



Full wwPDB EM Validation Report ⓘ

Sep 11, 2025 – 10:37 am BST

PDB ID : 9HQ4 / pdb_00009hq4
EMDB ID : EMD-52338
Title : TTLL11 bound to microtubule
Authors : Barinka, C.; Campbell, J.; Desfosses, A.; Gutsche, I.
Deposited on : 2024-12-16
Resolution : 3.28 Å(reported)
Based on initial model : .

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.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

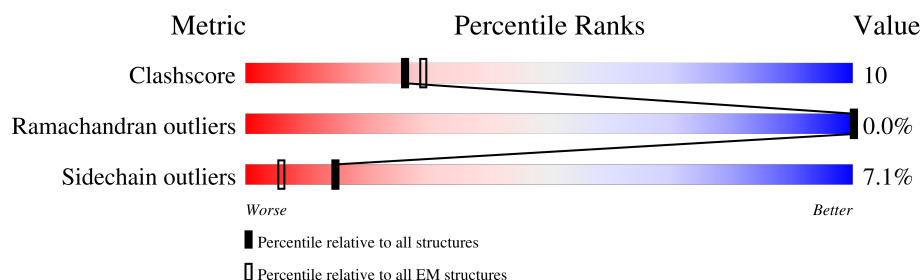
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	451	
1	C	451	
2	B	444	
2	D	444	
3	E	990	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17848 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		
1	C	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3346	2106	573	642	25		
2	D	427	Total	C	N	O	S	0	0
			3354	2110	574	645	25		

- Molecule 3 is a protein called Tubulin polyglutamylase TTLL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	517	Total	C	N	O	S	0	0
			4148	2672	704	747	25		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-279	MET	-	initiating methionine	UNP P0A3G4
E	-278	ALA	-	expression tag	UNP P0A3G4
E	-277	SER	-	expression tag	UNP P0A3G4
E	-276	ALA	-	expression tag	UNP P0A3G4
E	-275	TRP	-	expression tag	UNP P0A3G4
E	-274	SER	-	expression tag	UNP P0A3G4
E	-273	HIS	-	expression tag	UNP P0A3G4
E	-272	PRO	-	expression tag	UNP P0A3G4
E	-271	GLN	-	expression tag	UNP P0A3G4
E	-270	PHE	-	expression tag	UNP P0A3G4
E	-269	GLU	-	expression tag	UNP P0A3G4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-268	LYS	-	expression tag	UNP P0A3G4
E	-267	GLY	-	expression tag	UNP P0A3G4
E	-266	GLY	-	expression tag	UNP P0A3G4
E	-265	GLY	-	expression tag	UNP P0A3G4
E	-264	SER	-	expression tag	UNP P0A3G4
E	-263	GLY	-	expression tag	UNP P0A3G4
E	-262	GLY	-	expression tag	UNP P0A3G4
E	-261	GLY	-	expression tag	UNP P0A3G4
E	-260	SER	-	expression tag	UNP P0A3G4
E	-259	GLY	-	expression tag	UNP P0A3G4
E	-258	GLY	-	expression tag	UNP P0A3G4
E	-257	SER	-	expression tag	UNP P0A3G4
E	-256	ALA	-	expression tag	UNP P0A3G4
E	-255	TRP	-	expression tag	UNP P0A3G4
E	-254	SER	-	expression tag	UNP P0A3G4
E	-253	HIS	-	expression tag	UNP P0A3G4
E	-252	PRO	-	expression tag	UNP P0A3G4
E	-251	GLN	-	expression tag	UNP P0A3G4
E	-250	PHE	-	expression tag	UNP P0A3G4
E	-249	GLU	-	expression tag	UNP P0A3G4
E	-248	LYS	-	expression tag	UNP P0A3G4
E	-247	GLY	-	expression tag	UNP P0A3G4
E	-246	GLY	-	expression tag	UNP P0A3G4
E	-245	SER	-	expression tag	UNP P0A3G4
E	-244	GLY	-	expression tag	UNP P0A3G4
E	-243	GLY	-	expression tag	UNP P0A3G4
E	-242	SER	-	expression tag	UNP P0A3G4
E	-241	ASP	-	expression tag	UNP P0A3G4
E	-240	TYR	-	expression tag	UNP P0A3G4
E	-239	LYS	-	expression tag	UNP P0A3G4
E	-238	ASP	-	expression tag	UNP P0A3G4
E	-237	ASP	-	expression tag	UNP P0A3G4
E	-236	ASP	-	expression tag	UNP P0A3G4
E	-235	ASP	-	expression tag	UNP P0A3G4
E	-234	LYS	-	expression tag	UNP P0A3G4
E	-233	GLY	-	expression tag	UNP P0A3G4
E	-232	SER	-	expression tag	UNP P0A3G4
E	-231	GLY	-	expression tag	UNP P0A3G4
E	-230	SER	-	expression tag	UNP P0A3G4
E	-229	GLY	-	expression tag	UNP P0A3G4
E	-184	VAL	LEU	conflict	UNP P0A3G4
E	-173	THR	SER	conflict	UNP P0A3G4

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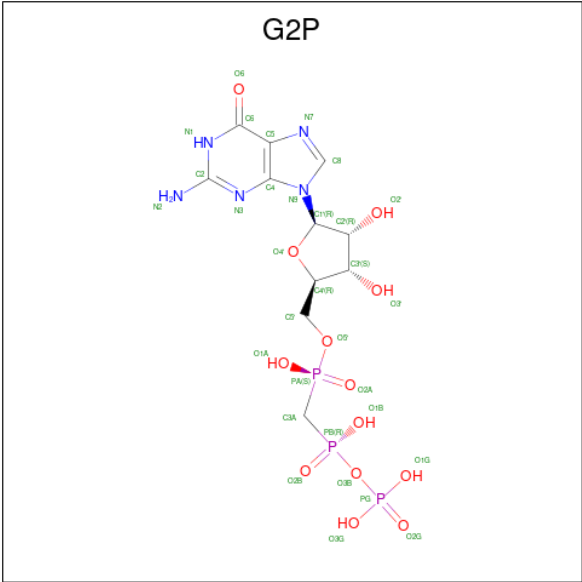
Chain	Residue	Modelled	Actual	Comment	Reference
E	-153	GLY	ASP	conflict	UNP P0A3G4
E	-144	PHE	TYR	conflict	UNP P0A3G4
E	-143	MET	LEU	conflict	UNP P0A3G4
E	-103	PHE	CYS	conflict	UNP P0A3G4
E	-76	THR	ALA	conflict	UNP P0A3G4
E	-71	LYS	GLU	conflict	UNP P0A3G4
E	-64	VAL	ALA	conflict	UNP P0A3G4
E	-59	THR	ALA	conflict	UNP P0A3G4
E	-56	MET	LYS	conflict	UNP P0A3G4
E	-55	GLY	CYS	conflict	UNP P0A3G4
E	-36	ASN	LYS	conflict	UNP P0A3G4
E	-7	GLU	ALA	conflict	UNP P0A3G4
E	-4	ASP	ASN	conflict	UNP P0A3G4
E	26	LYS	GLU	conflict	UNP P0A3G4
E	33	ALA	THR	conflict	UNP P0A3G4
E	41	ASN	HIS	conflict	UNP P0A3G4
E	42	LEU	TYR	conflict	UNP P0A3G4
E	60	SER	-	linker	UNP P0A3G4
E	61	THR	-	linker	UNP P0A3G4
E	62	LEU	-	linker	UNP P0A3G4
E	63	GLU	-	linker	UNP P0A3G4
E	64	ILE	-	linker	UNP P0A3G4
E	65	SER	-	linker	UNP P0A3G4
E	66	GLY	-	linker	UNP P0A3G4
E	67	GLU	-	linker	UNP P0A3G4
E	68	PRO	-	linker	UNP P0A3G4
E	69	THR	-	linker	UNP P0A3G4
E	70	THR	-	linker	UNP P0A3G4
E	71	GLU	-	linker	UNP P0A3G4
E	72	ASP	-	linker	UNP P0A3G4
E	73	LEU	-	linker	UNP P0A3G4
E	74	TYR	-	linker	UNP P0A3G4
E	75	PHE	-	linker	UNP P0A3G4
E	76	GLN	-	linker	UNP P0A3G4
E	77	SER	-	linker	UNP P0A3G4
E	78	ASP	-	linker	UNP P0A3G4
E	79	ASN	-	linker	UNP P0A3G4
E	80	ALA	-	linker	UNP P0A3G4
E	81	ILE	-	linker	UNP P0A3G4
E	82	ALA	-	linker	UNP P0A3G4
E	83	SER	-	linker	UNP P0A3G4
E	84	GLU	-	linker	UNP P0A3G4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	85	PHE	-	linker	UNP P0A3G4
E	86	CYS	-	linker	UNP P0A3G4
E	87	ARG	-	linker	UNP P0A3G4
E	88	TYR	-	linker	UNP P0A3G4
E	89	PRO	-	linker	UNP P0A3G4
E	90	ALA	-	linker	UNP P0A3G4
E	91	GLN	-	linker	UNP P0A3G4
E	92	TRP	-	linker	UNP P0A3G4
E	93	ARG	-	linker	UNP P0A3G4
E	94	PRO	-	linker	UNP P0A3G4
E	95	LEU	-	linker	UNP P0A3G4
E	96	GLU	-	linker	UNP P0A3G4
E	97	SER	-	linker	UNP P0A3G4
E	98	SER	-	linker	UNP P0A3G4
E	99	ARG	-	linker	UNP P0A3G4
E	100	HIS	-	linker	UNP P0A3G4
E	101	ASN	-	linker	UNP P0A3G4
E	102	GLN	-	linker	UNP P0A3G4
E	103	THR	-	linker	UNP P0A3G4
E	104	SER	-	linker	UNP P0A3G4
E	105	LEU	-	linker	UNP P0A3G4
E	106	TYR	-	linker	UNP P0A3G4
E	107	LYS	-	linker	UNP P0A3G4
E	108	LYS	-	linker	UNP P0A3G4
E	109	ALA	-	linker	UNP P0A3G4
E	110	GLY	-	linker	UNP P0A3G4
E	111	SER	-	linker	UNP P0A3G4
E	112	GLU	-	linker	UNP P0A3G4
E	113	ASN	-	linker	UNP P0A3G4
E	114	LEU	-	linker	UNP P0A3G4
E	115	TYR	-	linker	UNP P0A3G4
E	116	PHE	-	linker	UNP P0A3G4
E	117	GLN	-	linker	UNP P0A3G4
E	118	SER	-	linker	UNP P0A3G4
E	119	GLY	-	linker	UNP P0A3G4
E	120	GLY	-	linker	UNP P0A3G4
E	441	GLY	GLU	engineered mutation	UNP Q8NHH1

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	11	5	13	3	
4	B	1	Total	C	N	O	P	0
			32	11	5	13	3	
4	C	1	Total	C	N	O	P	0
			32	11	5	13	3	
4	D	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).

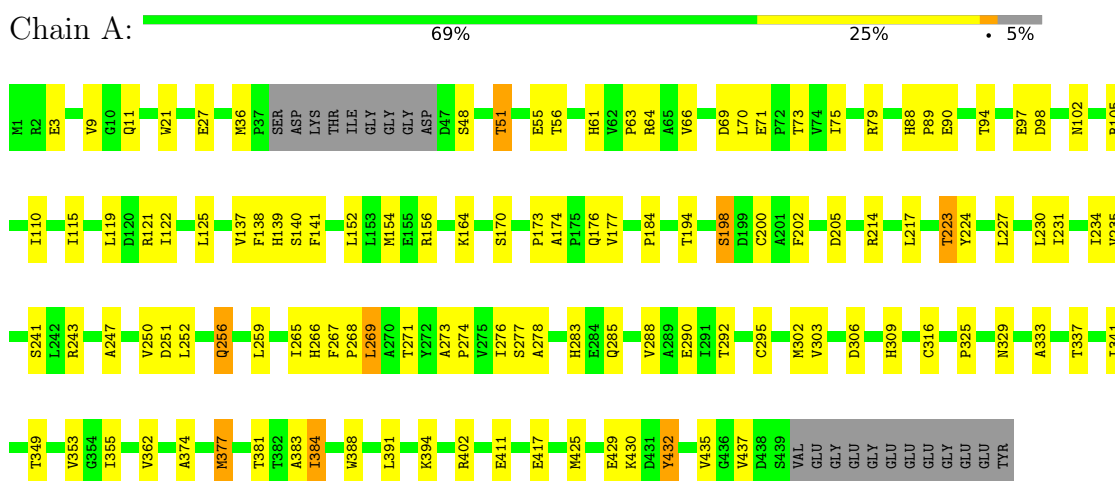


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total 62	C 47	N 1	O 14	0
6	D	1	Total 62	C 47	N 1	O 14	0

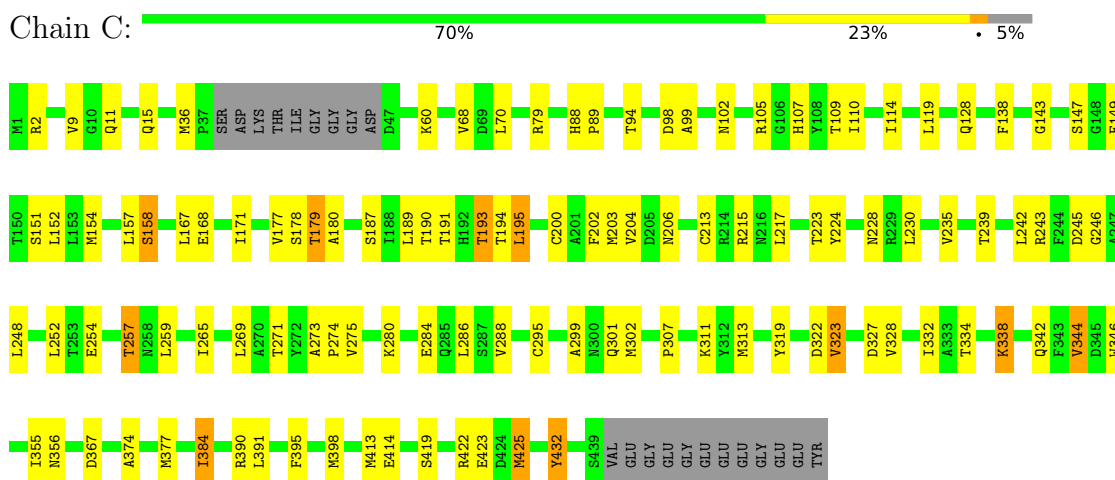
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Tubulin alpha-1B chain

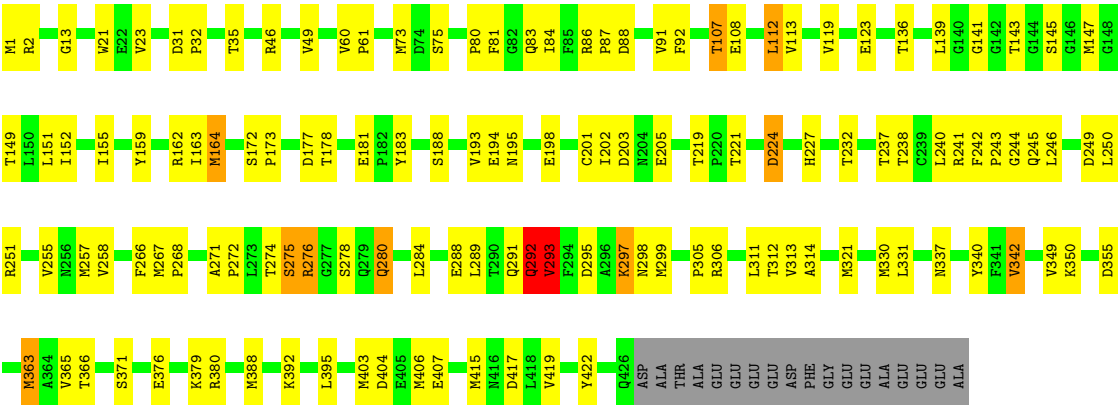


• Molecule 1: Tubulin alpha-1B chain



• Molecule 2: Tubulin beta chain

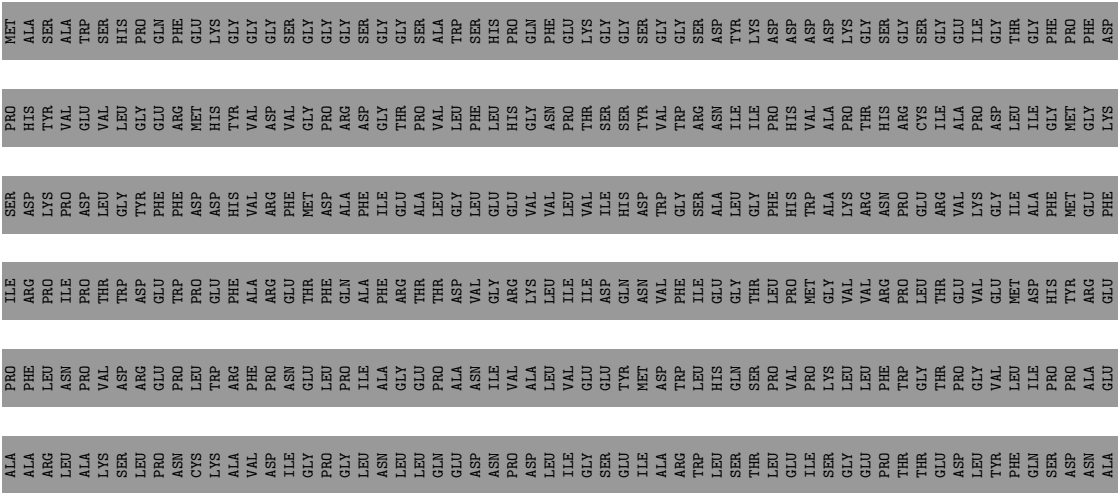
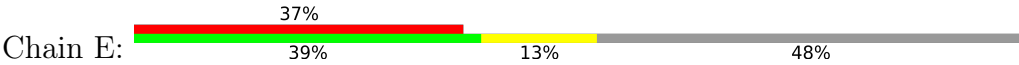




• Molecule 2: Tubulin beta chain



• Molecule 3: Tubulin polyglutamylase TTL11





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	239587	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.275	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0956	Depositor
Map size (Å)	647.52, 647.52, 647.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3490001, 1.3490001, 1.3490001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G2P, MG, TA1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/3449	0.32	0/4682
1	C	0.20	0/3449	0.39	1/4682 (0.0%)
2	B	0.41	0/3421	0.71	7/4637 (0.2%)
2	D	0.41	0/3429	0.70	10/4648 (0.2%)
3	E	0.13	0/4243	0.34	0/5735
All	All	0.28	0/17991	0.51	18/24384 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
2	D	0	4
3	E	0	1
All	All	0	8

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	SER	N-CA-C	-6.90	104.86	113.55
2	D	242	PHE	CB-CA-C	6.72	119.19	108.91
2	B	242	PHE	CA-CB-CG	6.59	120.39	113.80
2	B	243	PRO	N-CA-CB	-6.57	96.48	103.38
2	B	240	LEU	N-CA-C	-6.55	105.33	113.38
2	D	335	ASN	N-CA-C	-6.51	105.88	113.88
2	D	243	PRO	N-CA-CB	-6.37	95.65	102.85
2	B	83	GLN	N-CA-C	-6.01	105.25	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	240	LEU	N-CA-C	-5.94	106.37	113.97
2	B	293	VAL	N-CA-C	-5.83	107.13	112.96
2	D	47	ILE	N-CA-C	-5.81	105.45	113.00
2	B	292	GLN	CB-CA-C	-5.65	100.31	110.37
2	D	3	GLU	N-CA-CB	-5.42	102.05	110.29
2	D	276	ARG	N-CA-C	-5.29	106.99	113.50
2	D	126	SER	N-CA-C	-5.21	106.51	112.92
2	D	85	PHE	CB-CA-C	5.21	119.12	109.54
2	D	242	PHE	N-CA-CB	-5.14	100.44	110.10
2	B	243	PRO	CA-C-O	-5.08	115.58	122.08

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	241	ARG	Sidechain
2	B	276	ARG	Sidechain
2	B	46	ARG	Sidechain
2	D	156	ARG	Sidechain
2	D	241	ARG	Sidechain
2	D	276	ARG	Sidechain
2	D	46	ARG	Sidechain
3	E	601	ARG	Sidechain

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	3372	0	3286	65	0
1	C	3372	0	3286	72	0
2	B	3346	0	3239	65	0
2	D	3354	0	3243	69	0
3	E	4148	0	4232	84	0
4	A	32	0	14	0	0
4	B	32	0	14	0	0
4	C	32	0	14	4	0
4	D	32	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	62	0	51	4	0
6	D	62	0	51	3	0
All	All	17848	0	17444	348	0

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

All (348) 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)
3:E:574:ARG:HB3	3:E:574:ARG:NH1	1.86	0.91
2:B:173:PRO:HG3	2:B:380:ARG:HD2	1.59	0.85
2:D:253:LEU:O	2:D:257:MET:HB2	1.79	0.83
3:E:373:CYS:HB3	3:E:374:ARG:HH12	1.51	0.74
3:E:485:ASP:HB3	3:E:488:LYS:HD2	1.68	0.74
3:E:211:GLU:O	3:E:395:LYS:NZ	2.21	0.72
6:D:503:TA1:H472	6:D:503:TA1:H193	1.72	0.72
6:B:503:TA1:H193	6:B:503:TA1:H472	1.72	0.72
2:D:143:THR:O	2:D:147:MET:HB2	1.90	0.72
2:D:328:GLU:OE1	2:D:332:ASN:ND2	2.24	0.71
1:A:295:CYS:HB3	1:A:377:MET:HE2	1.73	0.69
2:D:116:VAL:HG11	2:D:151:LEU:HD11	1.74	0.69
2:B:249:ASP:OD2	2:B:250:LEU:N	2.25	0.69
1:A:227:LEU:O	1:A:231:ILE:HD12	1.92	0.69
1:C:319:TYR:HB3	1:C:323:VAL:HG11	1.74	0.68
2:B:194:GLU:OE2	2:B:194:GLU:N	2.26	0.68
1:C:246:GLY:HA3	1:C:356:ASN:HA	1.76	0.68
1:C:206:ASN:OD1	4:C:501:G2P:N2	2.28	0.66
2:D:289:LEU:HD13	2:D:365:VAL:CG2	2.25	0.66
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.13	0.66
3:E:370:SER:O	3:E:374:ARG:NH1	2.29	0.66
1:A:381:THR:HG23	1:A:383:ALA:H	1.61	0.66
2:D:31:ASP:OD1	2:D:32:PRO:HD2	1.95	0.66
3:E:544:ASN:OD1	3:E:547:ARG:NH2	2.29	0.64
3:E:473:LYS:O	3:E:477:ILE:HG12	1.97	0.64
1:A:388:TRP:HB3	1:A:425:MET:HE2	1.80	0.64
1:C:414:GLU:OE1	1:C:414:GLU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:373:CYS:SG	3:E:374:ARG:NH2	2.66	0.64
2:D:252:LYS:O	2:D:256:ASN:ND2	2.29	0.63
3:E:574:ARG:HB3	3:E:574:ARG:HH11	1.59	0.63
1:C:213:CYS:HA	1:C:217:LEU:HD12	1.79	0.63
1:C:398:MET:HE3	2:D:345:ILE:HG13	1.80	0.62
2:D:48:SER:O	2:D:62:ARG:NH2	2.28	0.62
2:D:396:HIS:HA	2:D:399:THR:HG22	1.81	0.62
2:D:248:ALA:HA	2:D:252:LYS:HE3	1.81	0.62
1:C:280:LYS:NZ	1:C:284:GLU:OE2	2.29	0.62
1:C:288:VAL:HG21	1:C:327:ASP:HB3	1.82	0.62
1:C:274:PRO:HG2	1:C:374:ALA:HA	1.83	0.61
2:D:100:ASN:HB3	2:D:103:LYS:HB2	1.80	0.61
1:A:214:ARG:HG2	1:A:214:ARG:HH11	1.64	0.61
3:E:287:LYS:HE3	3:E:287:LYS:O	2.01	0.61
1:C:191:THR:HG21	1:C:425:MET:HG2	1.82	0.61
3:E:133:SER:OG	3:E:154:GLU:OE2	2.17	0.61
1:C:334:THR:O	1:C:338:LYS:NZ	2.34	0.61
3:E:198:SER:O	3:E:202:ARG:HG3	2.01	0.61
2:B:177:ASP:N	2:B:177:ASP:OD1	2.35	0.60
3:E:449:ARG:O	3:E:473:LYS:NZ	2.32	0.60
1:A:176:GLN:HB3	2:B:331:LEU:HD21	1.82	0.60
2:B:330:MET:SD	2:B:349:VAL:HG11	2.41	0.60
2:B:406:MET:HA	2:B:406:MET:HE2	1.83	0.60
2:D:113:VAL:HG21	2:D:150:LEU:HD23	1.84	0.60
2:D:379:LYS:O	2:D:382:SER:OG	2.19	0.60
1:A:417:GLU:N	1:A:417:GLU:OE1	2.35	0.59
3:E:632:PHE:HB3	3:E:635:LEU:HD12	1.84	0.59
3:E:159:ARG:NH2	3:E:162:PRO:O	2.36	0.59
3:E:287:LYS:HZ3	3:E:433:LYS:HB3	1.67	0.59
2:B:232:THR:HG21	2:B:268:PRO:HB3	1.83	0.59
3:E:214:PHE:HE2	3:E:395:LYS:HD2	1.67	0.59
2:D:161:ASP:OD1	2:D:161:ASP:N	2.35	0.58
1:C:98:ASP:OD1	1:C:99:ALA:N	2.36	0.58
1:A:271:THR:HB	1:A:377:MET:HB3	1.85	0.58
3:E:307:LEU:HD22	3:E:401:THR:HG23	1.86	0.58
2:D:276:ARG:HH12	2:D:279:GLN:HE21	1.52	0.58
3:E:574:ARG:HB3	3:E:574:ARG:CZ	2.34	0.58
2:D:88:ASP:OD1	2:D:88:ASP:N	2.37	0.58
1:A:102:ASN:ND2	1:A:411:GLU:OE1	2.36	0.58
2:B:13:GLY:HA2	2:B:136:THR:HG22	1.85	0.58
1:C:367:ASP:OD1	1:C:367:ASP:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HG23	2:B:151:LEU:HD12	1.87	0.57
1:A:51:THR:HG21	1:A:243:ARG:HG2	1.87	0.57
3:E:148:ARG:HH11	3:E:148:ARG:HG2	1.70	0.57
2:B:21:TRP:CH2	2:B:61:PRO:HB3	2.40	0.57
3:E:188:MET:HA	3:E:191:MET:HG2	1.86	0.57
3:E:636:PRO:HG2	3:E:639:GLU:HB2	1.87	0.57
3:E:199:ARG:HH22	3:E:606:MET:HB3	1.70	0.57
3:E:568:LEU:HD11	3:E:572:GLY:HA3	1.87	0.57
3:E:388:ASP:O	3:E:392:VAL:HG13	2.05	0.56
1:A:11:GLN:HE22	2:B:246:LEU:HA	1.69	0.56
1:C:190:THR:O	1:C:194:THR:HG22	2.06	0.56
2:B:178:THR:HB	2:B:181:GLU:HB3	1.88	0.56
1:C:215:ARG:NH2	1:C:299:ALA:O	2.38	0.56
3:E:195:ILE:HD12	3:E:196:THR:H	1.69	0.56
3:E:397:VAL:O	3:E:401:THR:OG1	2.22	0.55
2:B:415:MET:O	2:B:419:VAL:HG23	2.07	0.55
3:E:539:TYR:HB3	3:E:542:GLN:HB3	1.88	0.55
1:A:139:HIS:ND1	1:A:140:SER:O	2.40	0.55
1:C:11:GLN:O	1:C:15:GLN:HG2	2.07	0.55
1:A:88:HIS:ND1	1:A:89:PRO:HD2	2.22	0.55
3:E:385:VAL:O	3:E:389:ILE:HG12	2.06	0.55
3:E:640:GLN:O	3:E:642:ALA:N	2.38	0.55
2:B:31:ASP:OD2	2:B:32:PRO:HD2	2.06	0.55
1:A:325:PRO:O	1:A:329:ASN:ND2	2.40	0.55
2:B:143:THR:O	2:B:147:MET:HB2	2.07	0.55
2:B:237:THR:HG22	2:B:250:LEU:HD11	1.89	0.54
3:E:195:ILE:HD12	3:E:196:THR:N	2.22	0.54
1:C:323:VAL:HG13	1:C:355:ILE:HG23	1.90	0.54
2:D:289:LEU:HD13	2:D:365:VAL:HG22	1.90	0.53
3:E:400:LEU:HD13	3:E:404:LEU:HD21	1.90	0.53
2:B:198:GLU:HG2	2:B:266:PHE:HE2	1.73	0.53
1:C:245:ASP:OD1	1:C:246:GLY:N	2.41	0.53
3:E:314:ILE:HD12	3:E:390:ILE:HG12	1.90	0.53
1:A:231:ILE:HA	1:A:234:ILE:HD12	1.90	0.53
3:E:147:ILE:HG22	3:E:148:ARG:HH12	1.74	0.53
1:C:70:LEU:HD11	1:C:114:ILE:HG21	1.89	0.53
1:C:98:ASP:O	1:C:105:ARG:NH1	2.42	0.53
1:C:102:ASN:HB3	1:C:105:ARG:HB2	1.91	0.53
2:D:290:THR:HG21	2:D:329:GLN:HG2	1.91	0.53
1:C:189:LEU:HD21	1:C:413:MET:HE1	1.91	0.53
1:A:98:ASP:O	1:A:105:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:231:GLN:HA	3:E:234:MET:HE2	1.91	0.52
3:E:159:ARG:HE	3:E:161:LEU:HB2	1.73	0.52
2:D:73:MET:HE2	2:D:92:PHE:HD2	1.74	0.52
3:E:248:VAL:HG22	3:E:281:VAL:HG22	1.91	0.52
1:A:97:GLU:OE1	2:B:251:ARG:NH1	2.43	0.52
1:A:290:GLU:OE2	1:C:128:GLN:NE2	2.42	0.52
1:C:204:VAL:HG12	1:C:302:MET:HB2	1.92	0.52
2:B:257:MET:HE2	2:B:314:ALA:HB2	1.91	0.52
2:D:257:MET:HE1	2:D:312:THR:O	2.10	0.52
3:E:393:VAL:O	3:E:397:VAL:HG23	2.10	0.52
3:E:479:ASP:HB2	3:E:532:LEU:HD12	1.91	0.52
2:D:271:ALA:HB3	2:D:365:VAL:HG23	1.92	0.52
1:C:328:VAL:O	1:C:332:ILE:HD13	2.10	0.51
2:D:309:ARG:NH1	2:D:339:SER:O	2.43	0.51
2:B:23:VAL:HG22	6:B:503:TA1:H321	1.91	0.51
2:D:272:PRO:HG3	2:D:364:ALA:HA	1.93	0.51
3:E:540:ALA:O	3:E:544:ASN:HB2	2.11	0.51
3:E:615:MET:HG2	3:E:619:ALA:HB3	1.91	0.51
2:B:313:VAL:HG12	2:B:349:VAL:HG13	1.92	0.51
1:A:79:ARG:HH22	1:A:94:THR:HG22	1.75	0.50
1:A:141:PHE:HB3	1:A:173:PRO:HD3	1.93	0.50
1:A:333:ALA:O	1:A:337:THR:HG23	2.12	0.50
2:B:321:MET:HB3	2:B:363:MET:HE2	1.94	0.50
1:C:147:SER:O	1:C:151:SER:OG	2.27	0.50
3:E:567:LYS:HB3	3:E:614:GLY:HA3	1.94	0.50
2:D:121:ARG:NH1	2:D:158:GLU:OE2	2.45	0.50
2:D:39:ASP:OD1	2:D:40:SER:N	2.45	0.50
2:B:244:GLY:HA2	2:B:355:ASP:OD1	2.12	0.50
2:D:289:LEU:HD13	2:D:365:VAL:HG23	1.93	0.50
3:E:305:LYS:HB3	3:E:311:GLU:HB2	1.93	0.50
2:B:292:GLN:O	2:B:298:ASN:ND2	2.45	0.49
2:B:311:LEU:HD23	2:B:342:VAL:HG21	1.93	0.49
2:D:73:MET:HE3	2:D:90:PHE:HD2	1.76	0.49
2:D:203:ASP:OD2	2:D:302:ALA:N	2.45	0.49
2:D:229:VAL:HG12	2:D:233:MET:HE2	1.94	0.49
3:E:574:ARG:CZ	3:E:574:ARG:CB	2.89	0.49
3:E:305:LYS:HG3	3:E:484:MET:HE2	1.94	0.49
3:E:573:PHE:CD2	3:E:615:MET:HE1	2.46	0.49
1:C:143:GLY:HA3	4:C:501:G2P:H3A2	1.95	0.49
2:D:390:ARG:HG2	2:D:391:ARG:H	1.76	0.49
2:D:293:VAL:HG22	2:D:367:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:OG1	1:A:224:TYR:N	2.44	0.49
1:A:269:LEU:HD11	1:A:381:THR:HG22	1.93	0.49
3:E:557:ILE:HA	3:E:560:LEU:HB2	1.94	0.49
2:B:274:THR:O	2:B:275:SER:HB3	2.13	0.49
1:C:191:THR:O	1:C:195:LEU:HB2	2.12	0.49
2:D:63:ALA:O	2:D:89:ASN:ND2	2.32	0.48
2:D:344:TRP:CD1	2:D:344:TRP:H	2.29	0.48
2:D:34:GLY:HA3	2:D:58:LYS:HG3	1.94	0.48
3:E:163:CYS:HB2	3:E:166:TYR:CZ	2.49	0.48
1:A:259:LEU:HD13	1:A:316:CYS:HB2	1.94	0.48
2:B:376:GLU:HA	2:B:379:LYS:HD2	1.95	0.48
1:C:223:THR:OG1	1:C:224:TYR:N	2.42	0.48
3:E:373:CYS:HB3	3:E:374:ARG:NH1	2.22	0.48
1:C:79:ARG:HH22	1:C:94:THR:HG21	1.79	0.48
3:E:152:TRP:HZ3	3:E:481:LEU:HD22	1.78	0.48
1:C:177:VAL:HG13	2:D:327:ASP:HB3	1.95	0.48
2:D:80:PRO:O	2:D:81:PHE:C	2.57	0.48
3:E:212:TYR:CZ	3:E:395:LYS:HG2	2.49	0.48
3:E:370:SER:O	3:E:374:ARG:HG2	2.14	0.48
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.44	0.48
3:E:269:ARG:O	3:E:275:GLN:NE2	2.47	0.48
3:E:291:ILE:HB	3:E:322:PHE:HE2	1.78	0.48
3:E:449:ARG:HG2	3:E:451:GLU:H	1.77	0.48
1:A:194:THR:HG22	1:A:267:PHE:HE2	1.78	0.47
1:A:283:HIS:ND1	1:C:89:PRO:HD3	2.29	0.47
2:B:267:MET:HE3	2:B:371:SER:HB3	1.95	0.47
1:C:15:GLN:HE21	4:C:501:G2P:C6	2.24	0.47
2:B:107:THR:OG1	2:B:108:GLU:OE1	2.32	0.47
2:B:404:ASP:OD1	2:B:407:GLU:HG3	2.14	0.47
1:C:273:ALA:HB2	1:C:295:CYS:SG	2.55	0.47
2:D:390:ARG:HG2	2:D:391:ARG:N	2.30	0.47
3:E:148:ARG:HA	3:E:148:ARG:CZ	2.45	0.47
1:A:234:ILE:HD11	1:A:302:MET:SD	2.54	0.47
1:C:254:GLU:HA	1:C:257:THR:HG22	1.97	0.47
1:C:395:PHE:CD2	1:C:422:ARG:HD3	2.50	0.47
1:A:115:ILE:HG12	1:A:152:LEU:HD22	1.97	0.47
2:D:10:GLY:O	2:D:14:ASN:ND2	2.41	0.47
2:B:227:HIS:NE2	6:B:503:TA1:O14	2.35	0.47
3:E:571:THR:HA	3:E:574:ARG:HD2	1.97	0.47
2:D:243:PRO:O	2:D:355:ASP:HB2	2.15	0.47
1:A:269:LEU:HD21	1:A:384:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ASP:OD1	2:B:224:ASP:N	2.47	0.46
3:E:204:MET:O	3:E:208:PHE:N	2.29	0.46
3:E:628:ALA:HB1	3:E:641:VAL:H	1.79	0.46
1:A:283:HIS:HB3	1:C:88:HIS:CD2	2.51	0.46
1:C:167:LEU:HD22	1:C:200:CYS:HB2	1.97	0.46
1:C:180:ALA:O	2:D:347:ASN:ND2	2.49	0.46
1:A:184:PRO:HA	1:A:391:LEU:HD21	1.98	0.46
2:B:164:MET:HB2	2:B:164:MET:HE2	1.64	0.46
1:A:137:VAL:HG11	1:A:154:MET:HE1	1.98	0.46
1:A:251:ASP:N	1:A:251:ASP:OD1	2.49	0.46
1:C:15:GLN:O	1:C:228:ASN:ND2	2.48	0.46
1:A:36:MET:HG3	1:A:61:HIS:NE2	2.31	0.46
2:B:306:ARG:HG3	2:B:340:TYR:CZ	2.51	0.46
2:B:155:ILE:HG22	2:B:164:MET:HE1	1.96	0.46
2:B:152:ILE:HG22	2:B:195:ASN:HB3	1.98	0.46
1:C:2:ARG:NH1	1:C:242:LEU:O	2.49	0.46
2:D:172:SER:OG	2:D:175:VAL:O	2.34	0.45
2:D:184:ASN:OD1	2:D:398:TYR:OH	2.21	0.45
2:B:271:ALA:HB3	2:B:272:PRO:HD3	1.97	0.45
1:C:171:ILE:HD13	1:C:204:VAL:HG23	1.98	0.45
1:C:311:LYS:HB3	1:C:344:VAL:HG13	1.99	0.45
1:C:269:LEU:HD13	1:C:384:ILE:HD11	1.98	0.45
2:D:107:THR:HG21	2:D:401:GLU:HB3	1.99	0.45
2:D:240:LEU:HD21	2:D:249:ASP:HB2	1.98	0.45
1:A:217:LEU:HA	1:A:277:SER:HB3	1.97	0.45
1:C:338:LYS:HE3	1:C:338:LYS:HB3	1.87	0.45
1:C:15:GLN:NE2	4:C:501:G2P:O6	2.38	0.45
2:D:207:LEU:HB3	2:D:225:LEU:HD22	1.99	0.45
3:E:385:VAL:HA	3:E:388:ASP:OD1	2.17	0.45
2:B:275:SER:OG	2:B:276:ARG:N	2.46	0.45
3:E:153:LYS:HE3	3:E:153:LYS:HB3	1.56	0.45
1:C:190:THR:O	1:C:193:THR:HG23	2.16	0.44
1:A:90:GLU:HB3	1:A:121:ARG:NH1	2.32	0.44
1:A:214:ARG:HG2	1:A:214:ARG:NH1	2.32	0.44
1:A:276:ILE:HG22	1:A:278:ALA:H	1.82	0.44
2:B:201:CYS:C	2:B:202:ILE:HD13	2.42	0.44
2:B:295:ASP:C	2:B:297:LYS:H	2.25	0.44
2:D:21:TRP:CZ2	2:D:63:ALA:HB2	2.53	0.44
3:E:358:ASP:HB3	3:E:467:LEU:HD12	1.99	0.44
2:B:299:MET:HE3	2:B:305:PRO:HG2	1.99	0.44
2:B:31:ASP:HB3	2:B:35:THR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:503:TA1:H472	6:D:503:TA1:H021	1.77	0.44
2:B:2:ARG:O	2:B:49:VAL:HG23	2.17	0.44
2:B:73:MET:HG3	2:B:92:PHE:HD1	1.83	0.44
1:C:265:ILE:HG21	1:C:313:MET:HE1	1.99	0.44
2:D:183:TYR:OH	2:D:388:MET:O	2.33	0.44
1:A:55:GLU:HG3	1:A:61:HIS:CE1	2.53	0.44
2:B:107:THR:OG1	2:B:108:GLU:N	2.50	0.44
1:C:68:VAL:HG11	1:C:149:PHE:CE2	2.53	0.44
2:B:141:GLY:O	2:B:145:SER:HB3	2.18	0.44
2:B:280:GLN:H	2:B:280:GLN:HG3	1.28	0.44
1:C:60:LYS:HE2	1:C:60:LYS:HB3	1.83	0.44
2:D:188:SER:O	2:D:189:VAL:C	2.61	0.44
1:A:241:SER:OG	1:A:250:VAL:O	2.28	0.44
2:D:297:LYS:HE3	2:D:297:LYS:H	1.83	0.44
3:E:406:VAL:HG21	3:E:617:LEU:HD22	2.00	0.44
1:A:285:GLN:O	1:A:285:GLN:HG2	2.18	0.43
1:A:306:ASP:HB3	1:A:309:HIS:CE1	2.53	0.43
2:B:80:PRO:O	2:B:81:PHE:C	2.61	0.43
2:B:139:LEU:HA	2:B:145:SER:HB2	2.00	0.43
2:B:159:TYR:HB3	2:B:162:ARG:HG2	2.00	0.43
3:E:626:PHE:CD1	3:E:626:PHE:C	2.96	0.43
2:B:271:ALA:HB1	2:B:289:LEU:HD22	2.00	0.43
2:B:403:MET:HE3	2:B:403:MET:HB3	1.90	0.43
3:E:159:ARG:NE	3:E:161:LEU:HB2	2.33	0.43
1:A:70:LEU:HB3	1:A:98:ASP:HA	2.01	0.43
1:C:98:ASP:OD2	2:D:252:LYS:HE2	2.18	0.43
2:D:173:PRO:HD3	2:D:380:ARG:NH2	2.33	0.43
3:E:551:ARG:O	3:E:554:ASN:ND2	2.48	0.43
1:A:69:ASP:OD1	1:A:70:LEU:N	2.51	0.43
1:C:398:MET:HG3	2:D:346:PRO:HD2	1.99	0.43
3:E:573:PHE:HD2	3:E:615:MET:HE1	1.81	0.43
1:A:252:LEU:O	1:A:256:GLN:HB2	2.18	0.43
2:D:267:MET:HA	2:D:268:PRO:HD3	1.79	0.43
1:C:273:ALA:O	1:C:275:VAL:N	2.41	0.43
6:D:503:TA1:H193	6:D:503:TA1:H021	1.83	0.43
3:E:652:LEU:HD12	3:E:652:LEU:HA	1.82	0.43
2:D:322:SER:OG	2:D:325:GLU:HG3	2.19	0.43
2:D:152:ILE:HG22	2:D:195:ASN:HB3	2.01	0.43
2:B:88:ASP:OD2	2:B:88:ASP:C	2.62	0.43
1:C:338:LYS:H	1:C:338:LYS:HG2	1.63	0.43
3:E:185:PHE:CB	3:E:188:MET:HE3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:242:TRP:CZ3	3:E:244:PRO:HG3	2.54	0.43
3:E:405:LYS:NZ	3:E:550:ASP:HB3	2.33	0.43
1:A:164:LYS:HE2	1:A:164:LYS:HB2	1.68	0.42
1:C:154:MET:HE2	1:C:168:GLU:OE2	2.19	0.42
1:C:200:CYS:HB3	1:C:202:PHE:HE1	1.84	0.42
1:A:174:ALA:HB3	1:A:177:VAL:O	2.20	0.42
2:D:203:ASP:OD1	2:D:206:ALA:N	2.43	0.42
6:B:503:TA1:H193	6:B:503:TA1:H021	1.85	0.42
1:C:301:GLN:HE21	1:C:307:PRO:HG3	1.84	0.42
1:A:205:ASP:HB2	1:A:303:VAL:HA	2.00	0.42
2:B:73:MET:HG3	2:B:92:PHE:CD1	2.54	0.42
1:C:239:THR:OG1	1:C:243:ARG:NH1	2.52	0.42
2:B:289:LEU:O	2:B:293:VAL:HB	2.20	0.42
1:C:178:SER:OG	1:C:179:THR:N	2.53	0.42
2:D:107:THR:OG1	2:D:108:GLU:N	2.53	0.42
3:E:168:HIS:N	3:E:183:ASN:OD1	2.41	0.42
2:D:112:LEU:O	2:D:116:VAL:HG23	2.19	0.42
1:A:198:SER:OG	1:A:200:CYS:O	2.38	0.42
2:D:152:ILE:HG23	2:D:164:MET:HE3	2.02	0.42
1:A:288:VAL:O	1:A:292:THR:OG1	2.26	0.42
1:C:288:VAL:HG21	1:C:327:ASP:CB	2.48	0.42
3:E:310:LEU:HD12	3:E:310:LEU:H	1.85	0.42
3:E:398:ILE:HD13	3:E:546:LEU:HB3	2.01	0.42
3:E:400:LEU:CD1	3:E:404:LEU:HD21	2.49	0.42
2:B:86:ARG:HG2	2:B:87:PRO:HD2	2.02	0.41
1:C:265:ILE:HG23	1:C:432:TYR:CE1	2.56	0.41
2:D:68:LEU:HD23	2:D:112:LEU:HD13	2.02	0.41
1:A:274:PRO:HG3	1:A:374:ALA:HA	2.02	0.41
3:E:201:VAL:HG11	3:E:215:TYR:CD2	2.55	0.41
1:A:119:LEU:HD21	1:A:156:ARG:HD3	2.01	0.41
2:B:172:SER:HB2	2:B:203:ASP:OD1	2.20	0.41
1:A:349:THR:O	1:A:349:THR:OG1	2.36	0.41
1:C:138:PHE:HZ	1:C:235:VAL:HG21	1.86	0.41
2:D:117:LEU:HD21	2:D:154:LYS:HB3	2.02	0.41
2:D:131:GLN:NE2	2:D:250:LEU:HB2	2.35	0.41
2:D:218:THR:O	2:D:220:PRO:HD3	2.20	0.41
3:E:635:LEU:HD23	3:E:635:LEU:HA	1.92	0.41
1:A:230:LEU:HD23	1:A:302:MET:HE2	2.03	0.41
1:C:138:PHE:CZ	1:C:235:VAL:HG21	2.56	0.41
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.53	0.41
1:A:266:HIS:C	1:A:268:PRO:HD3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:VAL:HG23	2:B:258:VAL:O	2.20	0.41
2:B:331:LEU:HD12	2:B:331:LEU:HA	1.88	0.41
1:C:9:VAL:HG22	1:C:68:VAL:HB	2.01	0.41
2:D:198:GLU:OE1	2:D:200:TYR:OH	2.29	0.41
3:E:630:ARG:HA	3:E:630:ARG:HD2	1.80	0.41
1:A:138:PHE:HE2	1:A:235:VAL:HG21	1.85	0.41
2:D:67:ASP:OD1	2:D:68:LEU:N	2.53	0.41
3:E:185:PHE:HB3	3:E:188:MET:HE3	2.02	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.41
2:B:183:TYR:OH	2:B:388:MET:O	2.36	0.41
2:B:284:LEU:HD12	2:B:288:GLU:OE2	2.21	0.41
1:C:313:MET:HG2	1:C:346:TRP:CZ2	2.56	0.41
1:C:419:SER:O	1:C:423:GLU:HG3	2.21	0.41
3:E:428:ASP:OD1	3:E:428:ASP:N	2.54	0.41
3:E:431:LEU:HD13	3:E:432:MET:O	2.20	0.41
1:A:247:ALA:HB3	1:A:355:ILE:HB	2.03	0.41
3:E:440:LEU:HB2	3:E:441:GLY:H	1.65	0.41
1:A:273:ALA:HB2	1:A:295:CYS:SG	2.61	0.40
3:E:148:ARG:HG2	3:E:148:ARG:NH1	2.35	0.40
1:A:11:GLN:NE2	2:B:245:GLN:O	2.54	0.40
2:B:112:LEU:HB3	2:B:147:MET:HE1	2.03	0.40
2:B:355:ASP:OD1	2:B:355:ASP:N	2.54	0.40
1:C:107:HIS:O	1:C:107:HIS:ND1	2.53	0.40
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.88	0.40
2:D:310:TYR:HA	2:D:371:SER:HB2	2.03	0.40
3:E:188:MET:HE1	3:E:404:LEU:HD22	2.03	0.40
1:C:252:LEU:HD12	1:C:252:LEU:HA	1.83	0.40
1:A:265:ILE:HG23	1:A:432:TYR:OH	2.21	0.40
2:D:164:MET:HG2	2:D:196:THR:HG22	2.02	0.40
1:A:402:ARG:HE	1:A:402:ARG:HB2	1.65	0.40
1:C:187:SER:OG	1:C:391:LEU:HD21	2.21	0.40
1:C:322:ASP:OD1	1:C:322:ASP:O	2.39	0.40
1:C:356:ASN:OD1	1:C:356:ASN:C	2.64	0.40
2:D:396:HIS:CE1	2:D:397:TRP:CD1	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/451 (94%)	405 (95%)	21 (5%)	0	100	100
1	C	426/451 (94%)	403 (95%)	23 (5%)	0	100	100
2	B	424/444 (96%)	392 (92%)	31 (7%)	1 (0%)	44	72
2	D	425/444 (96%)	396 (93%)	29 (7%)	0	100	100
3	E	513/990 (52%)	495 (96%)	18 (4%)	0	100	100
All	All	2214/2780 (80%)	2091 (94%)	122 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	275	SER

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	364/379 (96%)	338 (93%)	26 (7%)	12	36
1	C	364/379 (96%)	339 (93%)	25 (7%)	13	38
2	B	366/379 (97%)	329 (90%)	37 (10%)	6	23
2	D	367/379 (97%)	335 (91%)	32 (9%)	8	29
3	E	469/864 (54%)	452 (96%)	17 (4%)	30	57
All	All	1930/2380 (81%)	1793 (93%)	137 (7%)	15	36

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	48	SER
1	A	51	THR
1	A	56	THR
1	A	66	VAL
1	A	75	ILE
1	A	110	ILE
1	A	122	ILE
1	A	125	LEU
1	A	170	SER
1	A	198	SER
1	A	202	PHE
1	A	223	THR
1	A	256	GLN
1	A	269	LEU
1	A	341	ILE
1	A	353	VAL
1	A	362	VAL
1	A	377	MET
1	A	384	ILE
1	A	394	LYS
1	A	429	GLU
1	A	430	LYS
1	A	432	TYR
1	A	435	VAL
1	A	437	VAL
2	B	1	MET
2	B	60	VAL
2	B	75	SER
2	B	84	ILE
2	B	91	VAL
2	B	107	THR
2	B	112	LEU
2	B	119	VAL
2	B	123	GLU
2	B	149	THR
2	B	163	ILE
2	B	164	MET
2	B	188	SER
2	B	193	VAL
2	B	205	GLU
2	B	219	THR

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Mol	Chain	Res	Type
2	B	221	THR
2	B	224	ASP
2	B	238	THR
2	B	255	VAL
2	B	278	SER
2	B	280	GLN
2	B	291	GLN
2	B	292	GLN
2	B	293	VAL
2	B	297	LYS
2	B	312	THR
2	B	337	ASN
2	B	342	VAL
2	B	350	LYS
2	B	363	MET
2	B	365	VAL
2	B	366	THR
2	B	392	LYS
2	B	395	LEU
2	B	417	ASP
2	B	422	TYR
1	C	36	MET
1	C	109	THR
1	C	110	ILE
1	C	119	LEU
1	C	157	LEU
1	C	158	SER
1	C	179	THR
1	C	193	THR
1	C	195	LEU
1	C	203	MET
1	C	230	LEU
1	C	248	LEU
1	C	257	THR
1	C	259	LEU
1	C	271	THR
1	C	286	LEU
1	C	323	VAL
1	C	338	LYS
1	C	342	GLN
1	C	344	VAL
1	C	377	MET

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Mol	Chain	Res	Type
1	C	384	ILE
1	C	390	ARG
1	C	425	MET
1	C	432	TYR
2	D	19	LYS
2	D	44	LEU
2	D	47	ILE
2	D	83	GLN
2	D	84	ILE
2	D	88	ASP
2	D	147	MET
2	D	151	LEU
2	D	157	GLU
2	D	162	ARG
2	D	178	THR
2	D	219	THR
2	D	234	SER
2	D	243	PRO
2	D	247	ASN
2	D	274	THR
2	D	275	SER
2	D	276	ARG
2	D	293	VAL
2	D	297	LYS
2	D	306	ARG
2	D	312	THR
2	D	320	ARG
2	D	334	GLN
2	D	342	VAL
2	D	345	ILE
2	D	351	THR
2	D	362	LYS
2	D	365	VAL
2	D	395	LEU
2	D	396	HIS
2	D	415	MET
3	E	308	ASP
3	E	384	LYS
3	E	440	LEU
3	E	535	VAL
3	E	539	TYR
3	E	541	LYS

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Mol	Chain	Res	Type
3	E	548	LEU
3	E	552	MET
3	E	566	MET
3	E	574	ARG
3	E	589	MET
3	E	598	ASP
3	E	609	ASP
3	E	611	ARG
3	E	612	ASP
3	E	638	HIS
3	E	655	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	133	GLN
1	A	393	HIS
1	A	406	HIS
2	B	6	HIS
2	B	14	ASN
2	B	43	GLN
2	B	100	ASN
2	B	256	ASN
2	B	279	GLN
1	C	18	ASN
1	C	256	GLN
1	C	406	HIS
2	D	8	GLN
2	D	37	HIS
2	D	100	ASN
2	D	190	HIS
2	D	191	GLN
2	D	195	ASN
2	D	264	HIS
2	D	279	GLN
2	D	298	ASN
2	D	337	ASN
2	D	347	ASN
2	D	424	GLN
3	E	181	GLN
3	E	344	ASN

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Mol	Chain	Res	Type
3	E	534	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	G2P	C	501	5	27,34,34	1.75	6 (22%)	33,54,54	2.32	7 (21%)
4	G2P	B	501	5	27,34,34	1.77	6 (22%)	33,54,54	2.30	7 (21%)
4	G2P	A	501	5	27,34,34	1.77	6 (22%)	33,54,54	2.30	7 (21%)
4	G2P	D	501	5	27,34,34	1.77	6 (22%)	33,54,54	2.33	7 (21%)
6	TA1	B	503	-	68,68,68	0.66	1 (1%)	105,105,105	1.66	16 (15%)
6	TA1	D	503	-	68,68,68	0.65	1 (1%)	105,105,105	1.70	19 (18%)

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
4	G2P	C	501	5	-	5/15/38/38	0/3/3/3
4	G2P	B	501	5	-	9/15/38/38	0/3/3/3
4	G2P	A	501	5	-	3/15/38/38	0/3/3/3
4	G2P	D	501	5	-	3/15/38/38	0/3/3/3
6	TA1	B	503	-	-	9/41/127/127	0/7/7/7
6	TA1	D	503	-	-	6/41/127/127	0/7/7/7

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	G2P	PA-O5'	5.70	1.65	1.57
4	A	501	G2P	PA-O5'	5.61	1.65	1.57
4	B	501	G2P	PA-O5'	5.56	1.65	1.57
4	C	501	G2P	PA-O5'	5.45	1.65	1.57
4	A	501	G2P	C6-N1	4.05	1.40	1.33
4	B	501	G2P	C6-N1	4.03	1.40	1.33
4	C	501	G2P	C6-N1	4.02	1.40	1.33
4	D	501	G2P	C6-N1	3.97	1.39	1.33
4	C	501	G2P	C8-N7	-2.80	1.29	1.34
4	B	501	G2P	C8-N7	-2.74	1.29	1.34
4	D	501	G2P	C8-N7	-2.71	1.29	1.34
4	A	501	G2P	C8-N7	-2.69	1.29	1.34
4	A	501	G2P	PA-O1A	-2.44	1.50	1.56
4	A	501	G2P	PB-O3B	2.43	1.61	1.58
4	D	501	G2P	PB-O3B	2.41	1.61	1.58
4	B	501	G2P	PB-O3B	2.38	1.61	1.58
4	C	501	G2P	PA-O1A	-2.32	1.50	1.56
4	B	501	G2P	PB-O1B	-2.32	1.50	1.56
4	D	501	G2P	PA-O1A	-2.30	1.51	1.56
4	D	501	G2P	PB-O1B	-2.29	1.51	1.56
4	B	501	G2P	PA-O1A	-2.29	1.51	1.56
4	A	501	G2P	PB-O1B	-2.27	1.51	1.56
4	C	501	G2P	PB-O1B	-2.22	1.51	1.56
4	C	501	G2P	PB-O3B	2.16	1.60	1.58
6	D	503	TA1	C18-C10	2.13	1.62	1.57
6	B	503	TA1	C18-C10	2.06	1.61	1.57

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	G2P	C5-C6-N1	-9.20	110.84	123.43
4	B	501	G2P	C5-C6-N1	-9.13	110.95	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	G2P	C5-C6-N1	-9.10	110.98	123.43
4	A	501	G2P	C5-C6-N1	-9.05	111.05	123.43
6	B	503	TA1	C10-C18-C20	-6.41	105.27	116.31
4	D	501	G2P	C2-N1-C6	6.28	125.91	115.93
6	D	503	TA1	C10-C18-C20	-6.26	105.55	116.31
4	A	501	G2P	C2-N1-C6	6.25	125.86	115.93
4	C	501	G2P	C2-N1-C6	6.24	125.85	115.93
4	B	501	G2P	C2-N1-C6	6.16	125.72	115.93
6	B	503	TA1	O04-C11-C14	5.88	120.94	108.09
6	D	503	TA1	O04-C11-C14	5.80	120.77	108.09
6	D	503	TA1	C21-C24-C25	-5.22	113.06	120.40
6	B	503	TA1	C21-C24-C25	-5.19	113.11	120.40
6	D	503	TA1	O08-C20-C21	-4.55	113.37	119.30
6	B	503	TA1	O08-C20-C21	-4.45	113.50	119.30
6	B	503	TA1	C10-C18-C17	4.26	114.82	106.54
6	D	503	TA1	C10-C18-C17	4.24	114.80	106.54
6	B	503	TA1	O04-C11-C10	-3.97	102.88	109.24
6	B	503	TA1	O09-C21-C24	3.93	115.08	109.83
6	D	503	TA1	O04-C11-C10	-3.92	102.97	109.24
6	D	503	TA1	O09-C21-C24	3.60	114.64	109.83
6	D	503	TA1	C11-C10-C18	3.59	116.02	110.73
6	B	503	TA1	C11-C10-C18	3.31	115.60	110.73
6	D	503	TA1	O09-C21-C20	3.21	116.99	108.69
4	A	501	G2P	N3-C2-N1	-3.14	123.03	127.22
6	B	503	TA1	C47-C45-C46	-3.12	97.09	106.26
6	B	503	TA1	O09-C21-C20	3.11	116.73	108.69
4	C	501	G2P	N3-C2-N1	-3.10	123.08	127.22
6	D	503	TA1	C47-C45-C46	-3.06	97.25	106.26
4	D	501	G2P	N3-C2-N1	-2.96	123.28	127.22
4	B	501	G2P	N3-C2-N1	-2.85	123.43	127.22
6	D	503	TA1	C37-C29-N01	2.81	117.61	112.11
6	B	503	TA1	C19-C18-C17	-2.79	104.27	109.84
6	D	503	TA1	C19-C18-C17	-2.78	104.28	109.84
6	D	503	TA1	C18-C20-C21	2.75	127.72	121.44
6	B	503	TA1	C18-C20-C21	2.60	127.38	121.44
4	C	501	G2P	O1B-PB-O2B	2.46	118.29	110.07
4	D	501	G2P	O1B-PB-O2B	2.40	118.09	110.07
4	C	501	G2P	O1A-PA-O2A	2.36	117.94	110.07
4	B	501	G2P	O1B-PB-O2B	2.32	117.82	110.07
4	A	501	G2P	O1A-PA-O2A	2.31	117.79	110.07
6	B	503	TA1	C19-C18-C20	2.29	112.78	106.55
4	D	501	G2P	O1A-PA-O2A	2.27	117.66	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	G2P	O1A-PA-O2A	2.26	117.60	110.07
6	D	503	TA1	C11-O04-C12	2.24	124.85	119.06
6	D	503	TA1	C19-C18-C20	2.23	112.61	106.55
6	B	503	TA1	C11-O04-C12	2.20	124.75	119.06
4	A	501	G2P	O1B-PB-O2B	2.19	117.39	110.07
4	C	501	G2P	O3G-PG-O1G	2.19	116.00	107.64
4	A	501	G2P	C4-C5-C6	-2.18	118.72	120.80
6	D	503	TA1	C47-C45-C24	2.15	121.57	112.83
6	D	503	TA1	C45-C24-C21	2.14	125.97	118.78
4	B	501	G2P	O3G-PG-O1G	2.14	115.81	107.64
6	D	503	TA1	C29-N01-C30	2.13	125.70	122.28
6	B	503	TA1	C47-C45-C24	2.13	121.49	112.83
6	B	503	TA1	C45-C24-C21	2.12	125.90	118.78
4	C	501	G2P	C4-C5-C6	-2.11	118.78	120.80
4	B	501	G2P	PB-O3B-PG	-2.11	125.18	132.62
4	D	501	G2P	C4-C5-C6	-2.05	118.84	120.80
6	D	503	TA1	C42-C37-C29	2.05	124.04	120.78
4	D	501	G2P	O3G-PG-O1G	2.05	115.46	107.64
4	A	501	G2P	O3G-PG-O1G	2.02	115.37	107.64

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	G2P	PB-O3B-PG-O1G
4	A	501	G2P	C5'-O5'-PA-O2A
4	B	501	G2P	PB-O3B-PG-O3G
4	B	501	G2P	PA-C3A-PB-O3B
4	B	501	G2P	PA-C3A-PB-O2B
4	C	501	G2P	PA-C3A-PB-O3B
4	C	501	G2P	PA-C3A-PB-O1B
4	C	501	G2P	PA-C3A-PB-O2B
4	C	501	G2P	PB-C3A-PA-O2A
6	B	503	TA1	C15-C11-O04-C12
6	B	503	TA1	O05-C12-O04-C11
6	B	503	TA1	C13-C12-O04-C11
6	D	503	TA1	C14-C11-O04-C12
6	D	503	TA1	O05-C12-O04-C11
6	D	503	TA1	C13-C12-O04-C11
6	B	503	TA1	O14-C30-C31-C32
6	B	503	TA1	N01-C30-C31-C32
6	B	503	TA1	O14-C30-C31-C36

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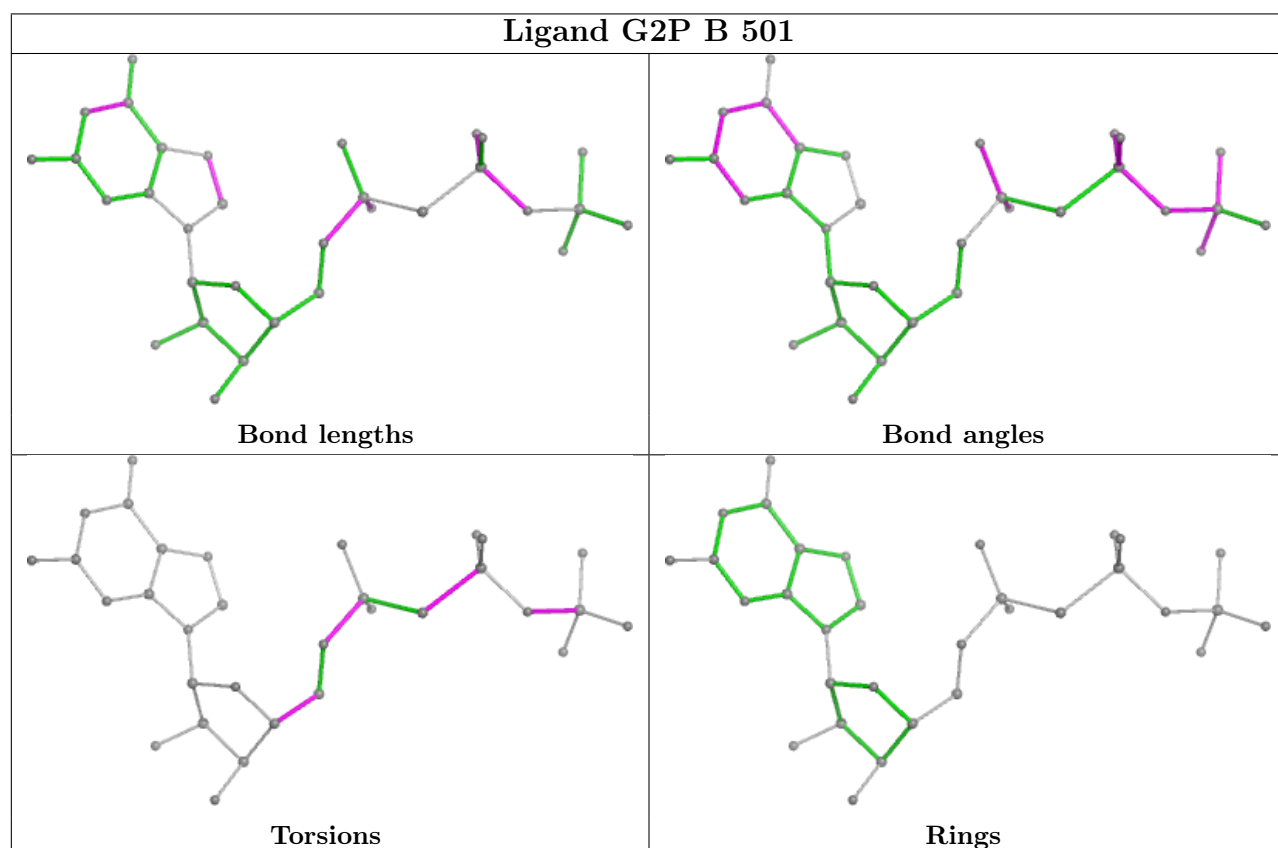
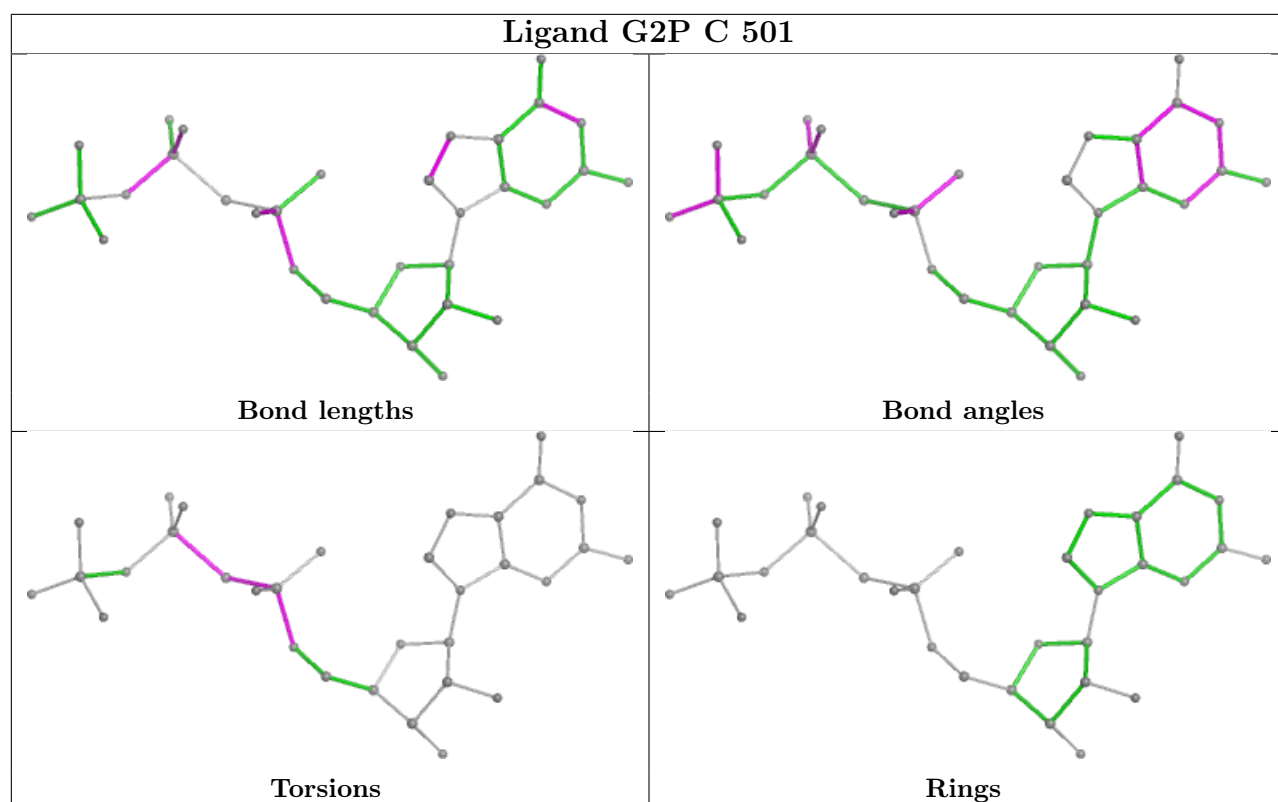
Mol	Chain	Res	Type	Atoms
6	B	503	TA1	N01-C30-C31-C36
4	B	501	G2P	O4'-C4'-C5'-O5'
4	B	501	G2P	C3'-C4'-C5'-O5'
4	D	501	G2P	C5'-O5'-PA-C3A
6	B	503	TA1	C14-C11-O04-C12
4	B	501	G2P	C5'-O5'-PA-O2A
4	B	501	G2P	PB-O3B-PG-O2G
6	D	503	TA1	C27-C28-C29-N01
4	C	501	G2P	C5'-O5'-PA-O2A
4	D	501	G2P	C5'-O5'-PA-O2A
4	B	501	G2P	PA-C3A-PB-O1B
4	A	501	G2P	C4'-C5'-O5'-PA
4	D	501	G2P	PB-C3A-PA-O2A
4	B	501	G2P	C5'-O5'-PA-O1A
6	B	503	TA1	C23-C22-O09-C21
6	D	503	TA1	C15-C11-O04-C12
6	D	503	TA1	C37-C29-N01-C30

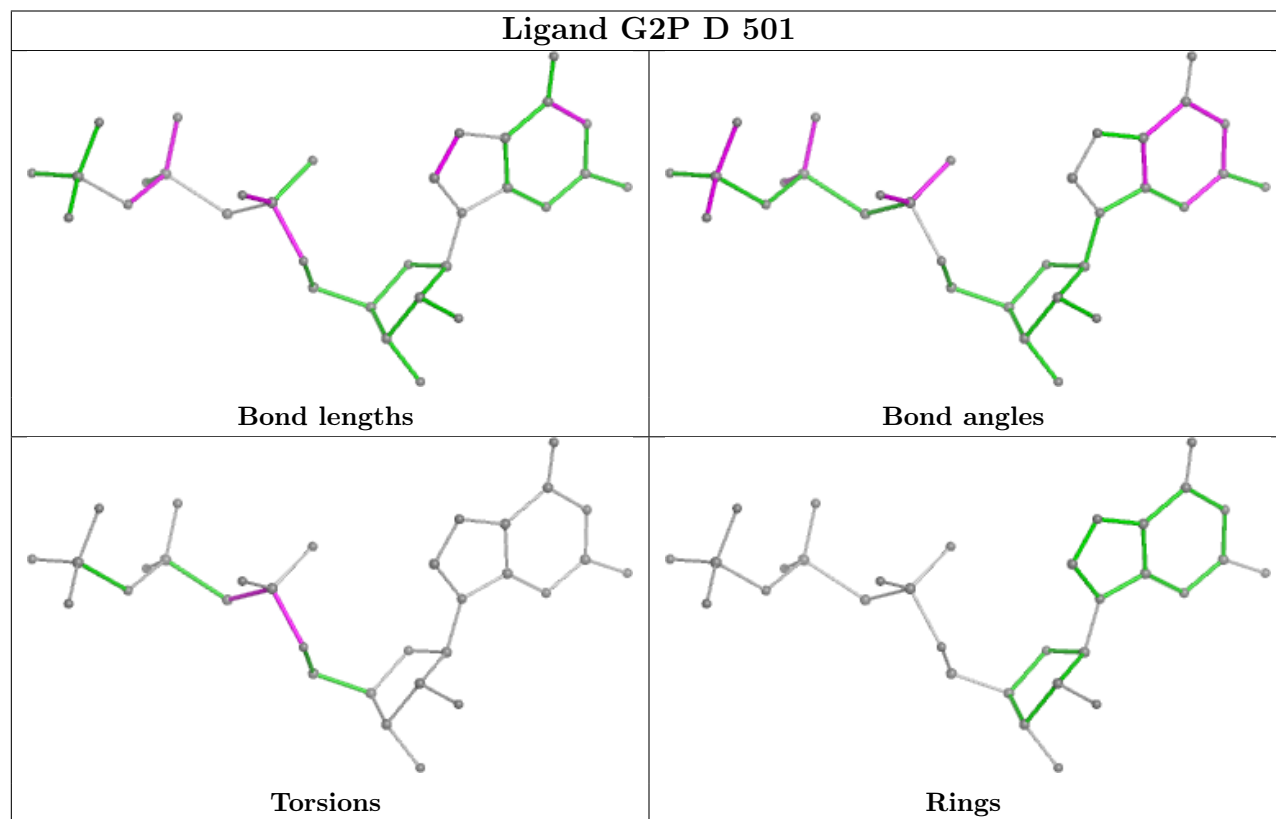
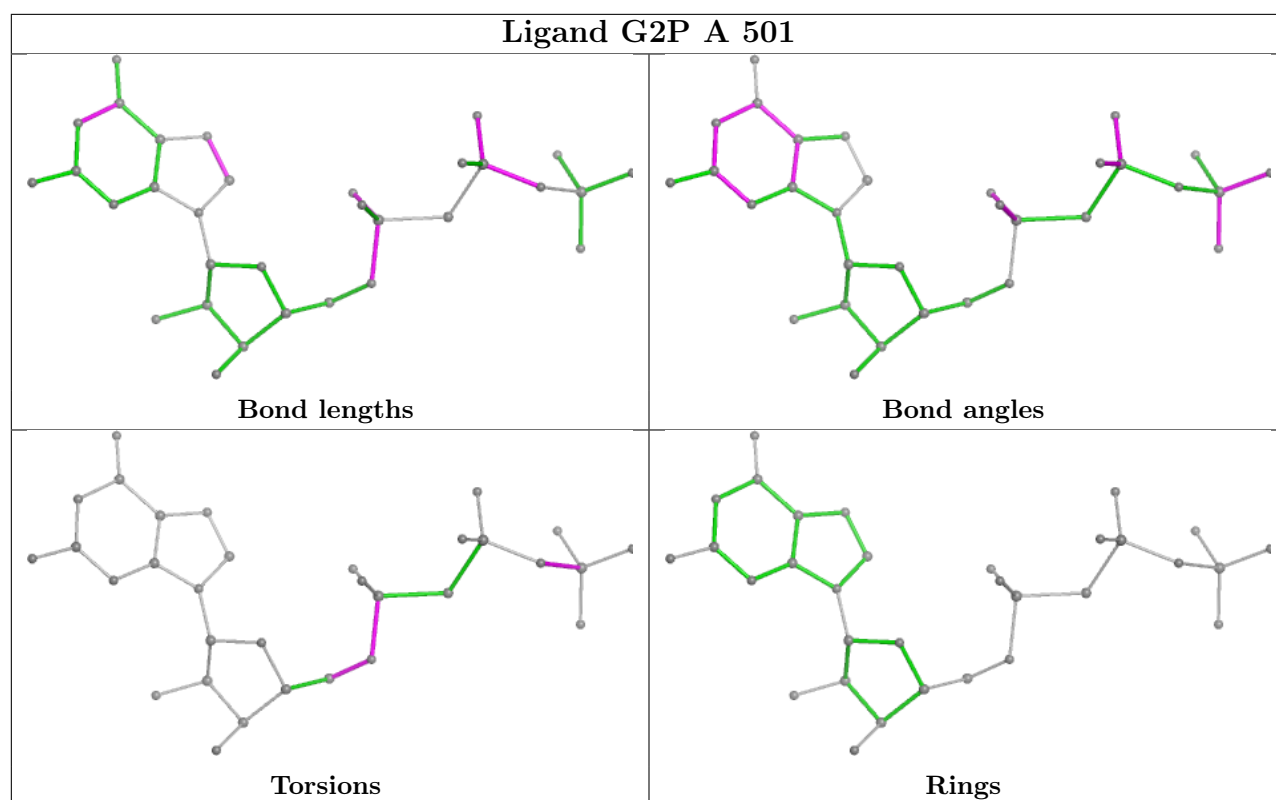
There are no ring outliers.

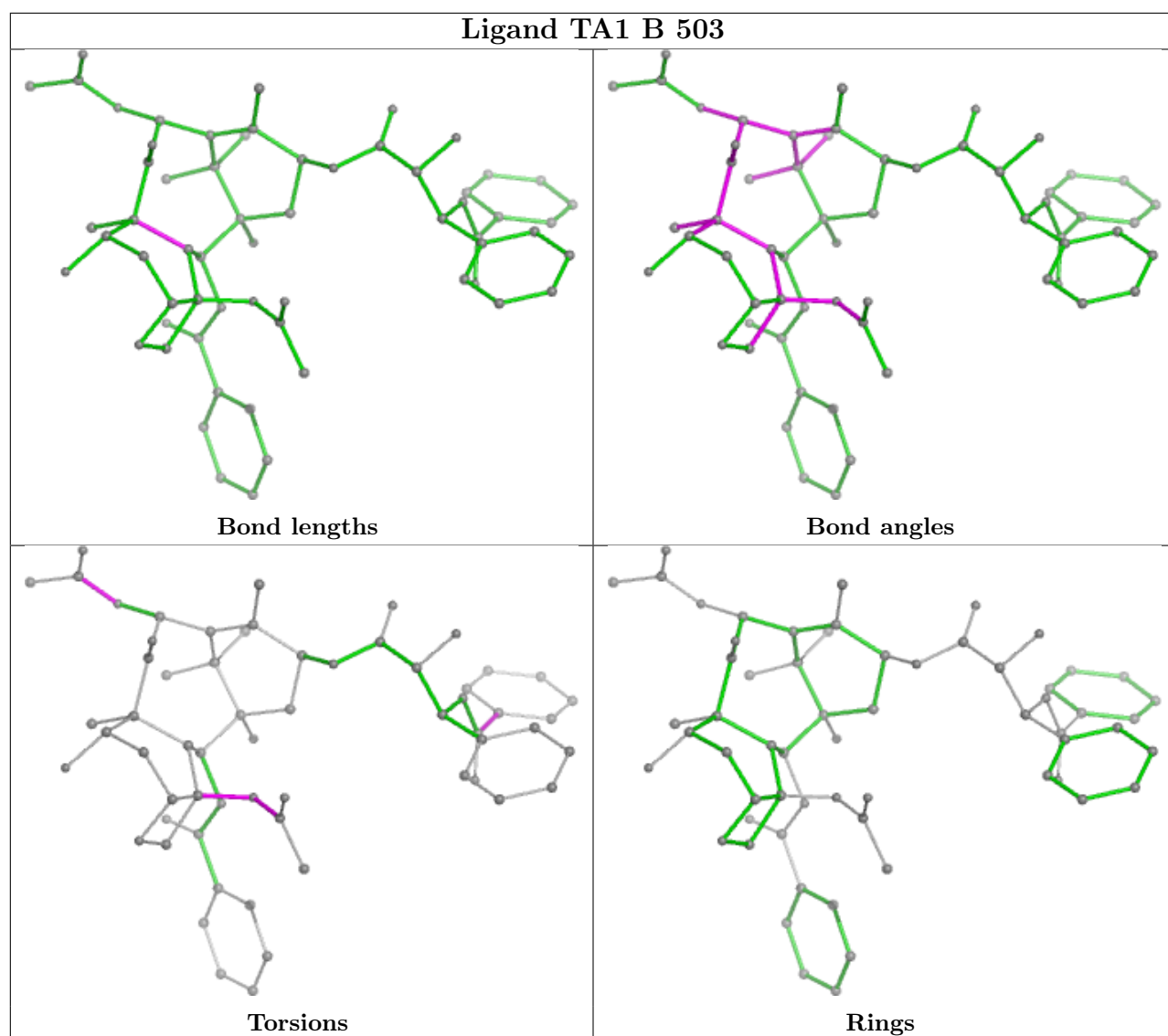
3 monomers are involved in 11 short contacts:

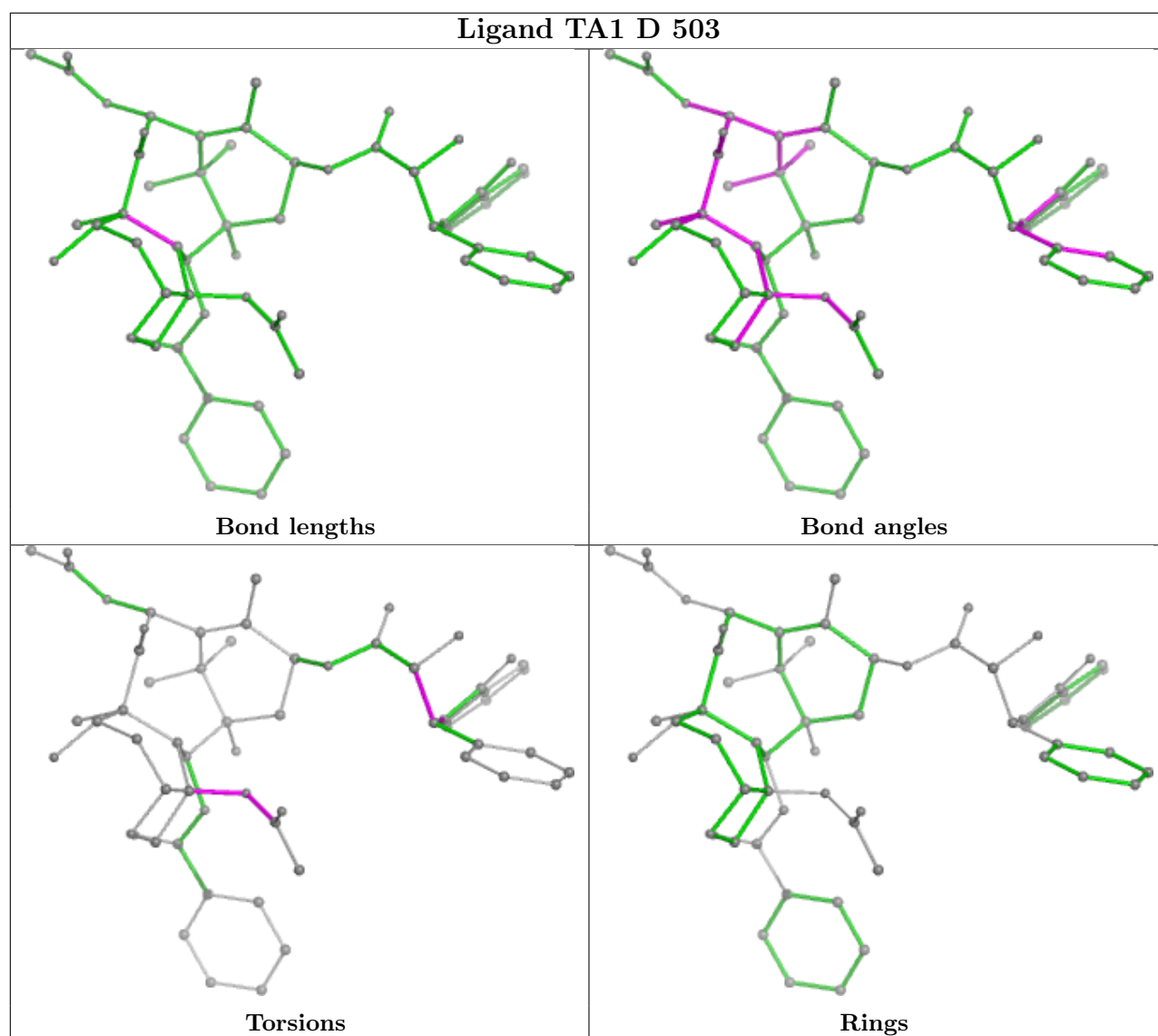
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	G2P	4	0
6	B	503	TA1	4	0
6	D	503	TA1	3	0

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









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.

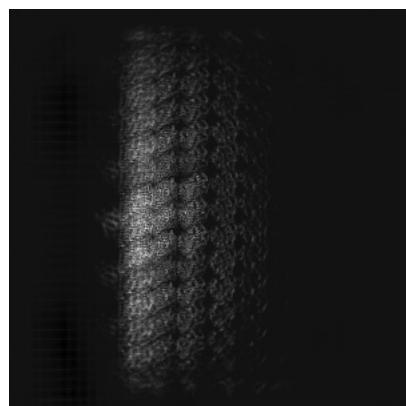
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52338. These allow visual inspection of the internal detail of the map and identification of artifacts.

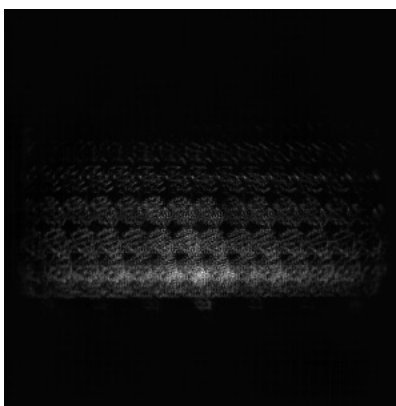
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

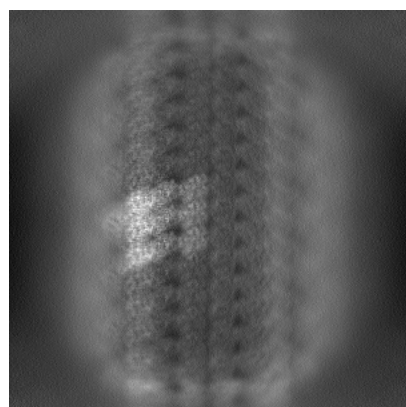


Y

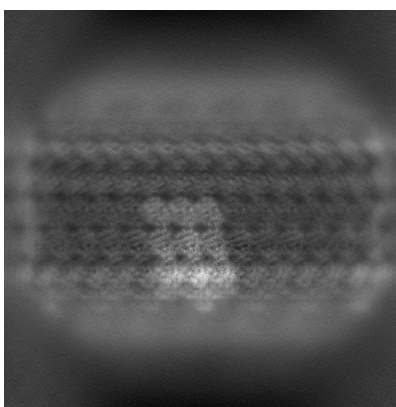


Z

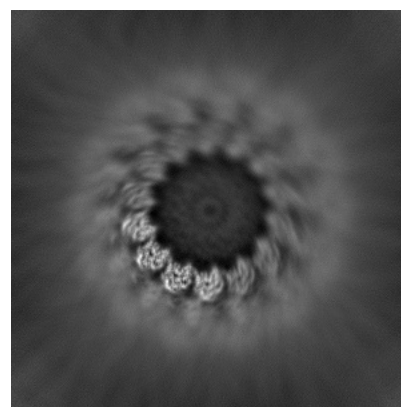
6.1.2 Raw map



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: 240

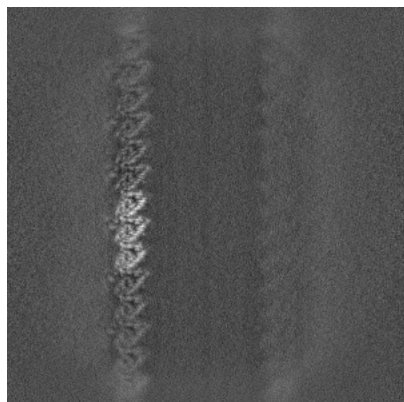


Y Index: 240

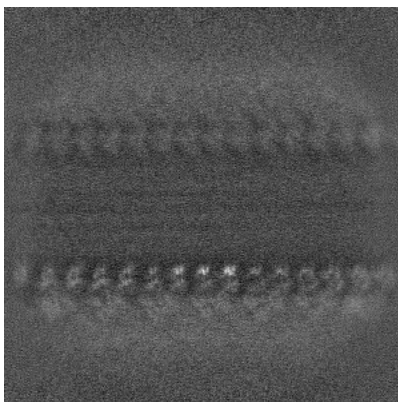


Z Index: 240

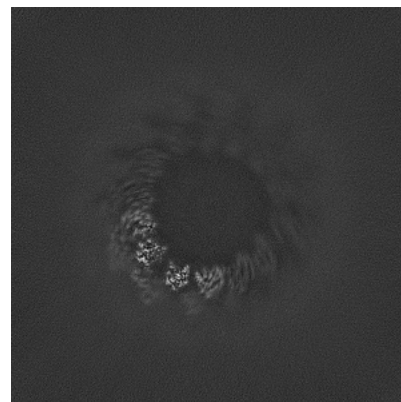
6.2.2 Raw map



X Index: 240



Y Index: 240

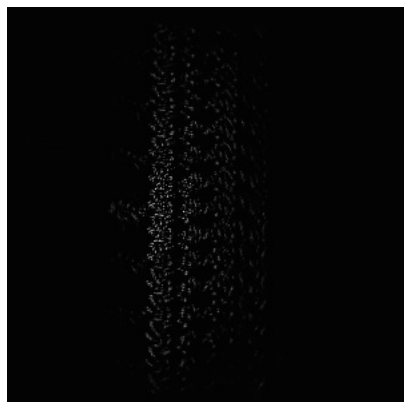


Z Index: 240

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: 162

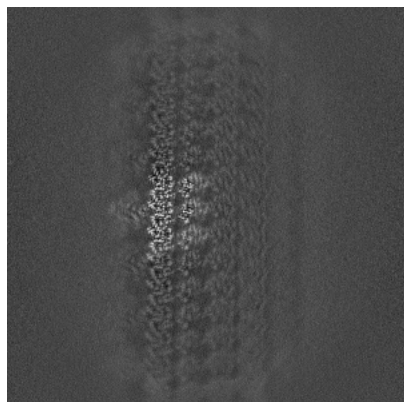


Y Index: 155

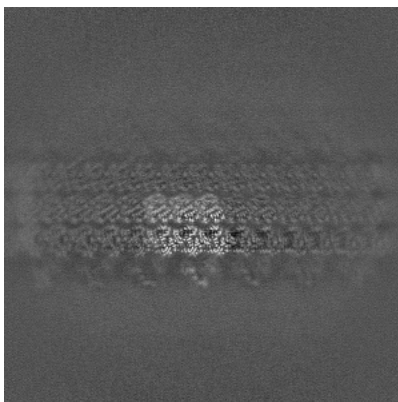


Z Index: 230

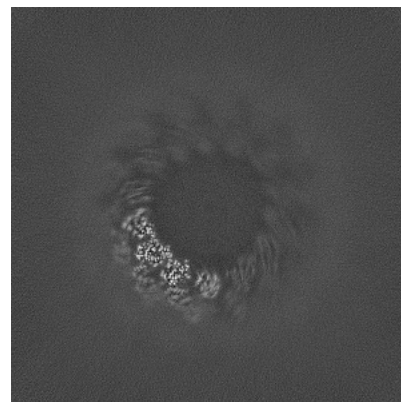
6.3.2 Raw map



X Index: 162



Y Index: 155

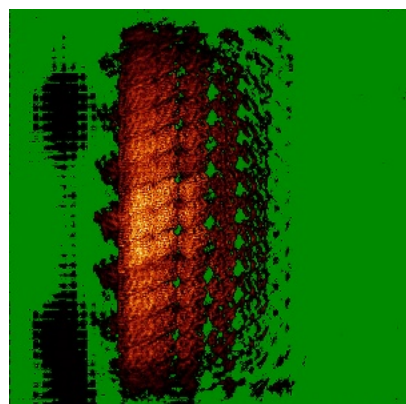


Z Index: 230

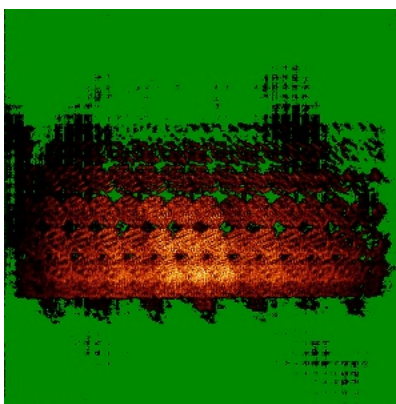
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

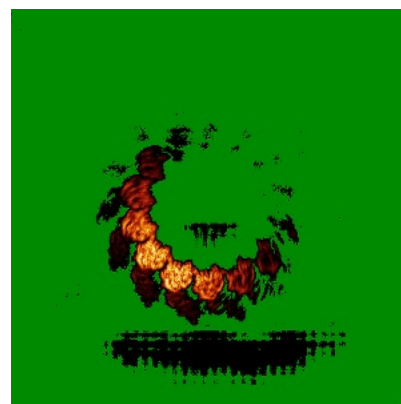
6.4.1 Primary map



X

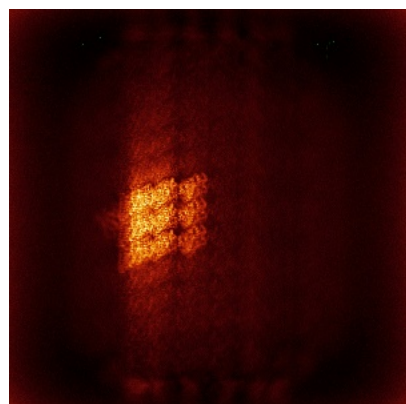


Y

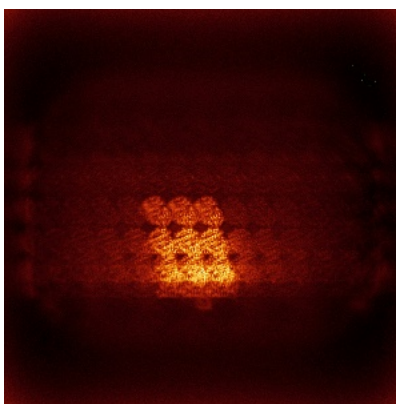


Z

6.4.2 Raw map



X



Y

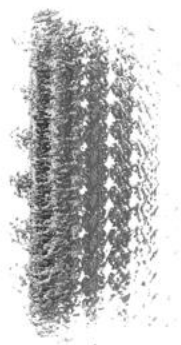


Z

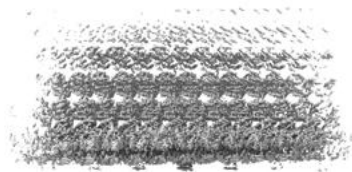
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



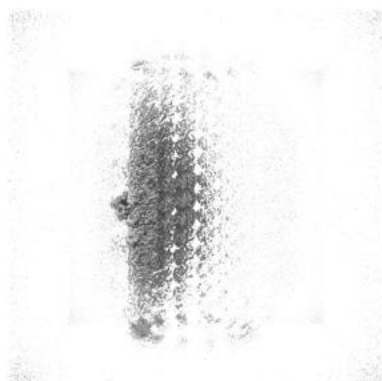
Y



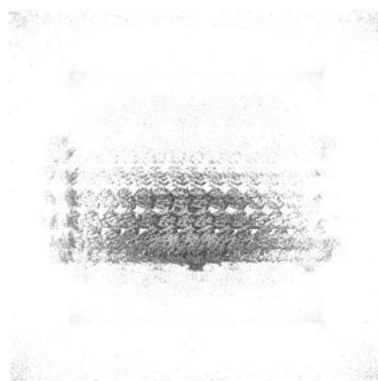
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0956. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

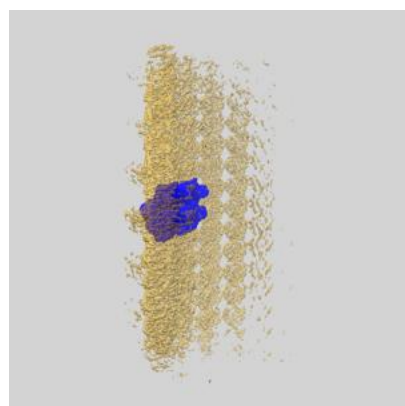
6.6 Mask visualisation [i](#)

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

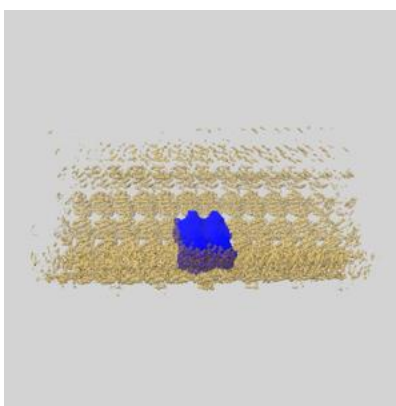
A mask typically either:

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

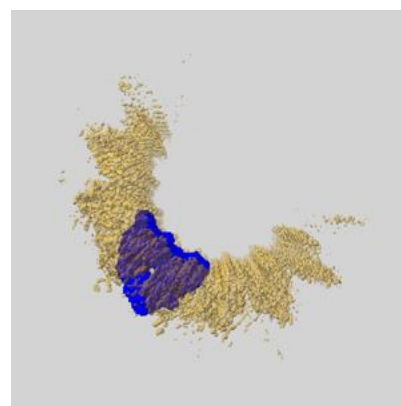
6.6.1 emd_52338_msk_1.map [i](#)



X



Y

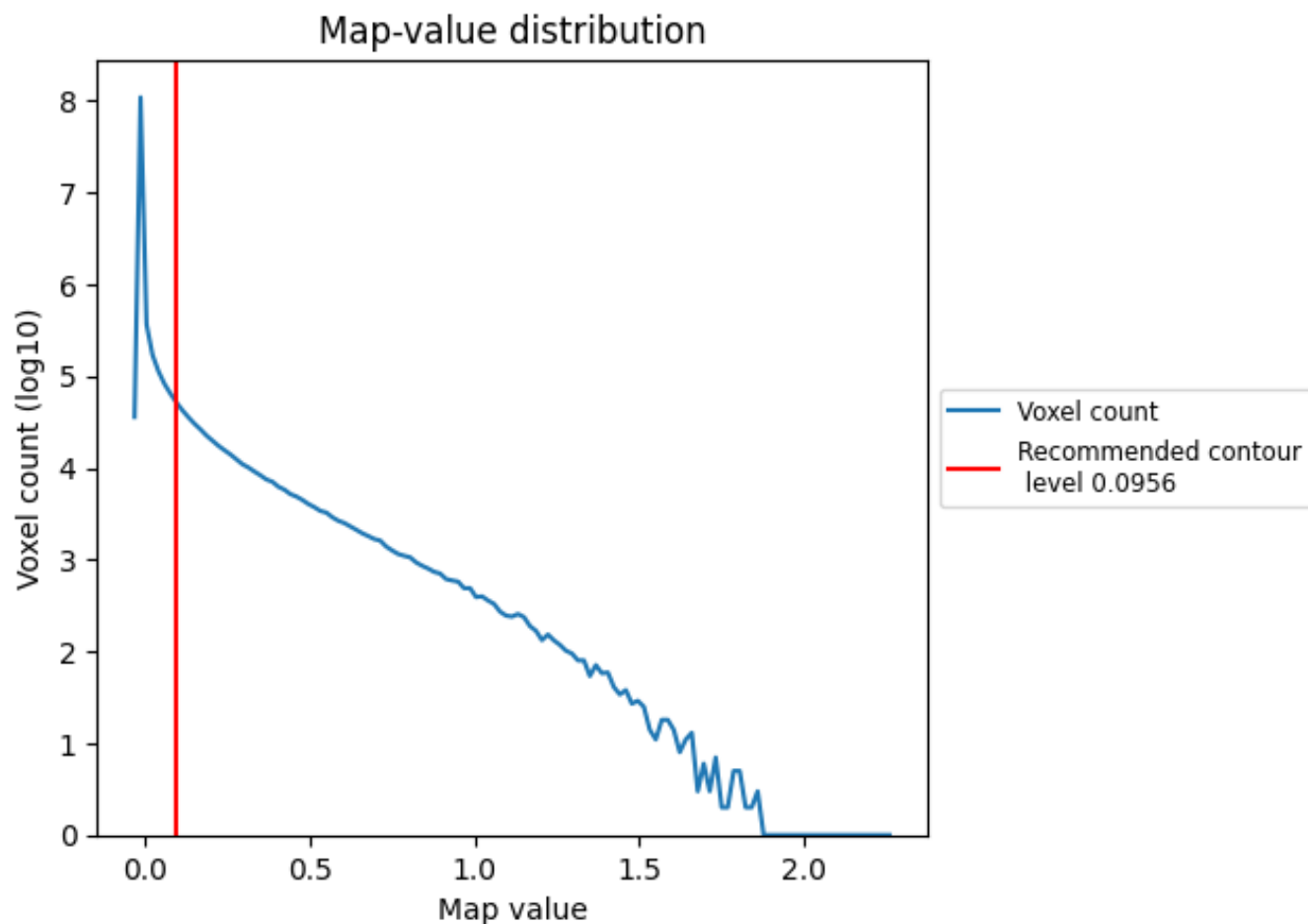


Z

7 Map analysis [i](#)

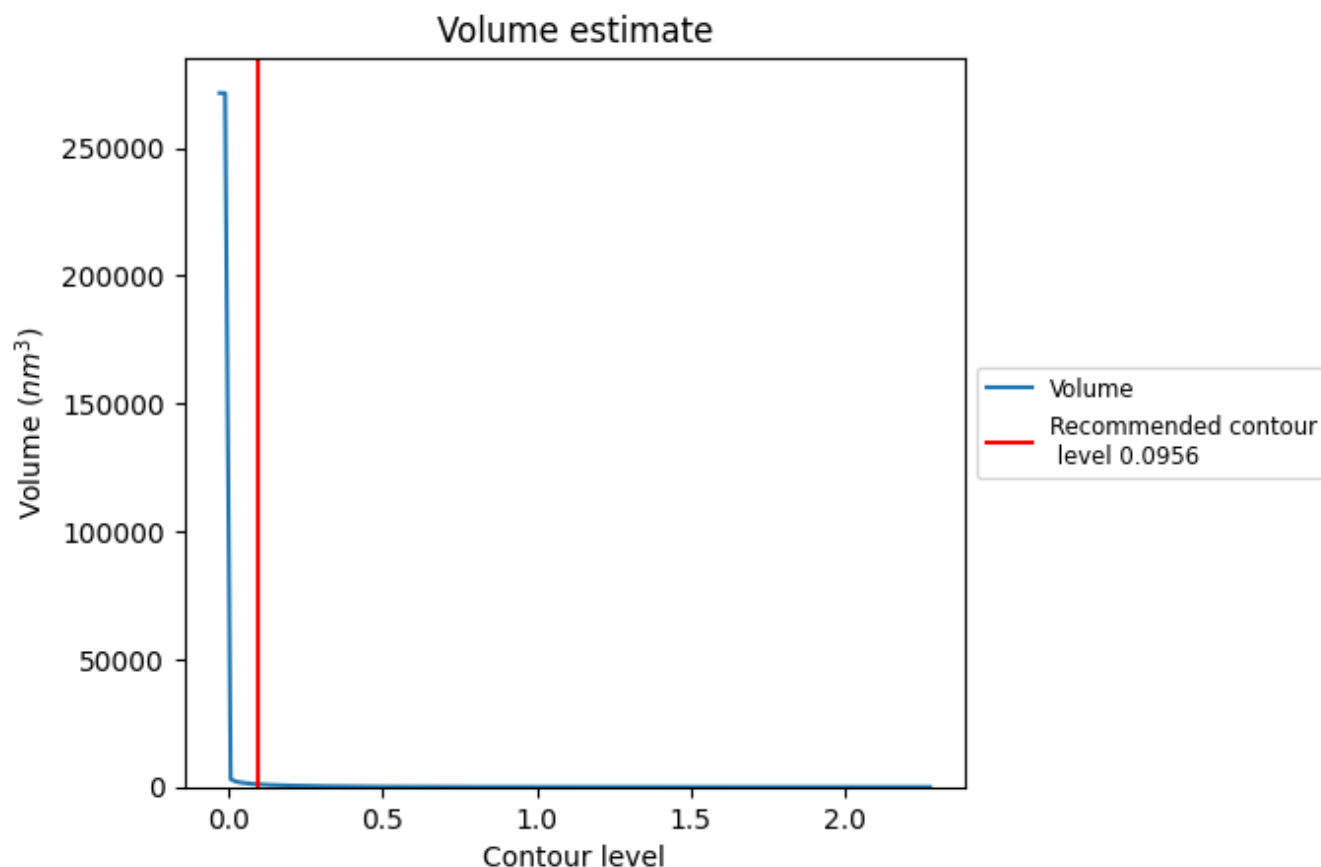
This section contains the results of statistical analysis of the map.

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.

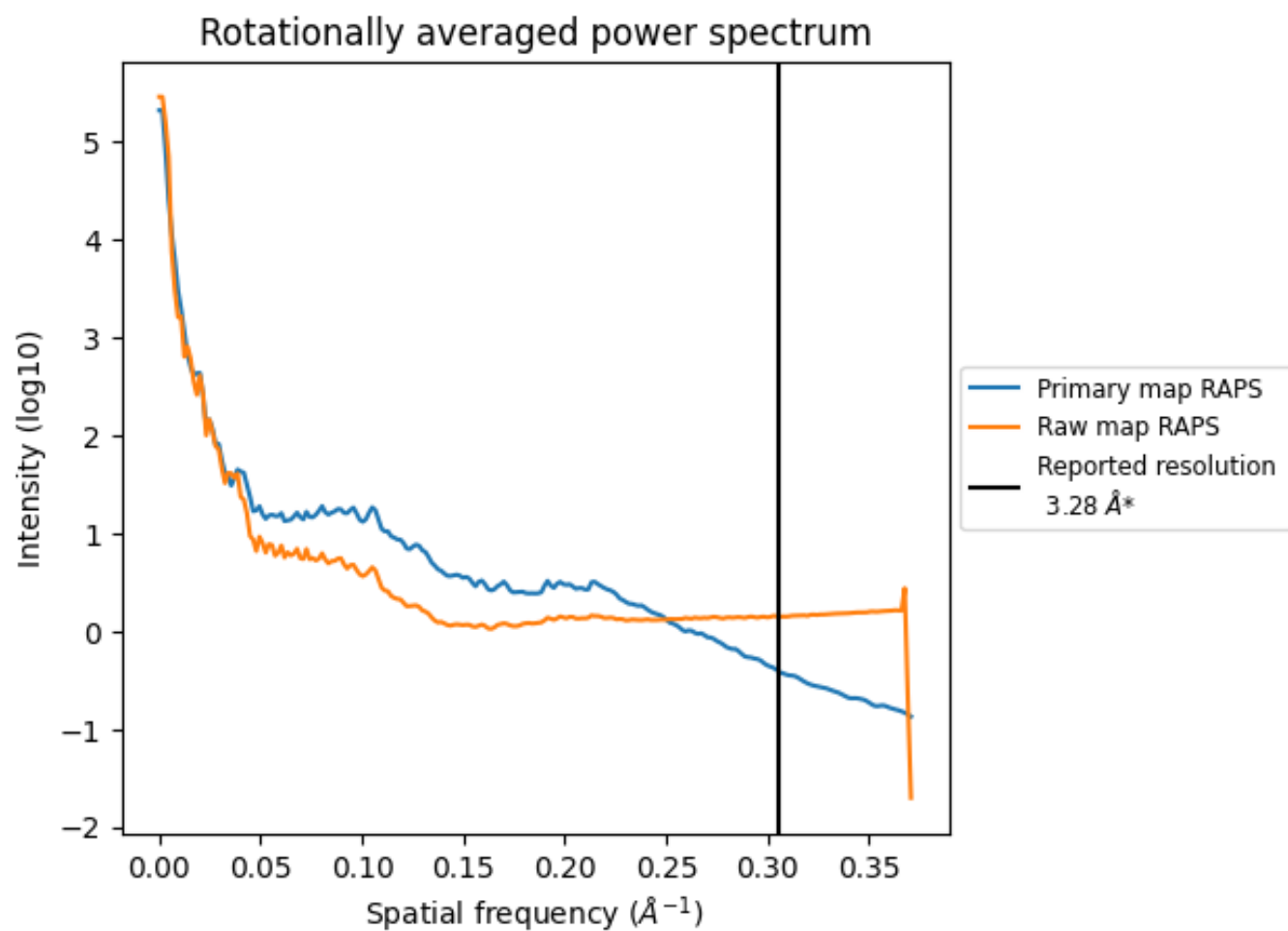
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1053 nm³; this corresponds to an approximate mass of 951 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 ⓘ

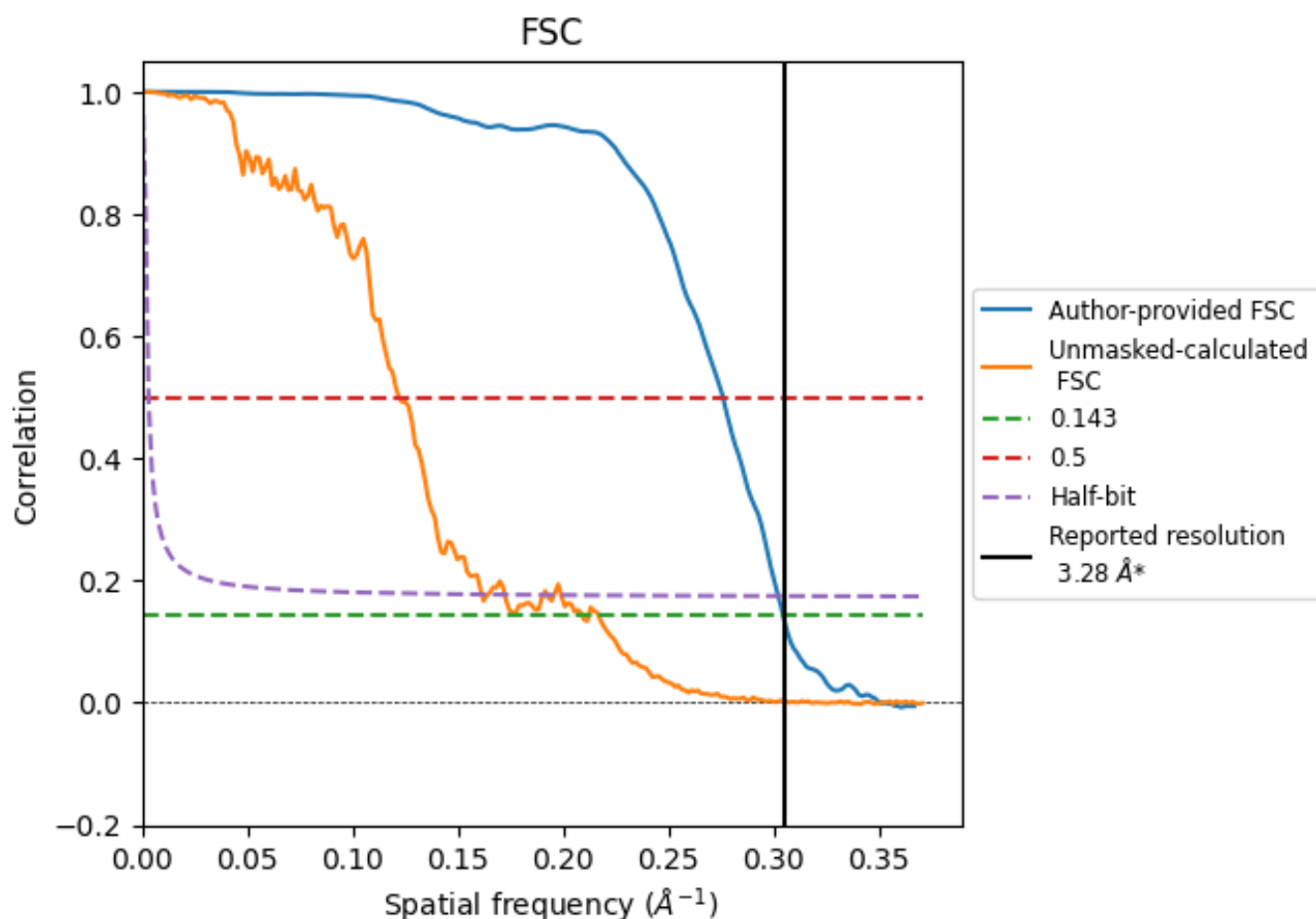


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

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 0.305 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.62	3.31
Unmasked-calculated*	4.78	8.20	6.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.78 differs from the reported value 3.28 by more than 10 %

9 Map-model fit [i](#)

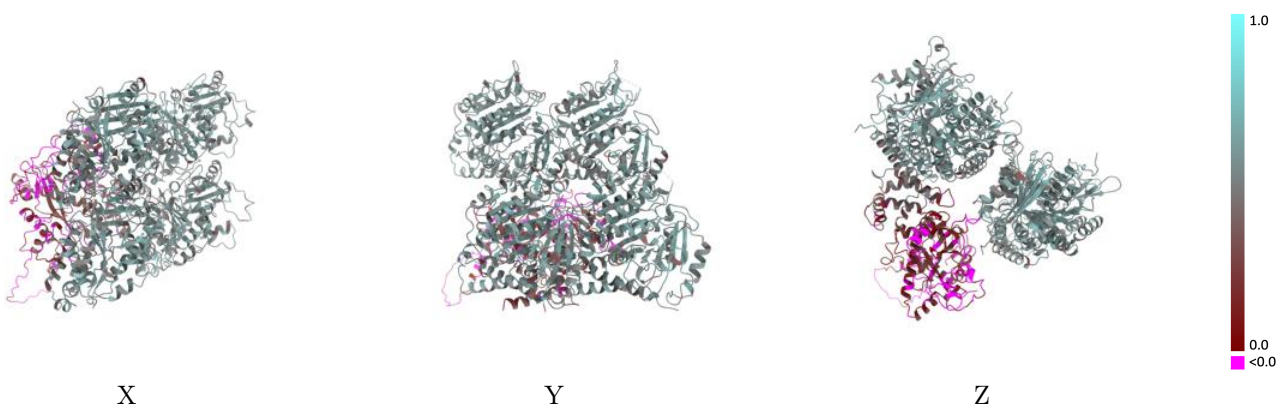
This section contains information regarding the fit between EMDB map EMD-52338 and PDB model 9HQ4. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



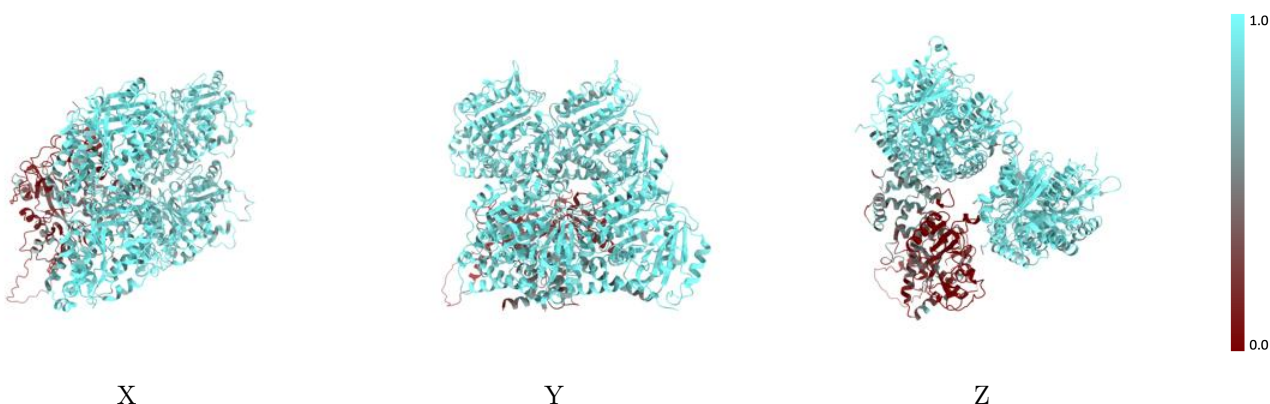
The images above show the 3D surface view of the map at the recommended contour level 0.0956 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



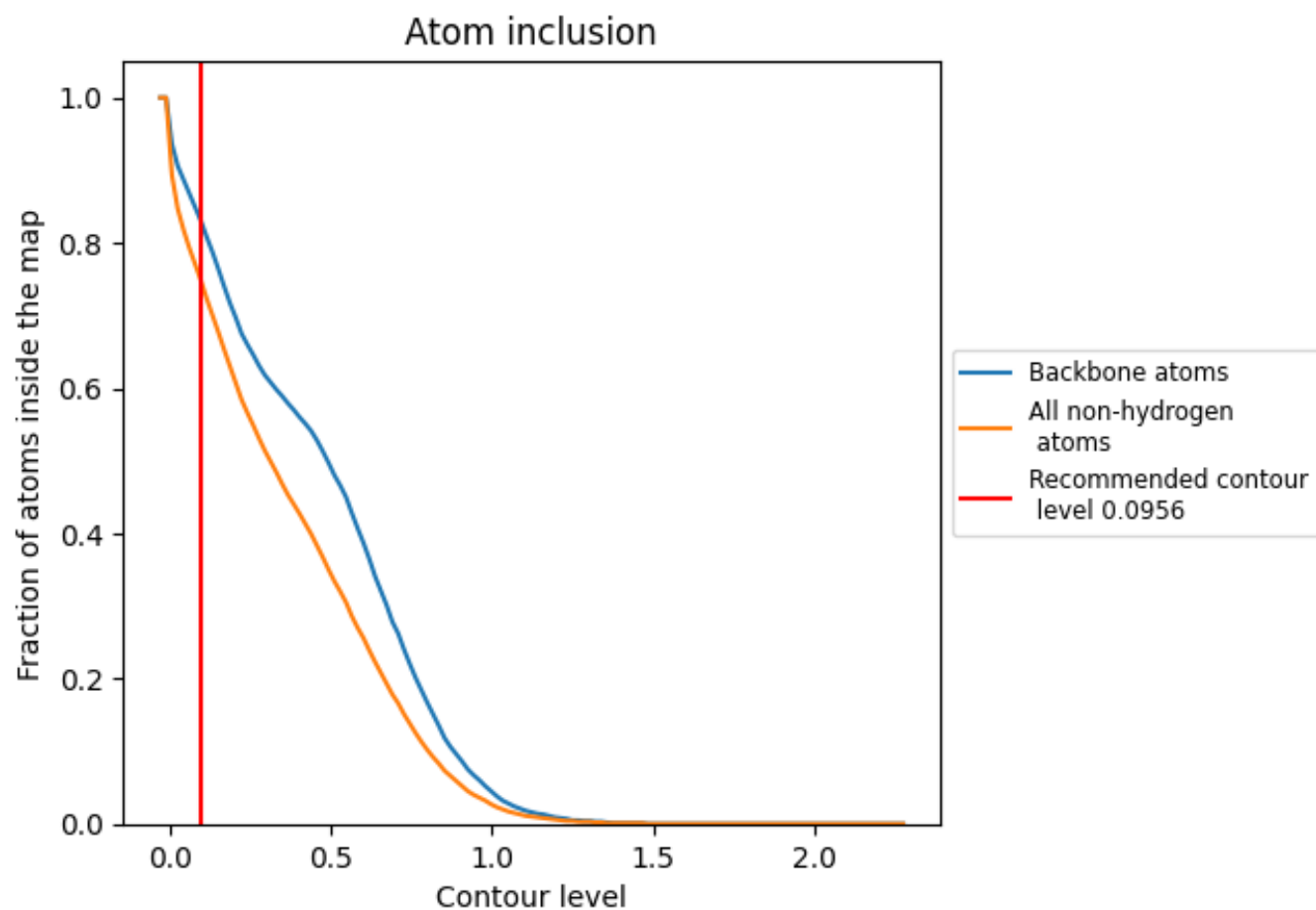
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0956).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.0956) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7500	<div></div> 0.4460
A	<div></div> 0.9050	<div></div> 0.5460
B	<div></div> 0.9000	<div></div> 0.5420
C	<div></div> 0.9120	<div></div> 0.5520
D	<div></div> 0.9060	<div></div> 0.5440
E	<div></div> 0.2330	<div></div> 0.1160

