P:245:ASN:C	2.62	0.41
1:U:239:SER:OG	1:U:240:GLY:N	2.53	0.41
2:C:244:LEU:O	2:C:245:ASN:C	2.62	0.41
2:F:146:ALA:HB3	2:F:147:PRO:HD3	2.02	0.41
2:H:244:LEU:O	2:H:245:ASN:C	2.62	0.41
1:I:337:ASN:O	1:I:338:TRP:C	2.63	0.41
2:L:340:ILE:HD12	1:Y:385:ARG:HD3	1.90	0.41
1:M:337:ASN:O	1:M:338:TRP:C	2.63	0.41
2:N:146:ALA:HB3	2:N:147:PRO:HD3	2.02	0.41
2:N:257:PRO:CG	1:a:388:PHE:CE1	2.97	0.41
2:P:95:ASP:OD1	2:P:95:ASP:C	2.61	0.41
1:Q:54:ASP:OD1	1:Q:54:ASP:N	2.49	0.41
1:S:337:ASN:O	1:S:338:TRP:C	2.63	0.41
1:U:337:ASN:O	1:U:338:TRP:C	2.63	0.41
1:W:236:LEU:HD23	1:W:236:LEU:HA	1.89	0.41
2:J:329:LYS:HE2	1:W:170:LYS:HZ2	1.82	0.41
2:J:352:LEU:HD12	2:J:352:LEU:HA	1.87	0.41
1:S:141:SER:HB2	1:S:184:THR:OG1	2.20	0.41
1:Y:67:PRO:HG3	1:Y:90:ALA:O	2.20	0.41
1:Y:337:ASN:O	1:Y:338:TRP:C	2.63	0.41
2:D:40:LYS:HZ1	2:C:305:LYS:CE	2.29	0.41
2:D:146:ALA:HB3	2:D:147:PRO:HD3	2.02	0.41
1:B:337:ASN:O	1:B:338:TRP:C	2.63	0.41
1:I:239:SER:OG	1:I:240:GLY:N	2.53	0.41
2:L:95:ASP:OD1	2:L:95:ASP:C	2.61	0.41
1:M:141:SER:HB2	1:M:184:THR:OG1	2.20	0.41
1:Q:141:SER:HB2	1:Q:184:THR:OG1	2.20	0.41
1:Q:239:SER:OG	1:Q:240:GLY:N	2.53	0.41
1:W:141:SER:HB2	1:W:184:THR:OG1	2.20	0.41
2:D:95:ASP:C	2:D:95:ASP:OD1	2.61	0.41
1:E:152:ARG:NH2	1:E:158:VAL:O	2.51	0.41
1:M:236:LEU:HD23	1:M:236:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:56:LYS:HZ2	1:O:427:TYR:HB3	1.85	0.41
2:P:146:ALA:HB3	2:P:147:PRO:HD3	2.02	0.41
1:Y:141:SER:HB2	1:Y:184:THR:OG1	2.20	0.41
1:K:141:SER:HB2	1:K:184:THR:OG1	2.20	0.41
1:Q:152:ARG:NH2	1:Q:158:VAL:O	2.51	0.41
1:S:67:PRO:HG3	1:S:90:ALA:O	2.20	0.41
1:U:67:PRO:HG3	1:U:90:ALA:O	2.20	0.41
2:L:40:LYS:NZ	2:N:305:LYS:HE3	2.35	0.41
1:W:67:PRO:HG3	1:W:90:ALA:O	2.20	0.41
2:F:321:HIS:CE1	1:S:218:LEU:CD1	3.02	0.41
2:H:321:HIS:HE1	1:U:218:LEU:HD12	1.86	0.41
2:J:399:MET:O	2:J:400:GLN:C	2.64	0.41
1:O:337:ASN:O	1:O:338:TRP:C	2.63	0.41
2:T:40:LYS:NZ	2:V:305:LYS:HE3	2.35	0.41
2:Z:399:MET:O	2:Z:400:GLN:C	2.64	0.41
2:C:146:ALA:HB3	2:C:147:PRO:HD3	2.02	0.41
2:N:40:LYS:CE	2:P:305:LYS:HE3	2.51	0.41
2:R:146:ALA:HB3	2:R:147:PRO:HD3	2.02	0.41
2:X:399:MET:O	2:X:400:GLN:C	2.64	0.41
1:G:67:PRO:HG3	1:G:90:ALA:O	2.20	0.40
1:G:141:SER:HB2	1:G:184:THR:OG1	2.20	0.40
1:Q:318:LYS:NZ	2:R:217:GLU:OE1	2.54	0.40
1:a:318:LYS:NZ	2:b:217:GLU:OE1	2.54	0.40
2:D:340:ILE:HD11	1:O:385:ARG:HH11	0.61	0.40
1:I:67:PRO:HG3	1:I:90:ALA:O	2.20	0.40
2:N:329:LYS:HE2	1:a:170:LYS:HZ2	1.80	0.40
2:N:399:MET:O	2:N:400:GLN:C	2.64	0.40
1:W:239:SER:OG	1:W:240:GLY:N	2.53	0.40
1:a:337:ASN:O	1:a:338:TRP:C	2.63	0.40
2:b:95:ASP:C	2:b:95:ASP:OD1	2.61	0.40
1:E:337:ASN:O	1:E:338:TRP:C	2.63	0.40
2:R:95:ASP:C	2:R:95:ASP:OD1	2.61	0.40
2:V:399:MET:O	2:V:400:GLN:C	2.64	0.40
1:A:152:ARG:NH2	1:A:158:VAL:O	2.51	0.40
1:a:32:ASP:HA	1:a:33:PRO:HD3	1.97	0.40
1:B:152:ARG:NH2	1:B:158:VAL:O	2.51	0.40
1:E:236:LEU:HD23	1:E:236:LEU:HA	1.89	0.40
2:L:322:SER:HB2	1:Y:208:GLU:OE2	2.21	0.40
2:N:3:ARG:HD3	1:a:91:ASP:O	2.21	0.40
1:U:152:ARG:NH2	1:U:158:VAL:O	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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 PDB entries followed by that with respect to all EM entries.

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	357/358 (100%)	357 (100%)	0	100	100
1	B	357/358 (100%)	357 (100%)	0	100	100
1	E	357/358 (100%)	357 (100%)	0	100	100
1	G	357/358 (100%)	357 (100%)	0	100	100
1	I	357/358 (100%)	357 (100%)	0	100	100
1	K	357/358 (100%)	357 (100%)	0	100	100
1	M	357/358 (100%)	357 (100%)	0	100	100
1	O	357/358 (100%)	357 (100%)	0	100	100
1	Q	357/358 (100%)	357 (100%)	0	100	100
1	S	357/358 (100%)	357 (100%)	0	100	100
1	U	357/358 (100%)	357 (100%)	0	100	100
1	W	357/358 (100%)	357 (100%)	0	100	100
1	Y	357/358 (100%)	357 (100%)	0	100	100
1	a	357/358 (100%)	357 (100%)	0	100	100
2	C	371/372 (100%)	371 (100%)	0	100	100
2	D	371/372 (100%)	371 (100%)	0	100	100
2	F	371/372 (100%)	371 (100%)	0	100	100
2	H	371/372 (100%)	371 (100%)	0	100	100
2	J	371/372 (100%)	371 (100%)	0	100	100
2	L	371/372 (100%)	371 (100%)	0	100	100
2	N	371/372 (100%)	371 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	371/372 (100%)	371 (100%)	0	100	100
2	R	371/372 (100%)	371 (100%)	0	100	100
2	T	371/372 (100%)	371 (100%)	0	100	100
2	V	371/372 (100%)	371 (100%)	0	100	100
2	X	371/372 (100%)	371 (100%)	0	100	100
2	Z	371/372 (100%)	371 (100%)	0	100	100
2	b	371/372 (100%)	371 (100%)	0	100	100
All	All	10192/10220 (100%)	10192 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	225	GLN
2	D	321	HIS
2	D	375	GLN
2	D	412	GLN
2	C	225	GLN
2	C	375	GLN
2	C	412	GLN
2	F	225	GLN
2	F	375	GLN
2	F	412	GLN
2	H	225	GLN
2	H	375	GLN
2	H	412	GLN
2	J	225	GLN
2	J	375	GLN
2	J	412	GLN
2	L	225	GLN
2	L	375	GLN
2	L	412	GLN
2	N	225	GLN
2	N	321	HIS
2	N	375	GLN
2	N	412	GLN
1	O	12	GLN
2	P	225	GLN

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Mol	Chain	Res	Type
2	P	375	GLN
2	P	412	GLN
2	R	225	GLN
2	R	375	GLN
2	R	412	GLN
2	T	225	GLN
2	T	375	GLN
2	T	412	GLN
2	V	225	GLN
2	V	375	GLN
2	V	412	GLN
2	X	225	GLN
2	X	375	GLN
2	X	412	GLN
2	Z	225	GLN
2	Z	375	GLN
2	Z	412	GLN
2	b	225	GLN
2	b	375	GLN
2	b	412	GLN

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](#)

14 ligands are modelled in this entry.

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	$\# Z > 2$
3	GDP	K	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	M	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	W	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	S	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	B	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.74	9 (20%)
3	GDP	O	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	a	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	G	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	A	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	Y	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	I	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	Q	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	U	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	9 (20%)
3	GDP	E	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.73	9 (20%)

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
3	GDP	K	501	-	-	3/16/32/32	0/3/3/3
3	GDP	M	501	-	-	3/16/32/32	0/3/3/3
3	GDP	W	501	-	-	3/16/32/32	0/3/3/3
3	GDP	S	501	-	-	3/16/32/32	0/3/3/3
3	GDP	B	501	-	-	3/16/32/32	0/3/3/3
3	GDP	O	501	-	-	3/16/32/32	0/3/3/3
3	GDP	a	501	-	-	3/16/32/32	0/3/3/3
3	GDP	G	501	-	-	3/16/32/32	0/3/3/3
3	GDP	A	501	-	-	3/16/32/32	0/3/3/3
3	GDP	Y	501	-	-	3/16/32/32	0/3/3/3
3	GDP	I	501	-	-	3/16/32/32	0/3/3/3
3	GDP	Q	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	U	501	-	-	3/16/32/32	0/3/3/3
3	GDP	E	501	-	-	3/16/32/32	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	501	GDP	C4-N3	2.73	1.40	1.34
3	Y	501	GDP	C4-N3	2.73	1.40	1.34
3	E	501	GDP	C4-N3	2.72	1.40	1.34
3	W	501	GDP	C4-N3	2.71	1.40	1.34
3	B	501	GDP	C4-N3	2.71	1.40	1.34
3	S	501	GDP	C4-N3	2.70	1.40	1.34
3	U	501	GDP	C4-N3	2.70	1.40	1.34
3	A	501	GDP	C4-N3	2.70	1.40	1.34
3	I	501	GDP	C4-N3	2.70	1.40	1.34
3	Q	501	GDP	C4-N3	2.69	1.40	1.34
3	G	501	GDP	C4-N3	2.69	1.40	1.34
3	M	501	GDP	C4-N3	2.68	1.40	1.34
3	K	501	GDP	C4-N3	2.68	1.40	1.34
3	O	501	GDP	C4-N3	2.67	1.40	1.34
3	a	501	GDP	O4'-C1'	2.19	1.47	1.42
3	O	501	GDP	O4'-C1'	2.18	1.47	1.42
3	B	501	GDP	C5-C4	2.18	1.44	1.38
3	Y	501	GDP	O4'-C1'	2.18	1.47	1.42
3	I	501	GDP	PB-O2B	2.18	1.62	1.54
3	W	501	GDP	PB-O2B	2.17	1.62	1.54
3	E	501	GDP	PB-O2B	2.17	1.62	1.54
3	G	501	GDP	PB-O2B	2.17	1.62	1.54
3	U	501	GDP	C5-C4	2.17	1.44	1.38
3	Q	501	GDP	C5-C4	2.17	1.44	1.38
3	S	501	GDP	C5-C4	2.17	1.44	1.38
3	Y	501	GDP	PB-O2B	2.17	1.62	1.54
3	M	501	GDP	C5-C4	2.17	1.44	1.38
3	O	501	GDP	C5-C4	2.16	1.44	1.38
3	W	501	GDP	C5-C4	2.16	1.44	1.38
3	M	501	GDP	O4'-C1'	2.16	1.47	1.42
3	A	501	GDP	PB-O2B	2.16	1.62	1.54
3	B	501	GDP	PB-O2B	2.16	1.62	1.54
3	S	501	GDP	PB-O2B	2.16	1.62	1.54
3	E	501	GDP	O4'-C1'	2.16	1.47	1.42
3	A	501	GDP	C5-C4	2.15	1.44	1.38
3	I	501	GDP	C5-C4	2.15	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	501	GDP	PB-O2B	2.15	1.62	1.54
3	Q	501	GDP	PB-O2B	2.15	1.62	1.54
3	G	501	GDP	C5-C4	2.15	1.44	1.38
3	A	501	GDP	O4'-C1'	2.15	1.47	1.42
3	B	501	GDP	O4'-C1'	2.15	1.47	1.42
3	G	501	GDP	O4'-C1'	2.15	1.47	1.42
3	S	501	GDP	O4'-C1'	2.15	1.47	1.42
3	K	501	GDP	PB-O2B	2.15	1.62	1.54
3	a	501	GDP	PB-O2B	2.14	1.62	1.54
3	U	501	GDP	PB-O2B	2.14	1.62	1.54
3	O	501	GDP	PB-O2B	2.14	1.62	1.54
3	K	501	GDP	C5-C4	2.14	1.44	1.38
3	K	501	GDP	O4'-C1'	2.14	1.46	1.42
3	E	501	GDP	C5-C4	2.14	1.44	1.38
3	a	501	GDP	C5-C4	2.14	1.44	1.38
3	W	501	GDP	O4'-C1'	2.13	1.46	1.42
3	U	501	GDP	O4'-C1'	2.13	1.46	1.42
3	Q	501	GDP	O4'-C1'	2.13	1.46	1.42
3	I	501	GDP	O4'-C1'	2.13	1.46	1.42
3	Y	501	GDP	C5-C4	2.13	1.44	1.38

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	501	GDP	C5-C4-N3	-5.44	119.72	128.39
3	B	501	GDP	C2-N3-C4	5.44	121.68	112.30
3	B	501	GDP	C5-C4-N3	-5.44	119.73	128.39
3	O	501	GDP	C5-C4-N3	-5.44	119.74	128.39
3	O	501	GDP	C2-N3-C4	5.44	121.67	112.30
3	W	501	GDP	C5-C4-N3	-5.43	119.74	128.39
3	S	501	GDP	C2-N3-C4	5.43	121.66	112.30
3	I	501	GDP	C2-N3-C4	5.43	121.66	112.30
3	Y	501	GDP	C5-C4-N3	-5.43	119.75	128.39
3	A	501	GDP	C5-C4-N3	-5.43	119.75	128.39
3	W	501	GDP	C2-N3-C4	5.43	121.65	112.30
3	A	501	GDP	C2-N3-C4	5.43	121.65	112.30
3	U	501	GDP	C5-C4-N3	-5.43	119.75	128.39
3	Q	501	GDP	C2-N3-C4	5.43	121.65	112.30
3	M	501	GDP	C5-C4-N3	-5.42	119.76	128.39
3	a	501	GDP	C2-N3-C4	5.42	121.64	112.30
3	E	501	GDP	C5-C4-N3	-5.42	119.76	128.39
3	S	501	GDP	C5-C4-N3	-5.42	119.76	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	501	GDP	C2-N3-C4	5.42	121.64	112.30
3	G	501	GDP	C5-C4-N3	-5.42	119.77	128.39
3	I	501	GDP	C5-C4-N3	-5.41	119.77	128.39
3	E	501	GDP	C2-N3-C4	5.41	121.62	112.30
3	G	501	GDP	C2-N3-C4	5.41	121.62	112.30
3	Q	501	GDP	C5-C4-N3	-5.41	119.78	128.39
3	K	501	GDP	C5-C4-N3	-5.41	119.78	128.39
3	M	501	GDP	C2-N3-C4	5.41	121.61	112.30
3	U	501	GDP	C2-N3-C4	5.40	121.61	112.30
3	Y	501	GDP	C2-N3-C4	5.40	121.60	112.30
3	B	501	GDP	N9-C4-N3	4.13	134.22	125.95
3	Q	501	GDP	N9-C4-N3	4.13	134.21	125.95
3	O	501	GDP	N9-C4-N3	4.13	134.21	125.95
3	K	501	GDP	N9-C4-N3	4.12	134.19	125.95
3	S	501	GDP	N9-C4-N3	4.12	134.19	125.95
3	M	501	GDP	N9-C4-N3	4.12	134.19	125.95
3	A	501	GDP	N9-C4-N3	4.12	134.18	125.95
3	U	501	GDP	N9-C4-N3	4.11	134.18	125.95
3	E	501	GDP	N9-C4-N3	4.11	134.17	125.95
3	W	501	GDP	N9-C4-N3	4.11	134.16	125.95
3	G	501	GDP	N9-C4-N3	4.10	134.15	125.95
3	I	501	GDP	N9-C4-N3	4.10	134.15	125.95
3	Y	501	GDP	N9-C4-N3	4.09	134.14	125.95
3	a	501	GDP	N9-C4-N3	4.09	134.14	125.95
3	B	501	GDP	C6-C5-N7	3.06	135.87	130.29
3	U	501	GDP	C6-C5-N7	3.06	135.86	130.29
3	M	501	GDP	C6-C5-N7	3.05	135.84	130.29
3	O	501	GDP	C6-C5-N7	3.05	135.83	130.29
3	W	501	GDP	C6-C5-N7	3.04	135.83	130.29
3	I	501	GDP	C6-C5-N7	3.04	135.82	130.29
3	S	501	GDP	C6-C5-N7	3.03	135.81	130.29
3	A	501	GDP	C6-C5-N7	3.03	135.81	130.29
3	Q	501	GDP	C6-C5-N7	3.03	135.81	130.29
3	a	501	GDP	C6-C5-N7	3.03	135.81	130.29
3	G	501	GDP	C6-C5-N7	3.03	135.80	130.29
3	Y	501	GDP	C6-C5-N7	3.02	135.79	130.29
3	E	501	GDP	C6-C5-N7	3.02	135.79	130.29
3	K	501	GDP	C6-C5-N7	3.01	135.77	130.29
3	B	501	GDP	C8-N7-C5	2.82	109.28	104.26
3	U	501	GDP	C8-N7-C5	2.81	109.26	104.26
3	K	501	GDP	C8-N7-C5	2.80	109.25	104.26
3	S	501	GDP	C8-N7-C5	2.80	109.24	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	501	GDP	C8-N7-C5	2.80	109.24	104.26
3	I	501	GDP	C8-N7-C5	2.79	109.23	104.26
3	W	501	GDP	C8-N7-C5	2.79	109.23	104.26
3	Y	501	GDP	C8-N7-C5	2.79	109.22	104.26
3	a	501	GDP	C8-N7-C5	2.79	109.22	104.26
3	O	501	GDP	C8-N7-C5	2.78	109.22	104.26
3	A	501	GDP	C8-N7-C5	2.78	109.22	104.26
3	Q	501	GDP	C8-N7-C5	2.78	109.21	104.26
3	E	501	GDP	C8-N7-C5	2.77	109.20	104.26
3	G	501	GDP	C8-N7-C5	2.76	109.18	104.26
3	O	501	GDP	O3B-PB-O3A	2.47	112.93	104.64
3	E	501	GDP	O3B-PB-O3A	2.47	112.92	104.64
3	Q	501	GDP	O3B-PB-O3A	2.47	112.91	104.64
3	M	501	GDP	O3B-PB-O3A	2.47	112.91	104.64
3	W	501	GDP	O3B-PB-O3A	2.46	112.90	104.64
3	A	501	GDP	O3B-PB-O3A	2.46	112.90	104.64
3	Y	501	GDP	O3B-PB-O3A	2.46	112.89	104.64
3	G	501	GDP	O3B-PB-O3A	2.46	112.89	104.64
3	S	501	GDP	O3B-PB-O3A	2.46	112.89	104.64
3	B	501	GDP	O3B-PB-O3A	2.45	112.87	104.64
3	I	501	GDP	O3B-PB-O3A	2.45	112.86	104.64
3	U	501	GDP	O3B-PB-O3A	2.45	112.86	104.64
3	a	501	GDP	O3B-PB-O3A	2.45	112.85	104.64
3	K	501	GDP	O3B-PB-O3A	2.44	112.83	104.64
3	U	501	GDP	C4-C5-N7	-2.38	106.89	110.67
3	a	501	GDP	C4-C5-N7	-2.38	106.90	110.67
3	W	501	GDP	C4-C5-N7	-2.38	106.90	110.67
3	Y	501	GDP	C4-C5-N7	-2.37	106.91	110.67
3	B	501	GDP	C4-C5-N7	-2.37	106.92	110.67
3	M	501	GDP	C4-C5-N7	-2.37	106.92	110.67
3	O	501	GDP	C4-C5-N7	-2.36	106.92	110.67
3	A	501	GDP	C4-C5-N7	-2.36	106.93	110.67
3	G	501	GDP	C4-C5-N7	-2.35	106.94	110.67
3	K	501	GDP	C4-C5-N7	-2.35	106.95	110.67
3	S	501	GDP	C4-C5-N7	-2.35	106.95	110.67
3	I	501	GDP	C4-C5-N7	-2.34	106.95	110.67
3	E	501	GDP	C4-C5-N7	-2.34	106.96	110.67
3	Q	501	GDP	C4-C5-N7	-2.33	106.97	110.67
3	O	501	GDP	C2-N1-C6	-2.25	121.02	125.11
3	E	501	GDP	C2-N1-C6	-2.25	121.03	125.11
3	Y	501	GDP	C2-N1-C6	-2.24	121.05	125.11
3	W	501	GDP	C2-N1-C6	-2.24	121.06	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	501	GDP	C2-N1-C6	-2.23	121.06	125.11
3	G	501	GDP	C2-N1-C6	-2.23	121.06	125.11
3	M	501	GDP	C2-N1-C6	-2.23	121.07	125.11
3	U	501	GDP	C2-N1-C6	-2.23	121.07	125.11
3	Q	501	GDP	C2-N1-C6	-2.23	121.07	125.11
3	A	501	GDP	C2-N1-C6	-2.23	121.07	125.11
3	B	501	GDP	C2-N1-C6	-2.22	121.09	125.11
3	I	501	GDP	C2-N1-C6	-2.22	121.09	125.11
3	K	501	GDP	C2-N1-C6	-2.21	121.10	125.11
3	a	501	GDP	C2-N1-C6	-2.20	121.12	125.11
3	O	501	GDP	C5-C6-N1	2.16	118.74	113.25
3	B	501	GDP	C5-C6-N1	2.15	118.73	113.25
3	U	501	GDP	C5-C6-N1	2.15	118.72	113.25
3	E	501	GDP	C5-C6-N1	2.15	118.72	113.25
3	G	501	GDP	C5-C6-N1	2.15	118.72	113.25
3	M	501	GDP	C5-C6-N1	2.15	118.72	113.25
3	W	501	GDP	C5-C6-N1	2.15	118.72	113.25
3	I	501	GDP	C5-C6-N1	2.15	118.72	113.25
3	Q	501	GDP	C5-C6-N1	2.14	118.71	113.25
3	S	501	GDP	C5-C6-N1	2.14	118.70	113.25
3	A	501	GDP	C5-C6-N1	2.14	118.70	113.25
3	Y	501	GDP	C5-C6-N1	2.14	118.70	113.25
3	a	501	GDP	C5-C6-N1	2.13	118.67	113.25
3	K	501	GDP	C5-C6-N1	2.12	118.65	113.25

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GDP	PA-O3A-PB-O3B
3	B	501	GDP	PA-O3A-PB-O3B
3	E	501	GDP	PA-O3A-PB-O3B
3	G	501	GDP	PA-O3A-PB-O3B
3	I	501	GDP	PA-O3A-PB-O3B
3	K	501	GDP	PA-O3A-PB-O3B
3	M	501	GDP	PA-O3A-PB-O3B
3	O	501	GDP	PA-O3A-PB-O3B
3	Q	501	GDP	PA-O3A-PB-O3B
3	S	501	GDP	PA-O3A-PB-O3B
3	U	501	GDP	PA-O3A-PB-O3B
3	W	501	GDP	PA-O3A-PB-O3B
3	Y	501	GDP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	a	501	GDP	PA-O3A-PB-O3B
3	A	501	GDP	PA-O3A-PB-O2B
3	B	501	GDP	PA-O3A-PB-O2B
3	E	501	GDP	PA-O3A-PB-O2B
3	G	501	GDP	PA-O3A-PB-O2B
3	I	501	GDP	PA-O3A-PB-O2B
3	K	501	GDP	PA-O3A-PB-O2B
3	M	501	GDP	PA-O3A-PB-O2B
3	O	501	GDP	PA-O3A-PB-O2B
3	Q	501	GDP	PA-O3A-PB-O2B
3	S	501	GDP	PA-O3A-PB-O2B
3	U	501	GDP	PA-O3A-PB-O2B
3	W	501	GDP	PA-O3A-PB-O2B
3	Y	501	GDP	PA-O3A-PB-O2B
3	a	501	GDP	PA-O3A-PB-O2B
3	A	501	GDP	PA-O3A-PB-O1B
3	B	501	GDP	PA-O3A-PB-O1B
3	E	501	GDP	PA-O3A-PB-O1B
3	G	501	GDP	PA-O3A-PB-O1B
3	I	501	GDP	PA-O3A-PB-O1B
3	K	501	GDP	PA-O3A-PB-O1B
3	M	501	GDP	PA-O3A-PB-O1B
3	O	501	GDP	PA-O3A-PB-O1B
3	Q	501	GDP	PA-O3A-PB-O1B
3	S	501	GDP	PA-O3A-PB-O1B
3	U	501	GDP	PA-O3A-PB-O1B
3	W	501	GDP	PA-O3A-PB-O1B
3	Y	501	GDP	PA-O3A-PB-O1B
3	a	501	GDP	PA-O3A-PB-O1B

There are no ring outliers.

14 monomers are involved in 14 short contacts:

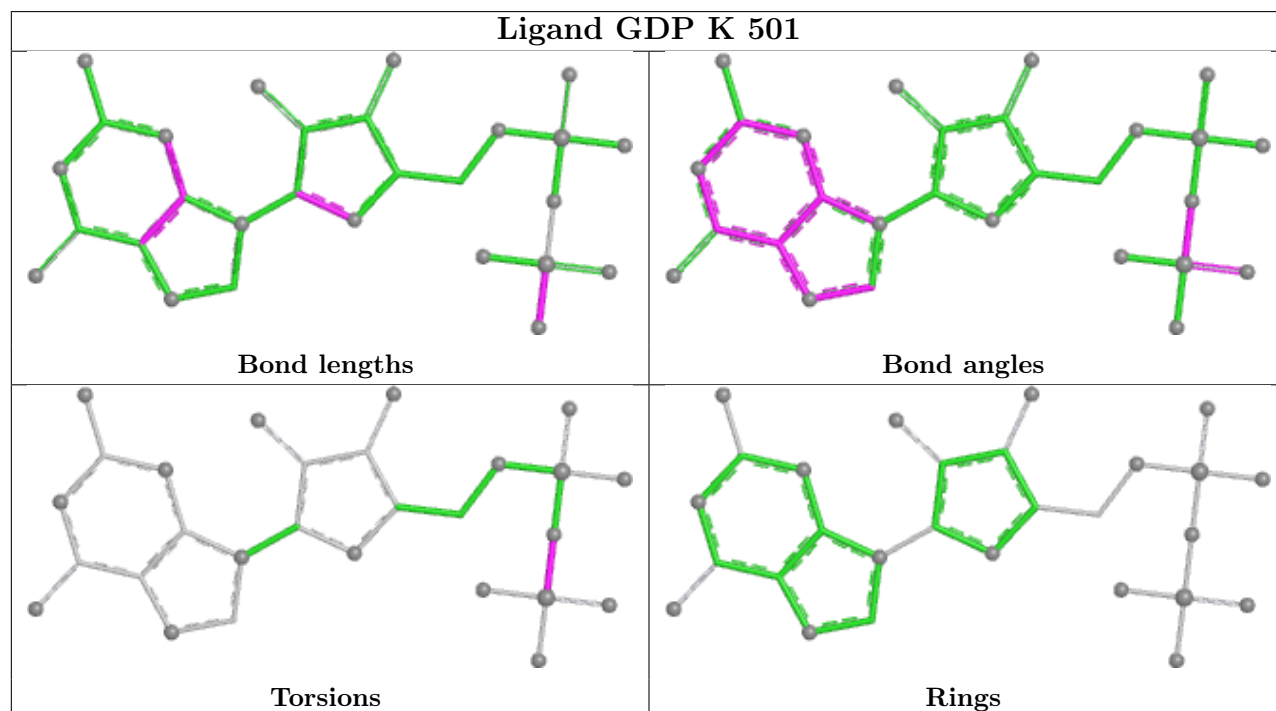
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	501	GDP	1	0
3	M	501	GDP	1	0
3	W	501	GDP	1	0
3	S	501	GDP	1	0
3	B	501	GDP	1	0
3	O	501	GDP	1	0
3	a	501	GDP	1	0
3	G	501	GDP	1	0

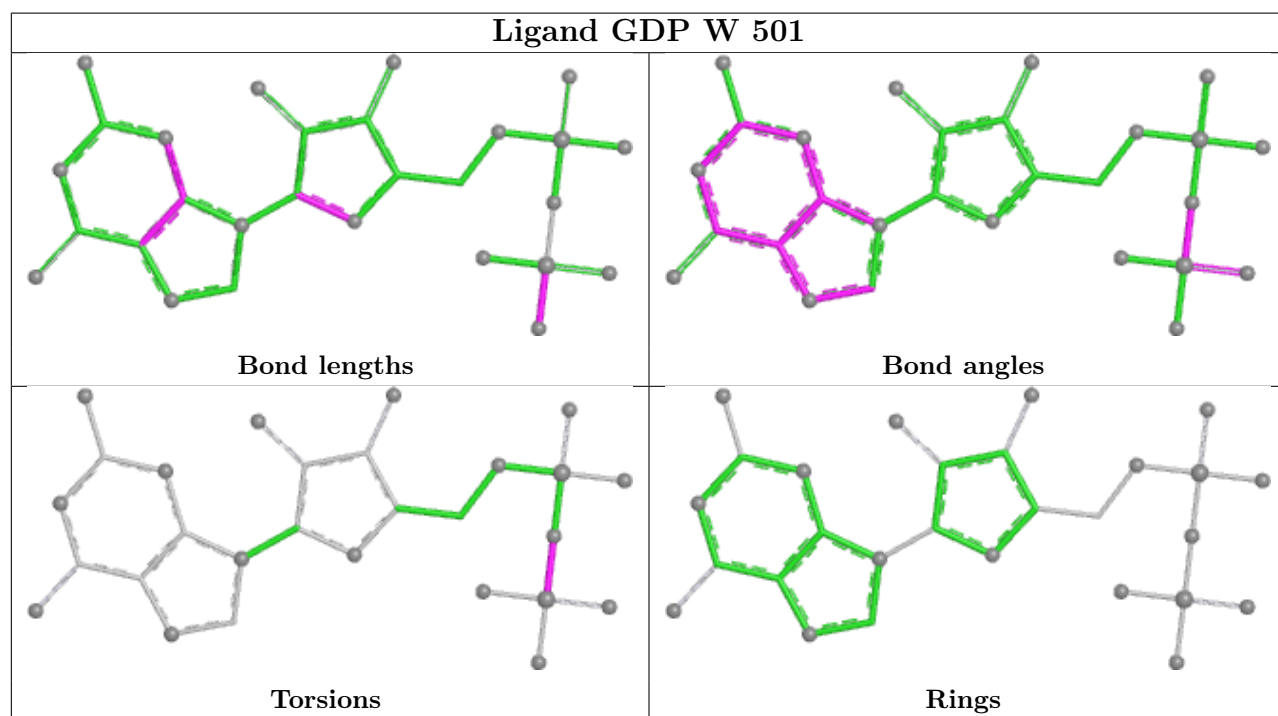
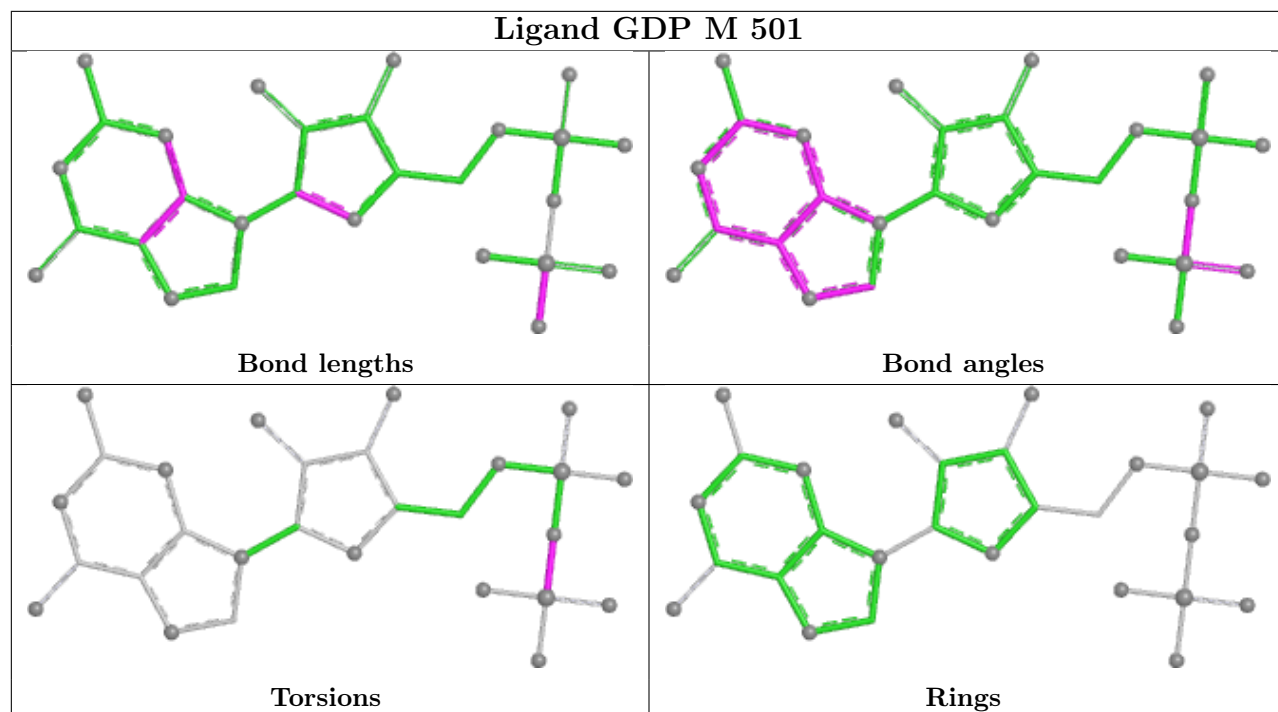
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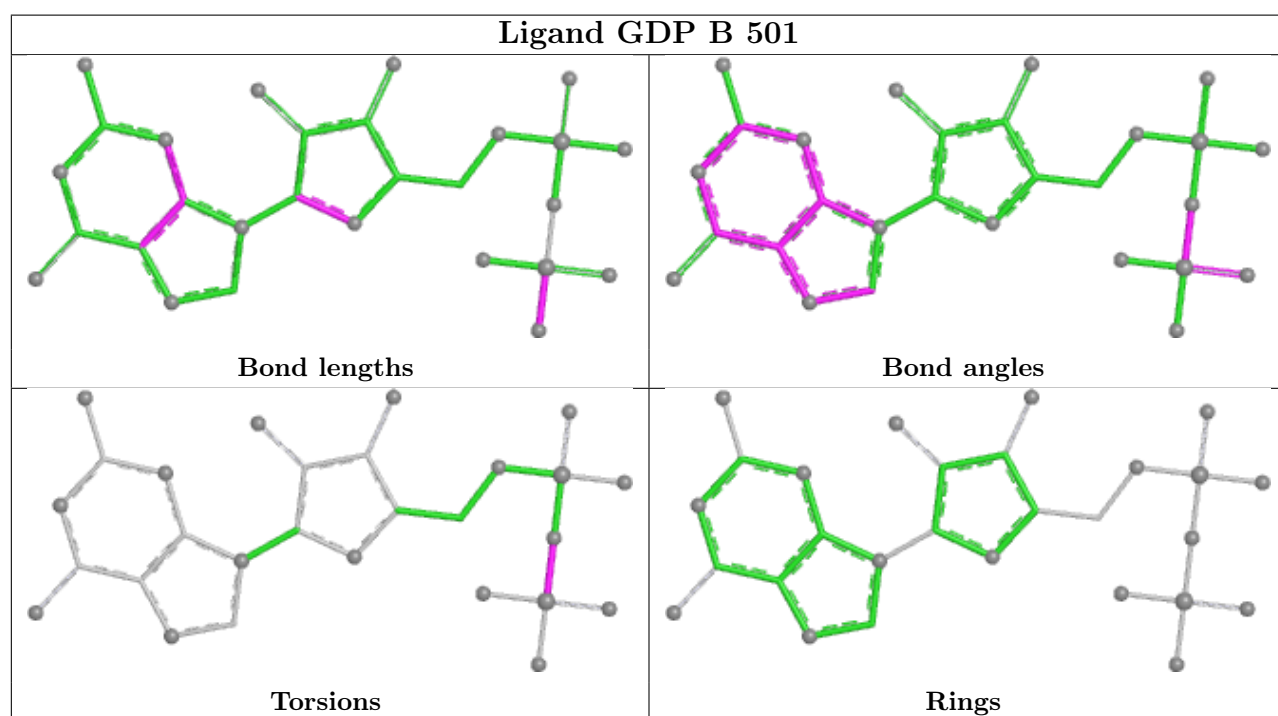
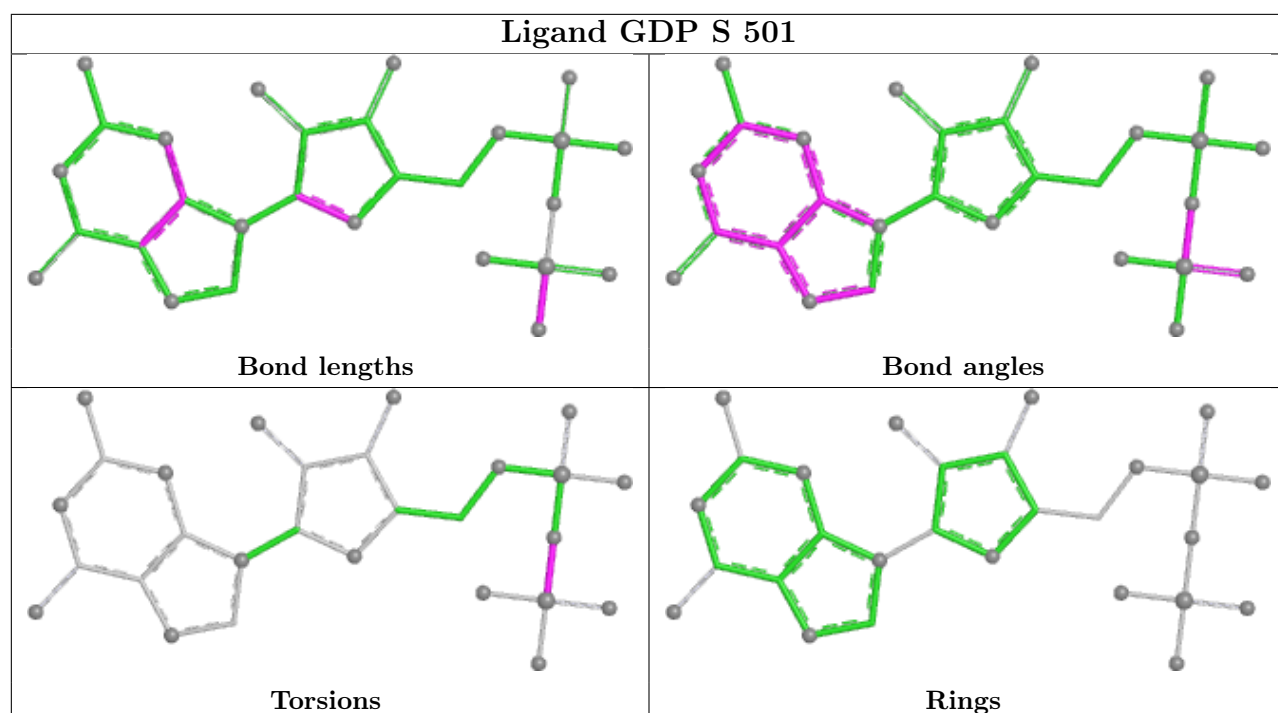
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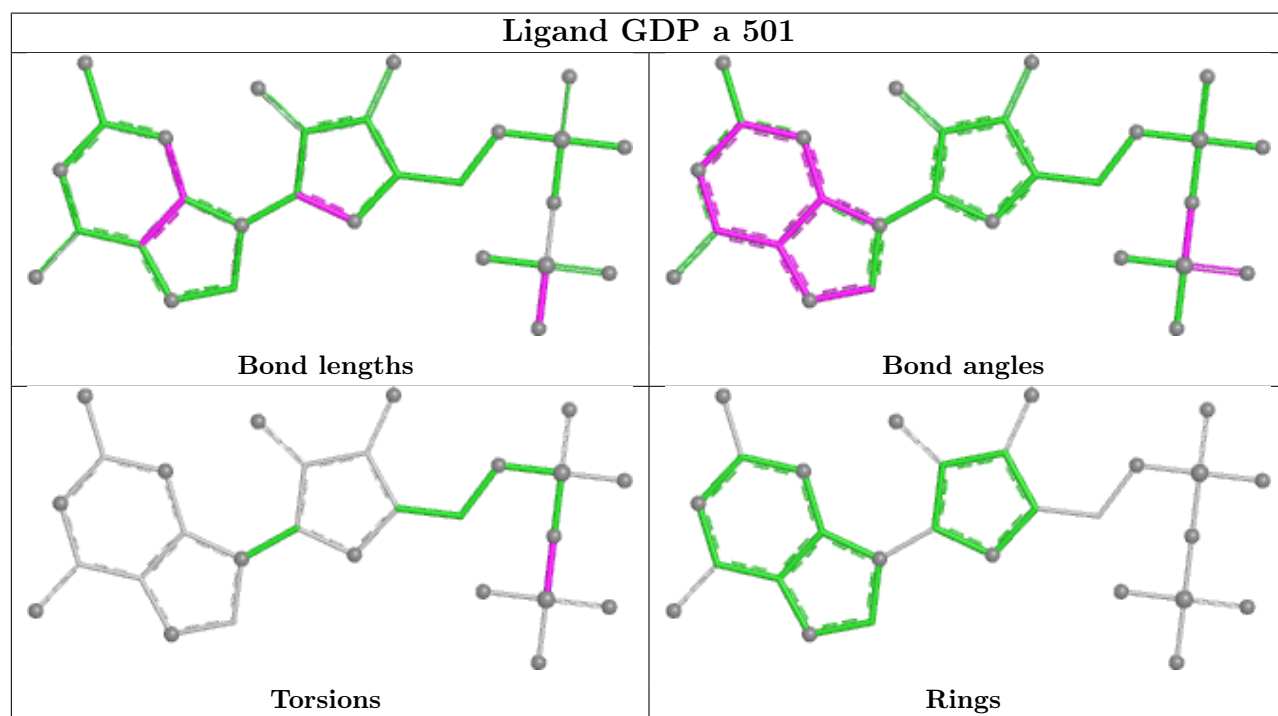
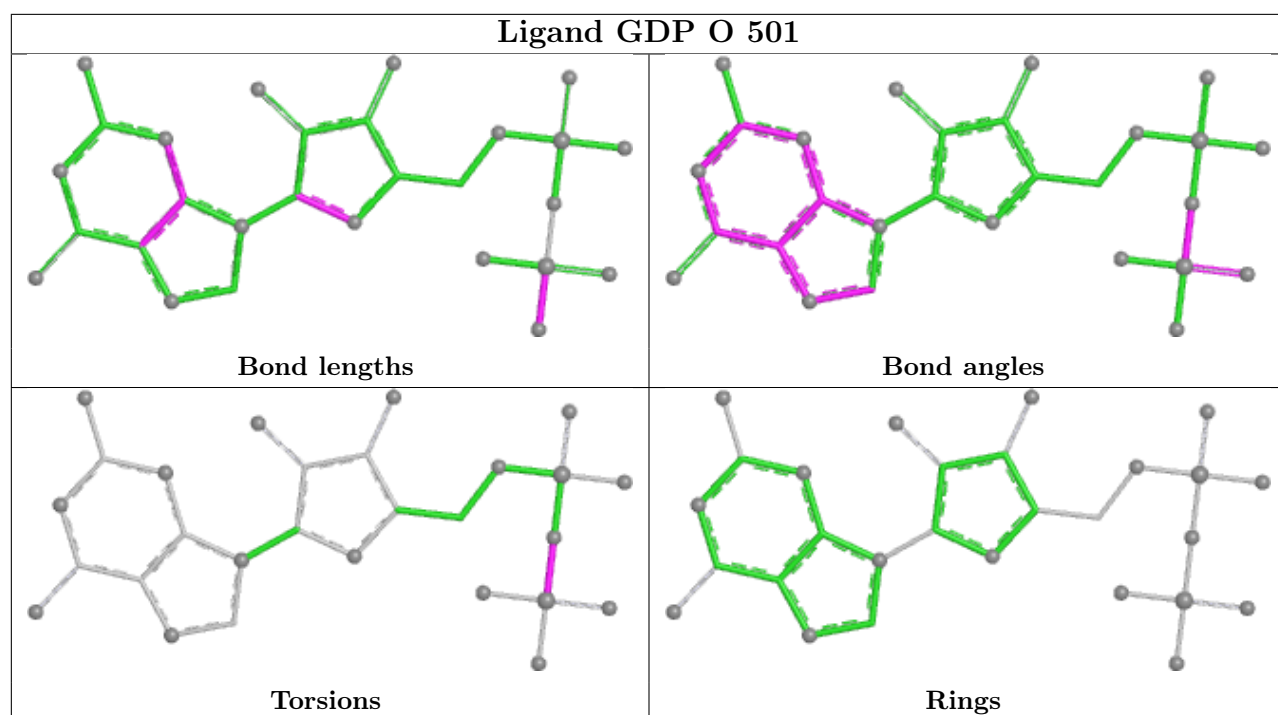
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GDP	1	0
3	Y	501	GDP	1	0
3	I	501	GDP	1	0
3	Q	501	GDP	1	0
3	U	501	GDP	1	0
3	E	501	GDP	1	0

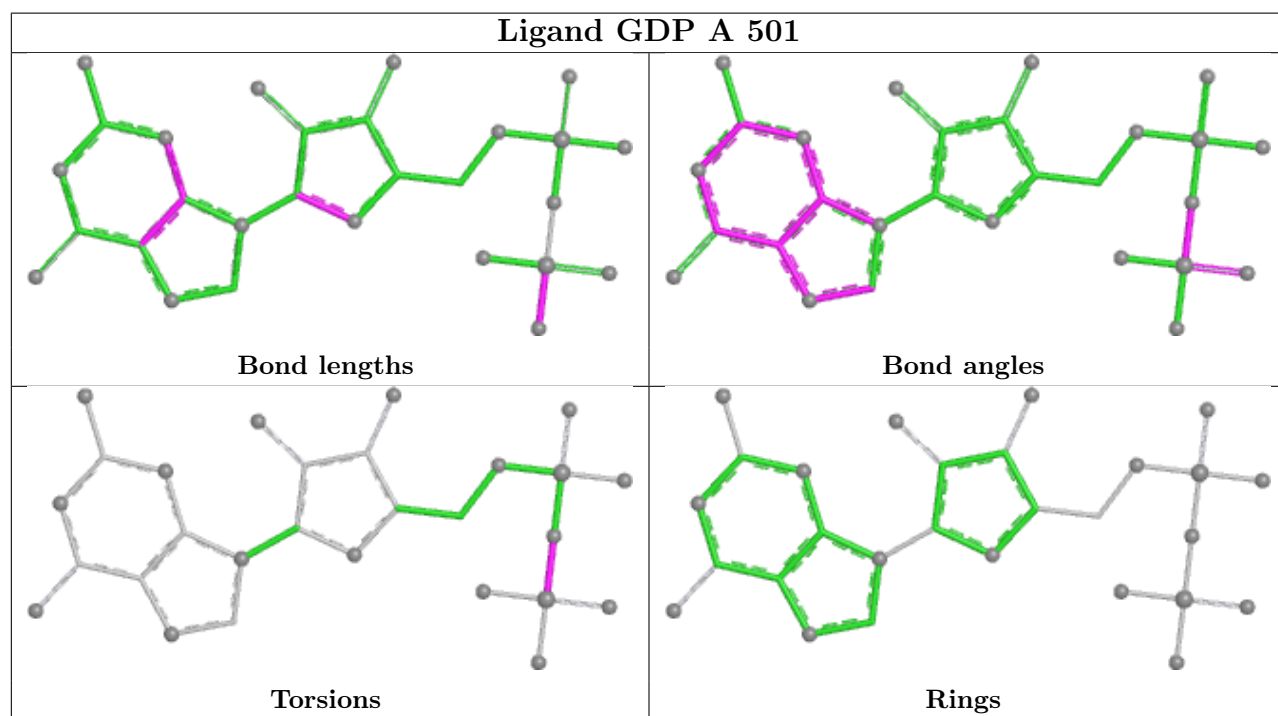
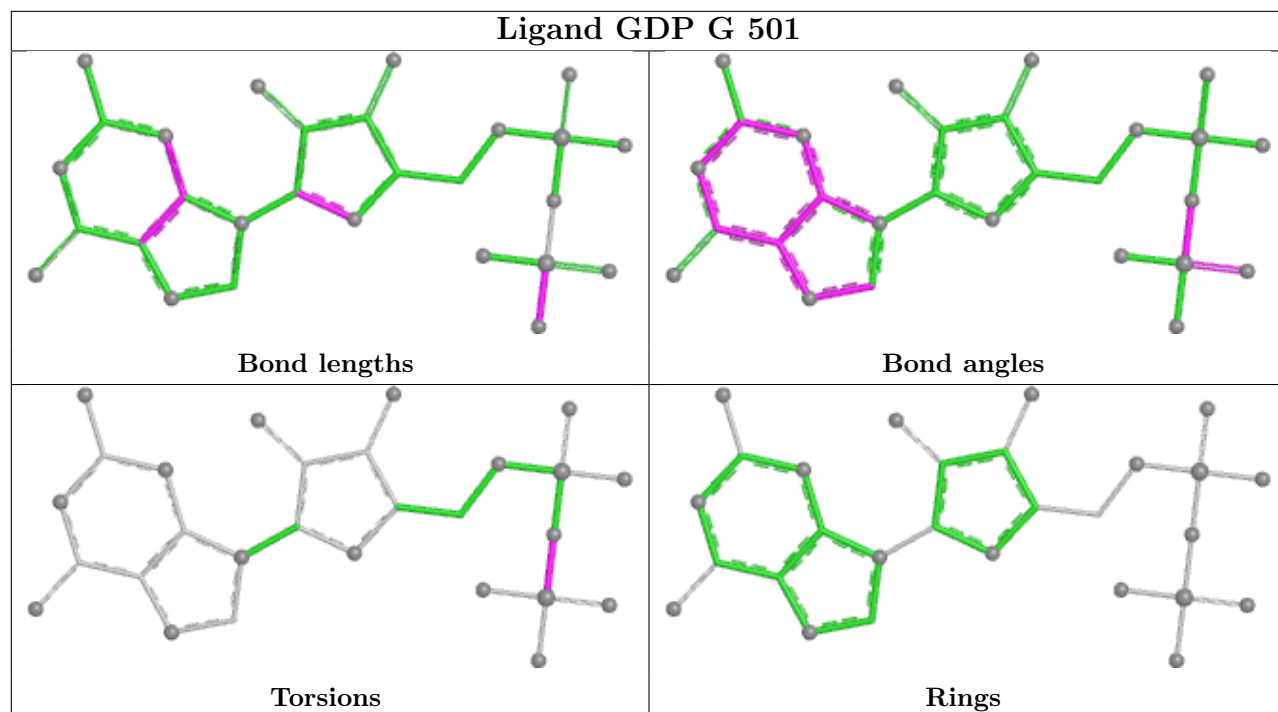
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

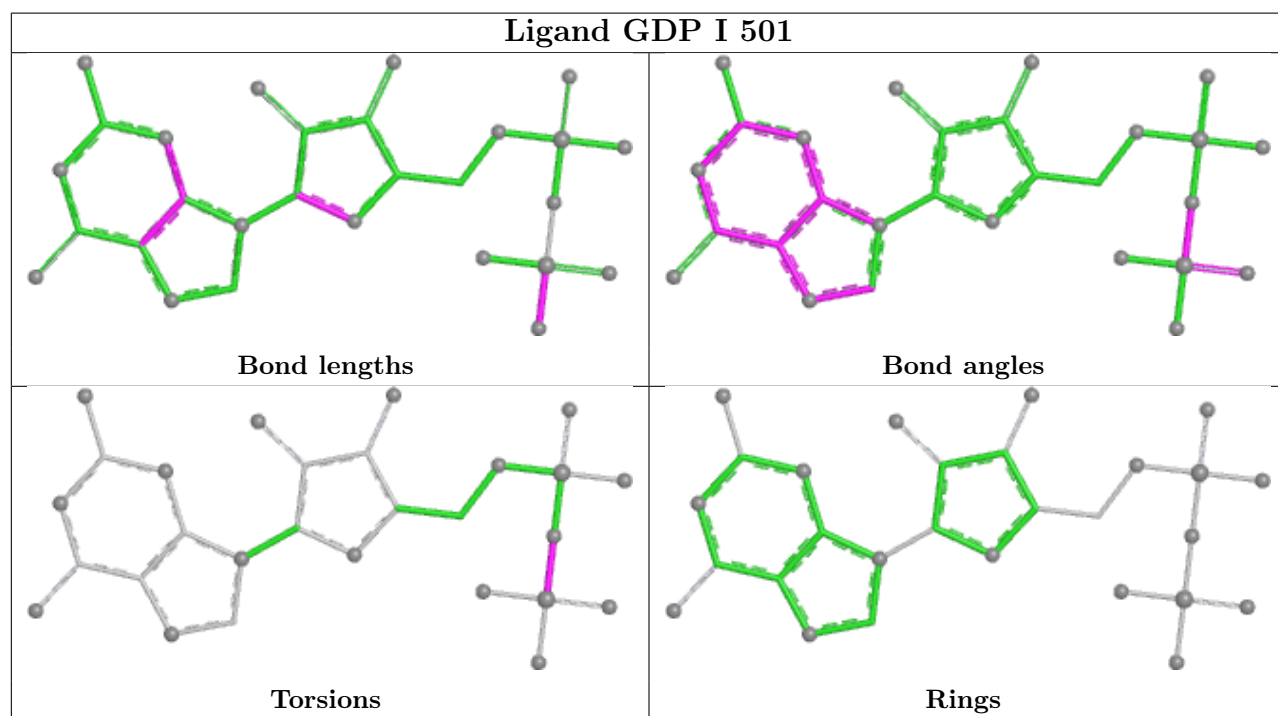
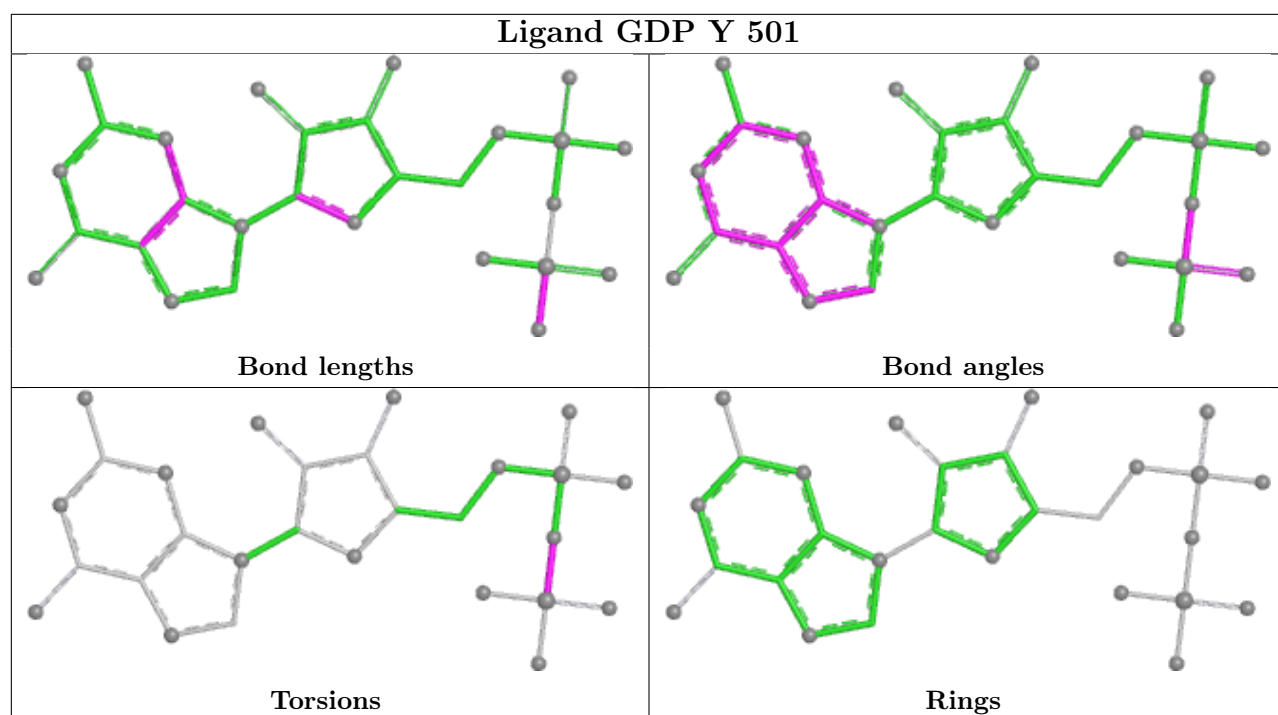


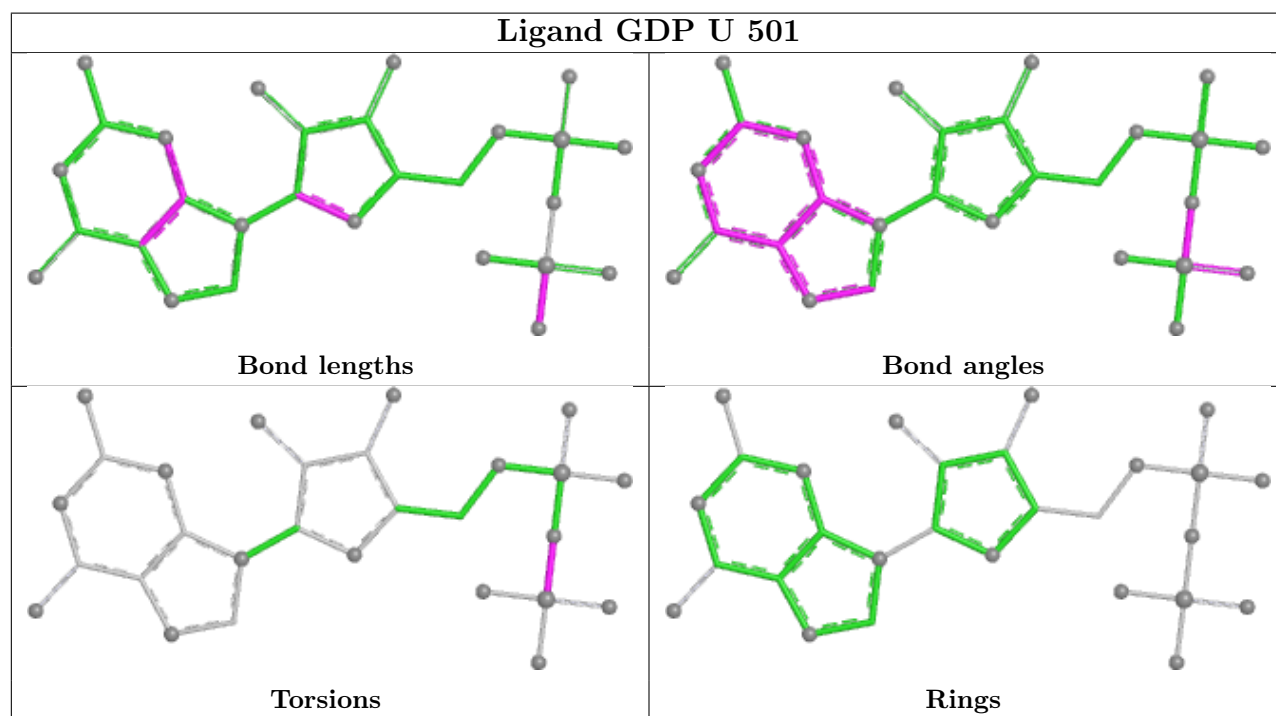
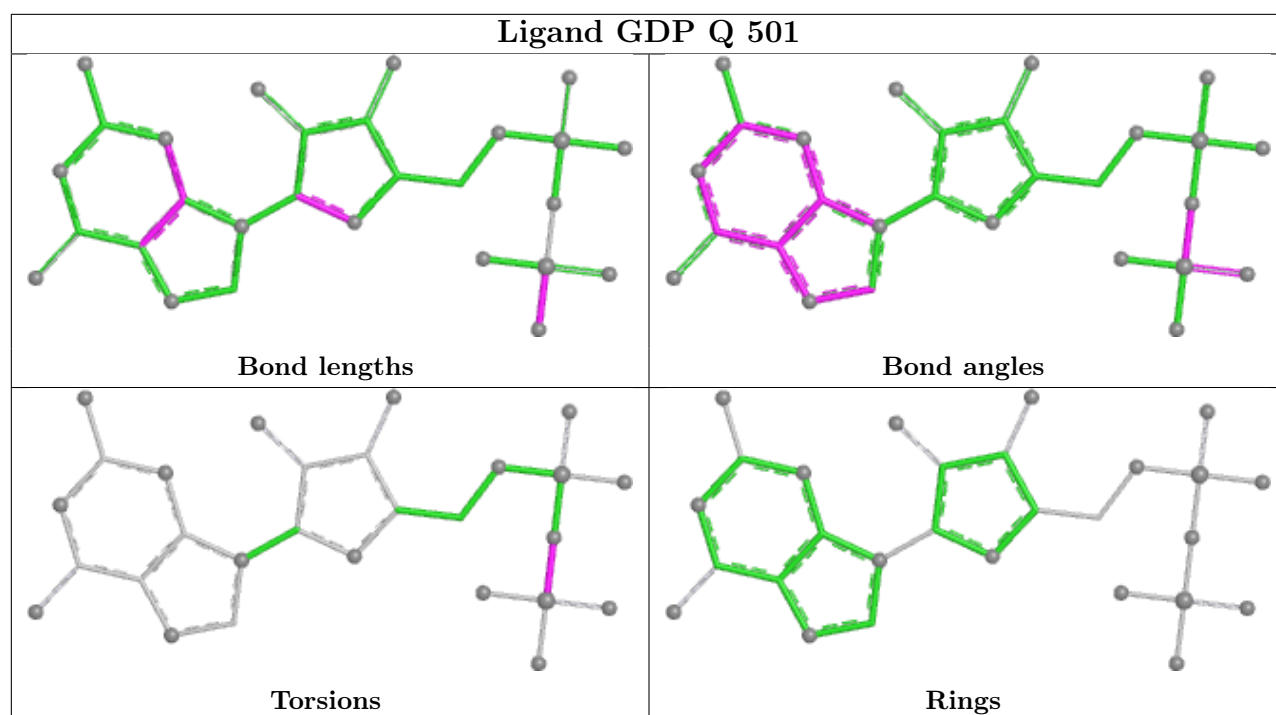


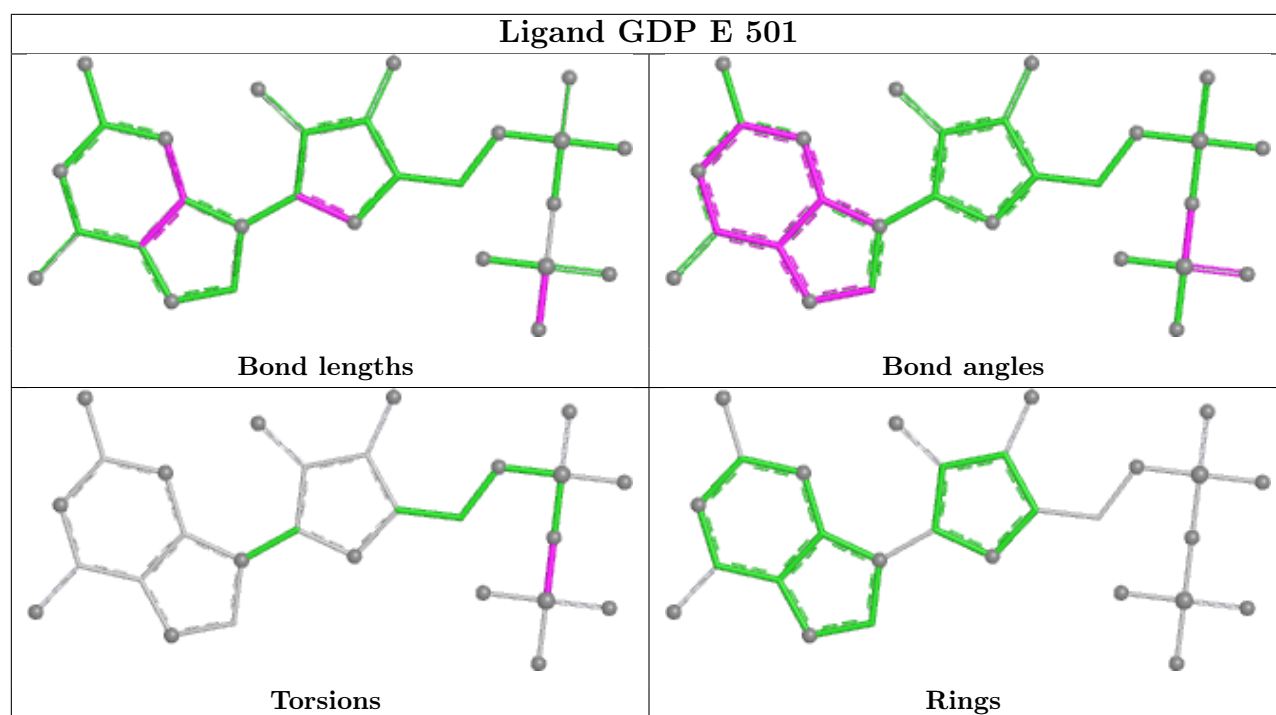












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

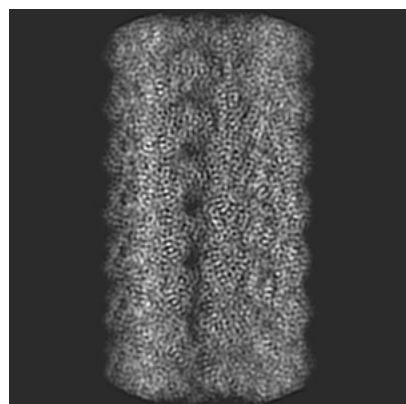
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52463. These allow visual inspection of the internal detail of the map and identification of artifacts.

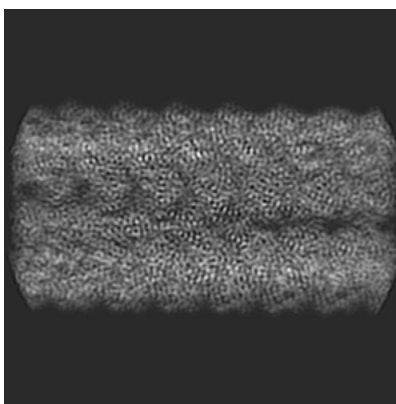
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

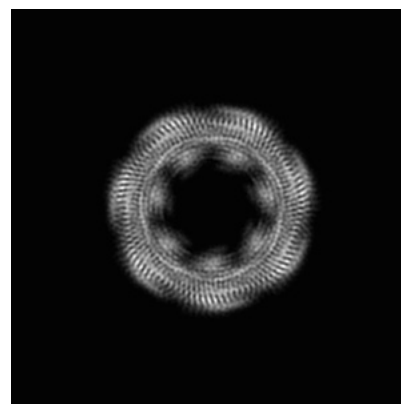
6.1.1 Primary map



X

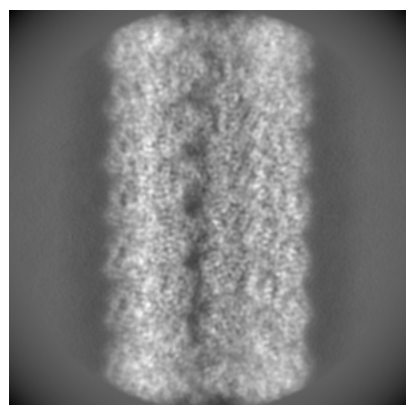


Y

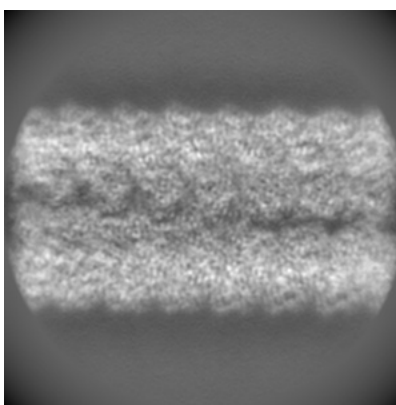


Z

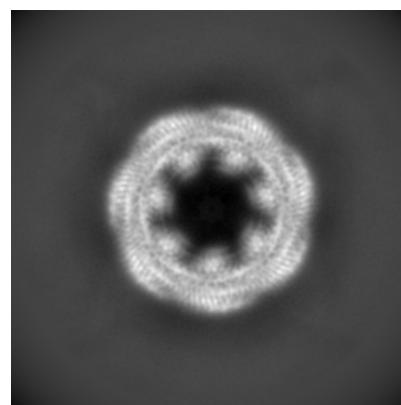
6.1.2 Raw map



X



Y

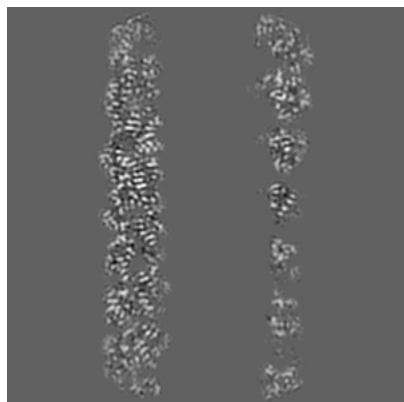


Z

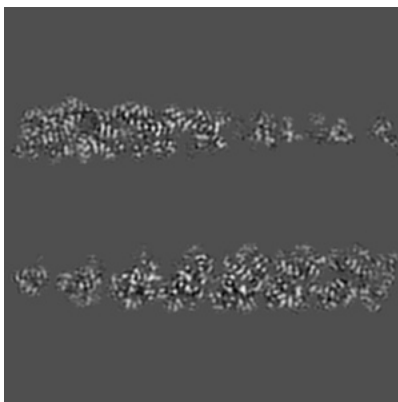
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

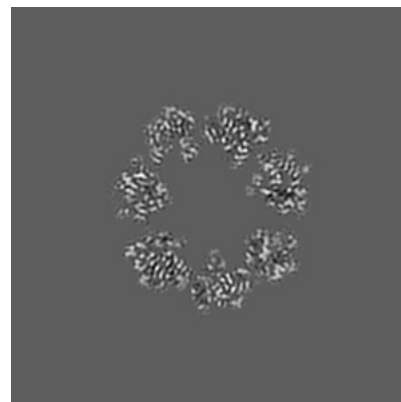
6.2.1 Primary map



X Index: 120

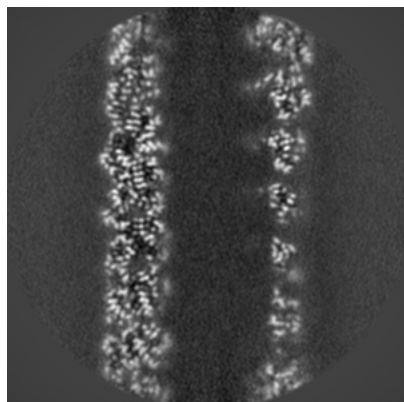


Y Index: 120

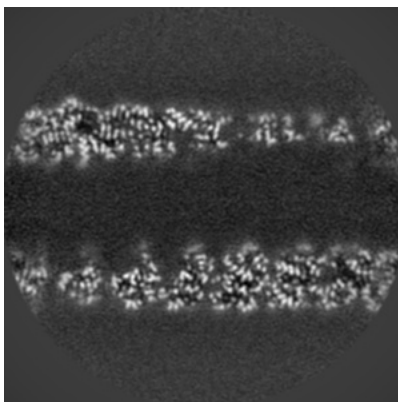


Z Index: 120

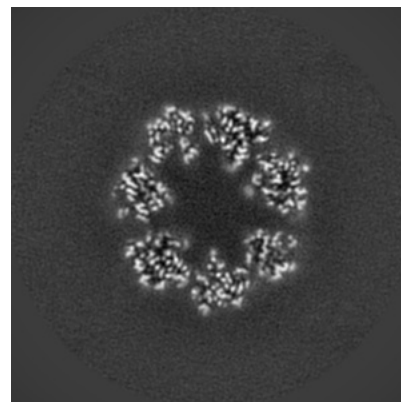
6.2.2 Raw map



X Index: 120



Y Index: 120

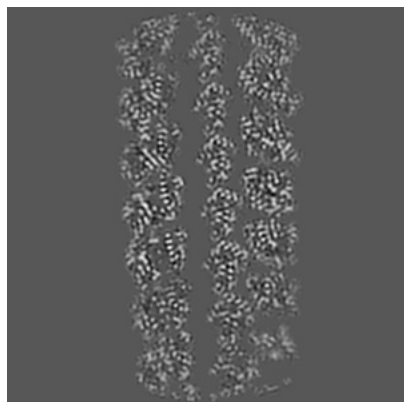


Z Index: 120

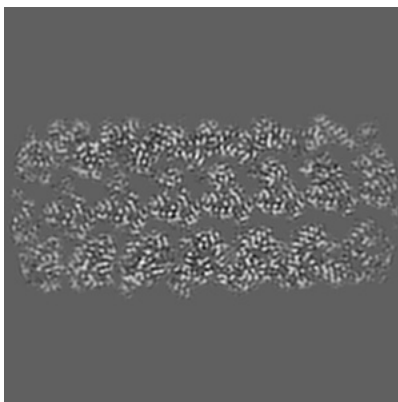
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

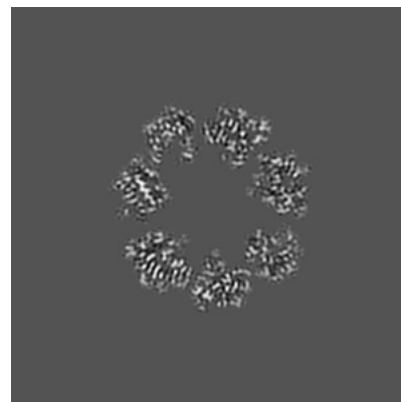
6.3.1 Primary map



X Index: 87

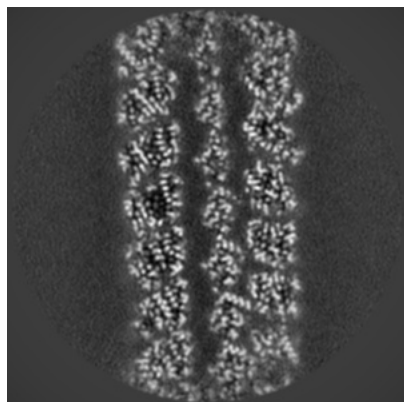


Y Index: 84

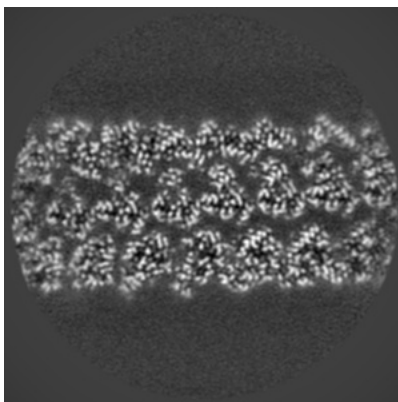


Z Index: 121

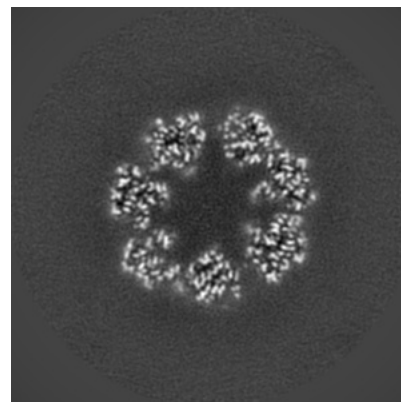
6.3.2 Raw map



X Index: 89



Y Index: 84

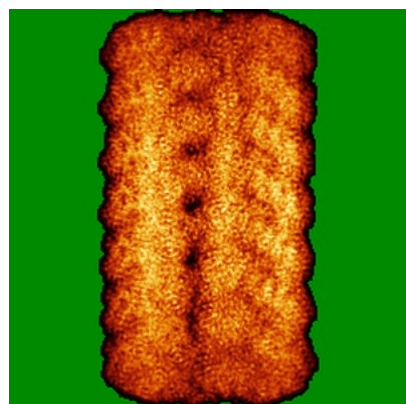


Z Index: 107

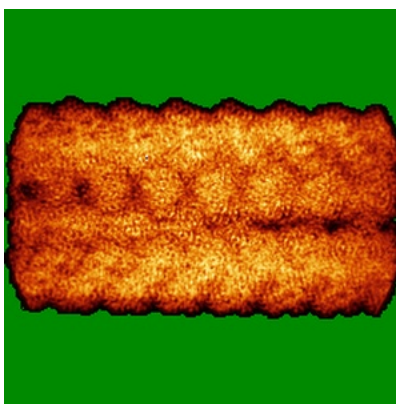
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

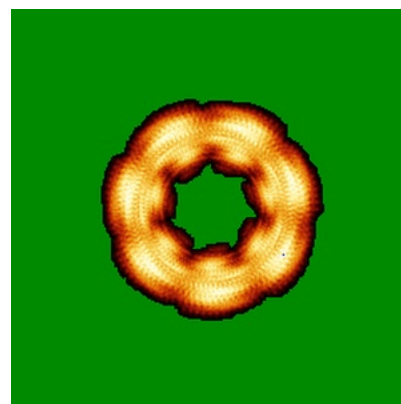
6.4.1 Primary map



X

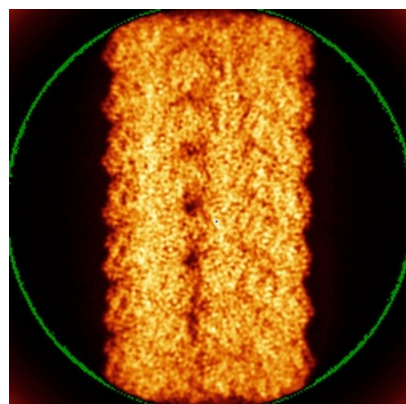


Y

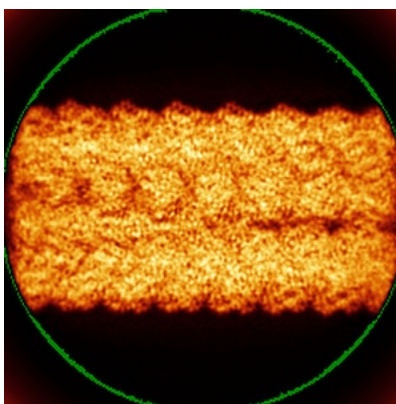


Z

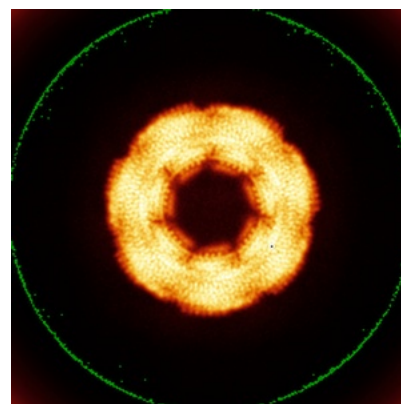
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

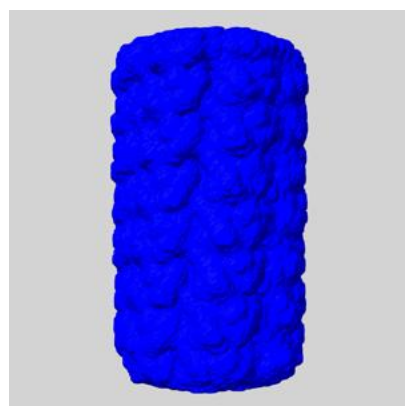
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

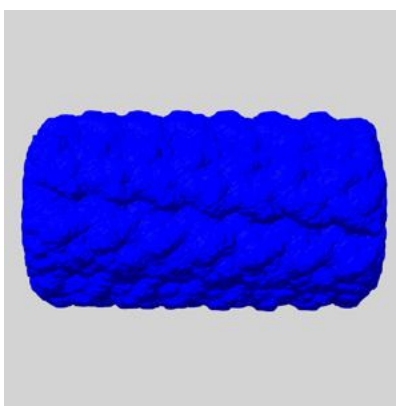
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

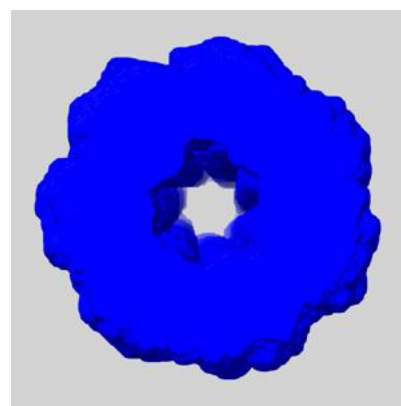
6.6.1 emd_52463_msk_1.map [i](#)



X



Y

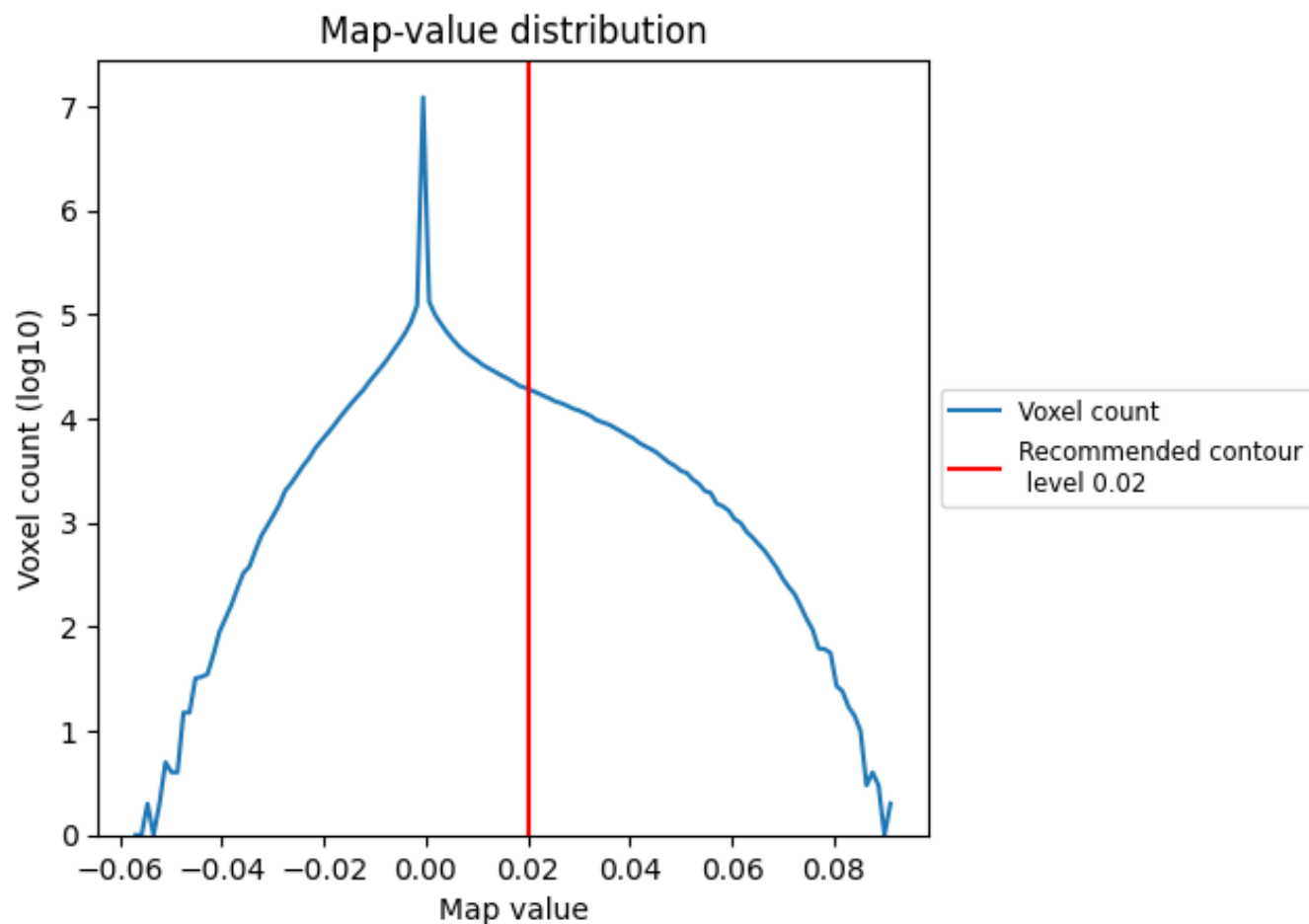


Z

7 Map analysis [i](#)

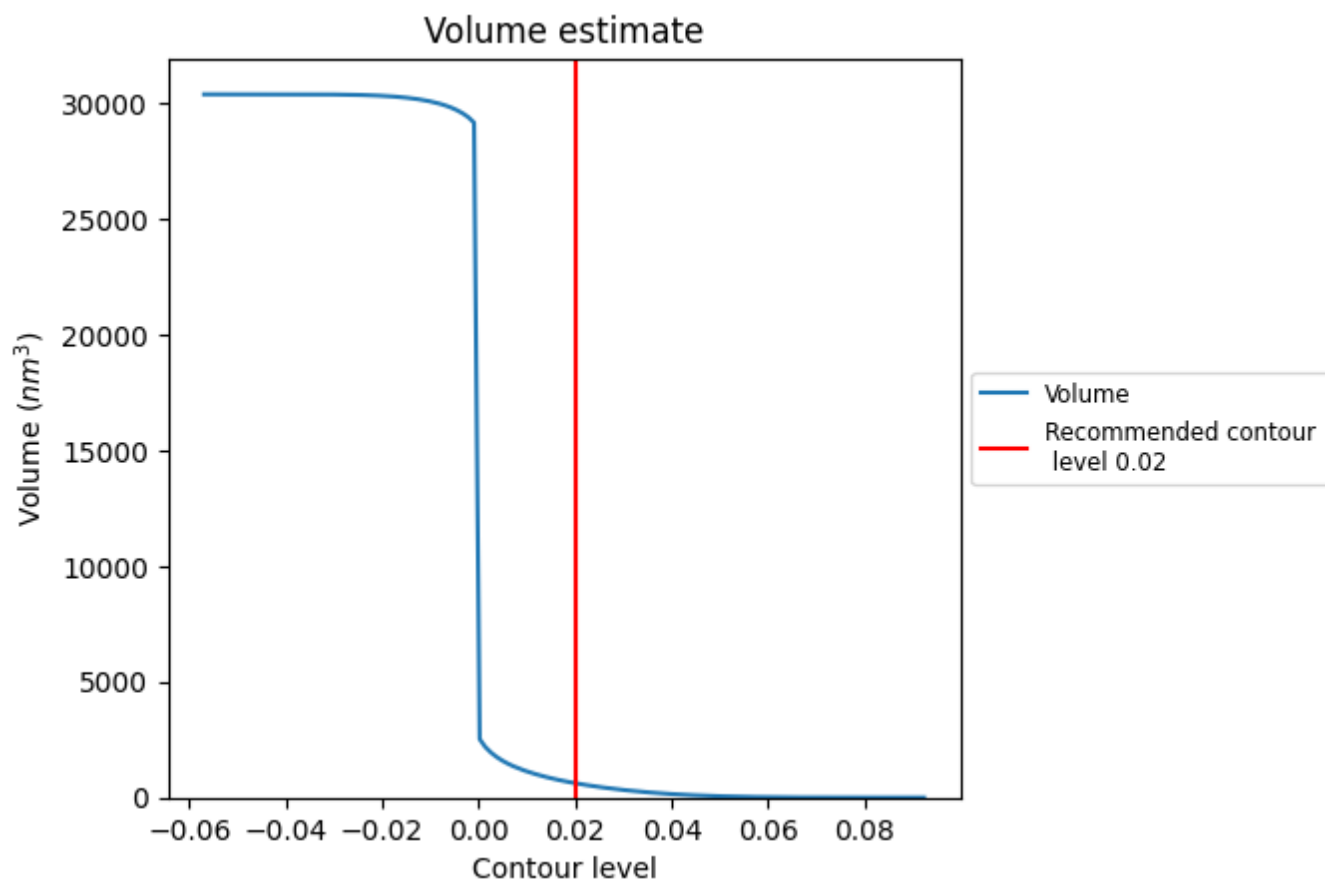
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

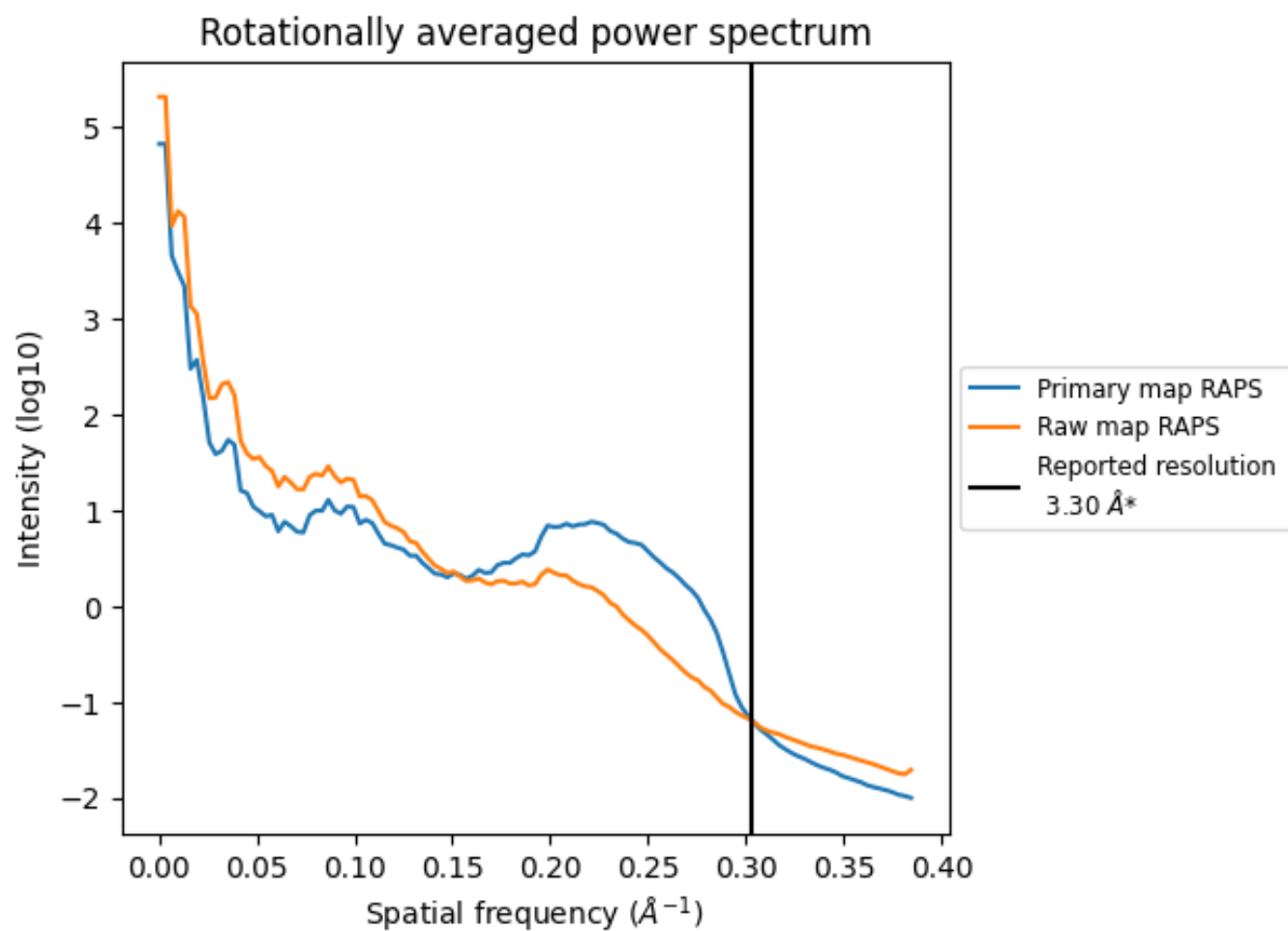
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm³; this corresponds to an approximate mass of 561 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

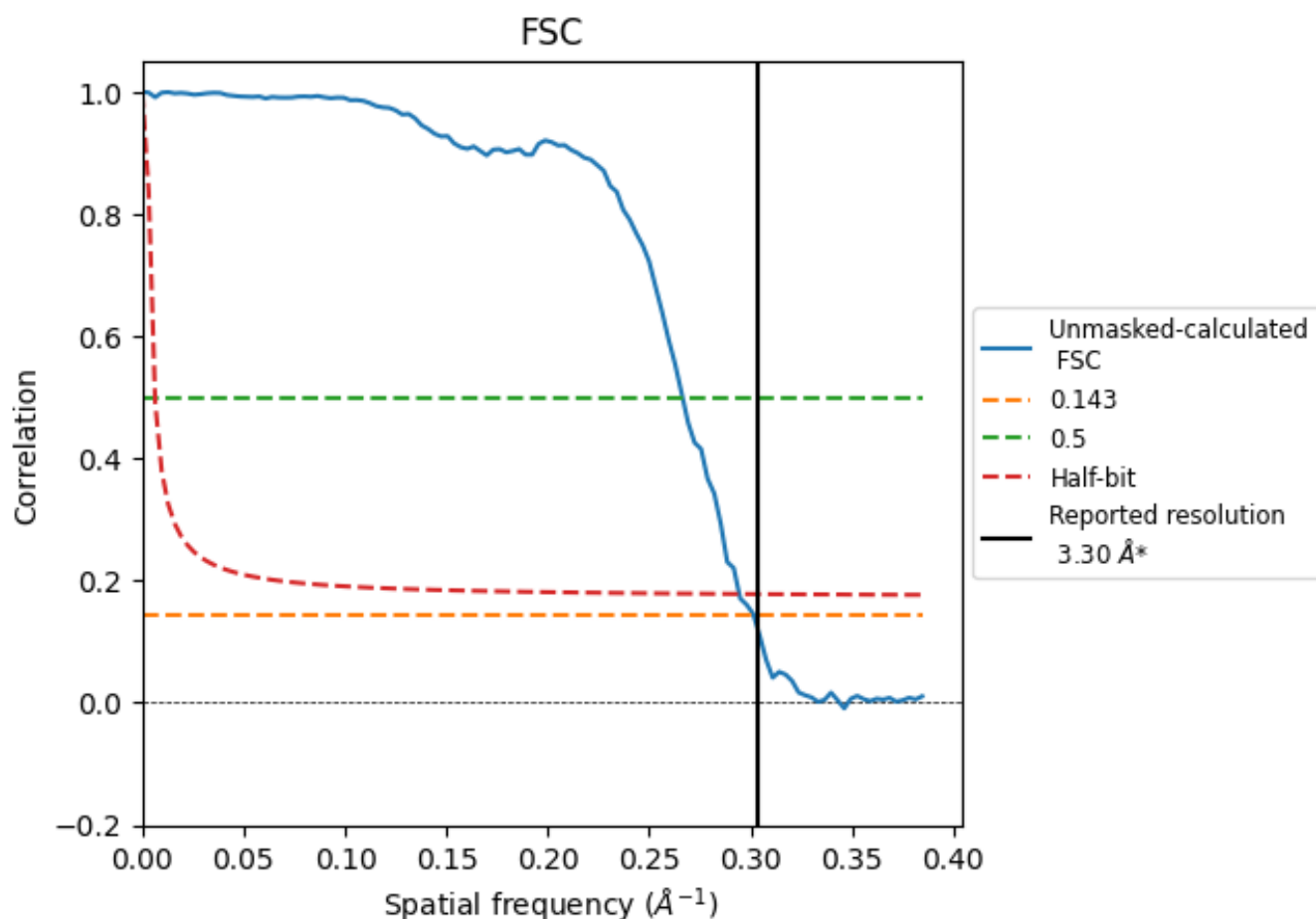


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

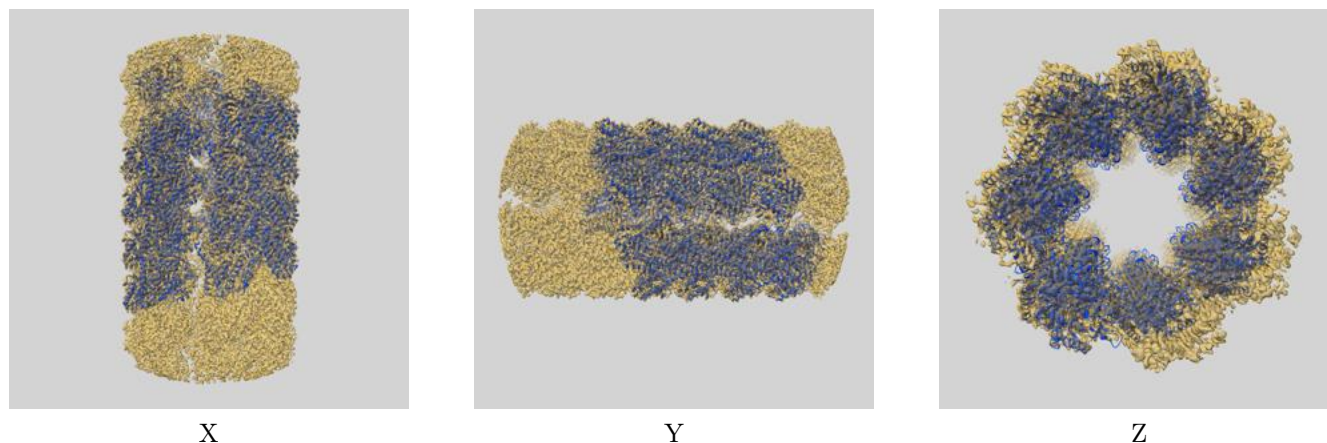
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.32	3.75	3.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

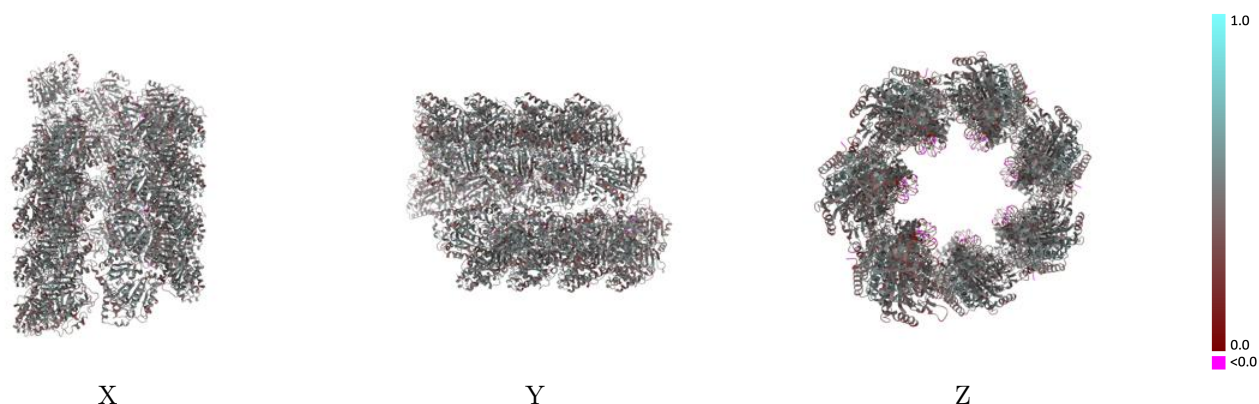
This section contains information regarding the fit between EMDB map EMD-52463 and PDB model 9HXC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

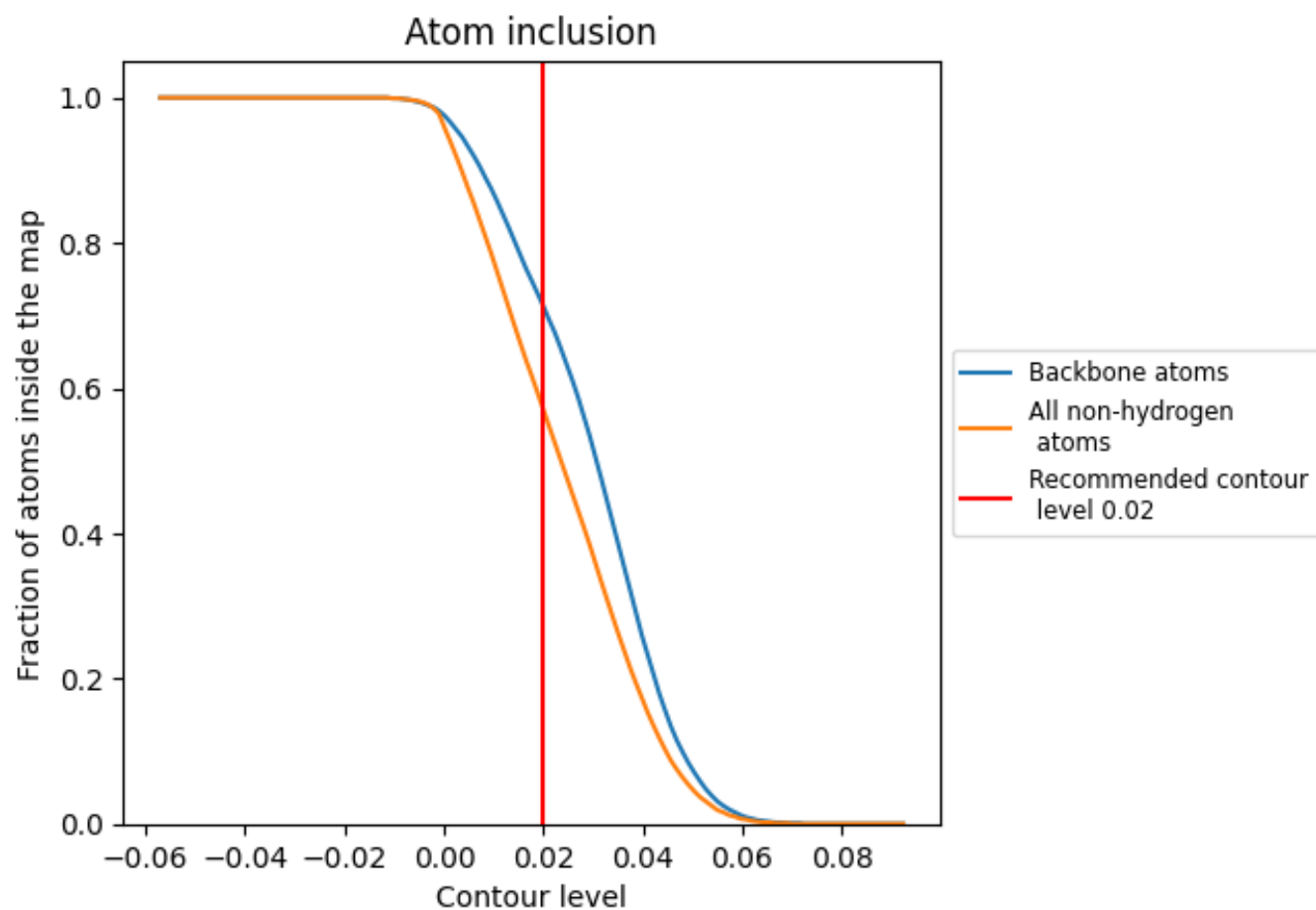


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5710	 0.4440
A	 0.5380	 0.4180
B	 0.5730	 0.4450
C	 0.6000	 0.4610
D	 0.5850	 0.4460
E	 0.5780	 0.4440
F	 0.5930	 0.4590
G	 0.5830	 0.4450
H	 0.5970	 0.4570
I	 0.5830	 0.4480
J	 0.5970	 0.4560
K	 0.5920	 0.4480
L	 0.5910	 0.4540
M	 0.5950	 0.4460
N	 0.5910	 0.4560
O	 0.5800	 0.4350
P	 0.5810	 0.4490
Q	 0.5910	 0.4450
R	 0.5730	 0.4480
S	 0.5850	 0.4440
T	 0.5610	 0.4470
U	 0.5740	 0.4440
V	 0.5510	 0.4460
W	 0.5710	 0.4370
X	 0.5310	 0.4360
Y	 0.5610	 0.4380
Z	 0.5090	 0.4300
a	 0.5500	 0.4360
b	 0.4660	 0.4160

