



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:45 AM UTC

PDB ID : 5ND4 / pdb_00005nd4
EMDB ID : EMD-3622
Title : Microtubule-bound MKLP2 motor domain in the presence of ADP.AIFx
Authors : Atherton, J.; Yu, I.-M.; Cook, A.; Muretta, J.M.; Joseph, A.P.; Major, J.; Sourigues, Y.; Clause, J.; Topf, M.; Rosenfeld, S.S.; Houdusse, A.; Moores, C.A.
Deposited on : 2017-03-07
Resolution : 4.40 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

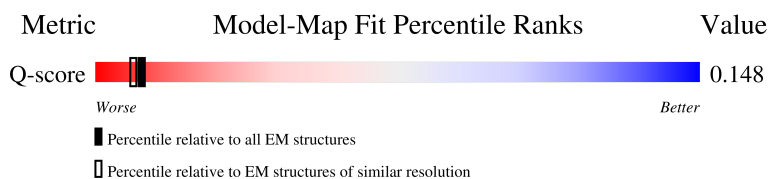
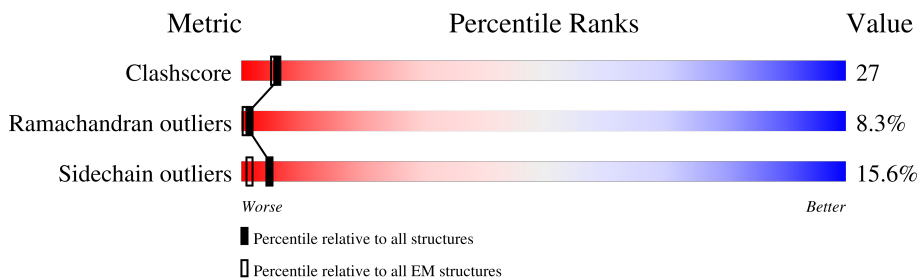
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	C	501	
2	A	412	
3	B	426	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	C	601	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9435 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 Kinesin-like protein KIF20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	337	Total	C	N	O	S	0	0
			2701	1704	487	498	12		

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP F2Z4C1
A	?	-	MET	deletion	UNP F2Z4C1
A	?	-	PRO	deletion	UNP F2Z4C1
A	?	-	SER	deletion	UNP F2Z4C1
A	?	-	ASP	deletion	UNP F2Z4C1
A	?	-	LYS	deletion	UNP F2Z4C1
A	?	-	THR	deletion	UNP F2Z4C1
A	?	-	ILE	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	ASP	deletion	UNP F2Z4C1
A	?	-	ASP	deletion	UNP F2Z4C1
A	?	-	SER	deletion	UNP F2Z4C1
A	?	-	PHE	deletion	UNP F2Z4C1
A	?	-	ASN	deletion	UNP F2Z4C1
A	?	-	THR	deletion	UNP F2Z4C1
A	?	-	PHE	deletion	UNP F2Z4C1
A	?	-	PHE	deletion	UNP F2Z4C1
A	?	-	SER	deletion	UNP F2Z4C1
A	?	-	GLU	deletion	UNP F2Z4C1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	ALA	deletion	UNP F2Z4C1
A	?	-	GLY	deletion	UNP F2Z4C1
A	?	-	LYS	deletion	UNP F2Z4C1
A	136	SER	LEU	conflict	UNP F2Z4C1
A	265	GLY	ILE	conflict	UNP F2Z4C1
A	358	GLU	GLN	conflict	UNP F2Z4C1

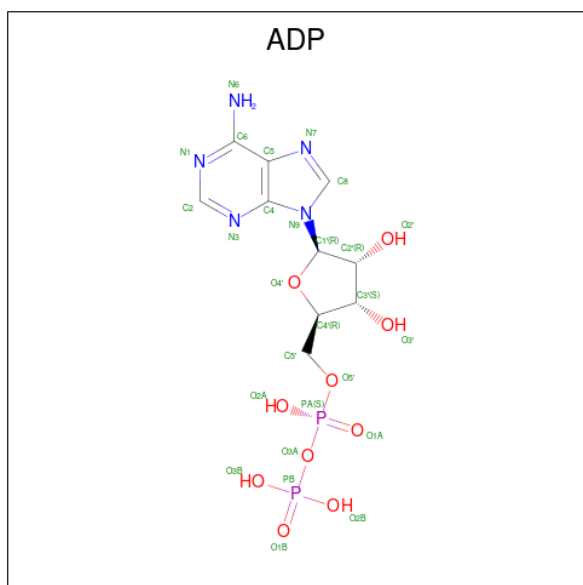
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	ALA	THR	conflict	UNP Q6B856
B	172	VAL	MET	conflict	UNP Q6B856
B	298	ALA	SER	conflict	UNP Q6B856
B	318	VAL	ILE	conflict	UNP Q6B856

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

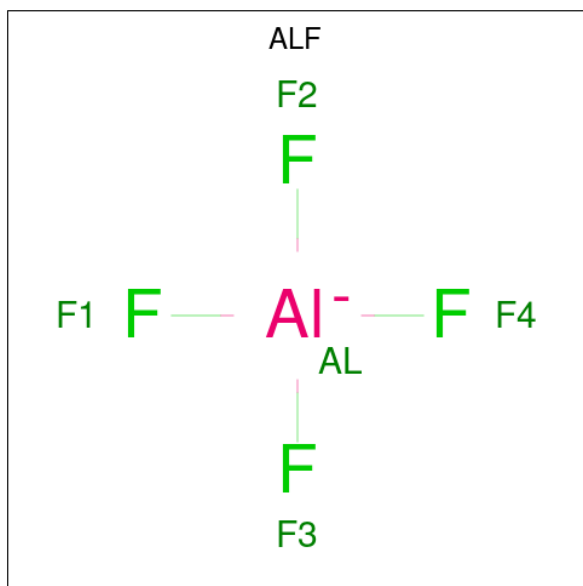


Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

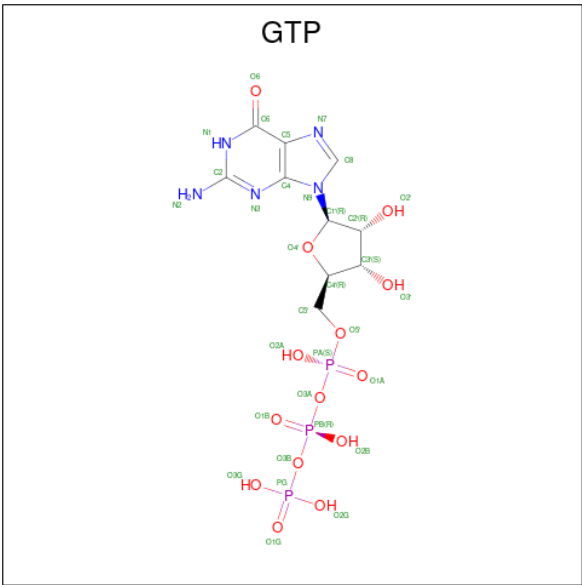
Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	

- Molecule 6 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4^-).



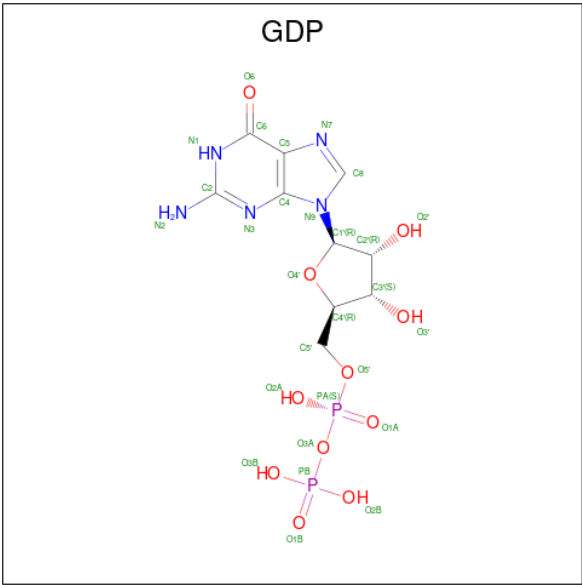
Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	Al	F	0
			5	1	4	

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



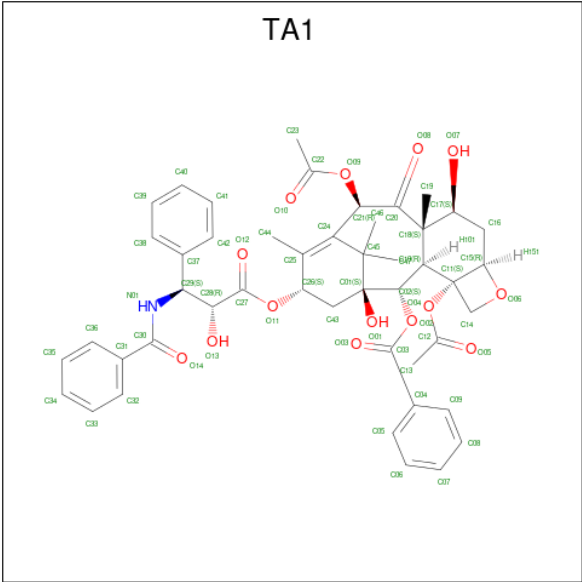
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

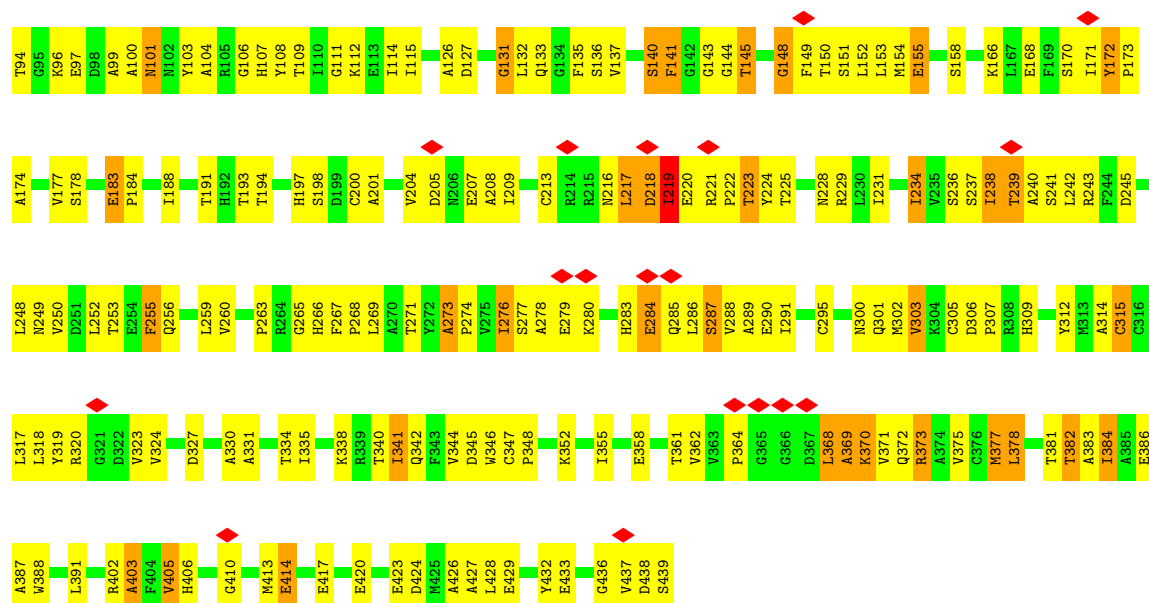


Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

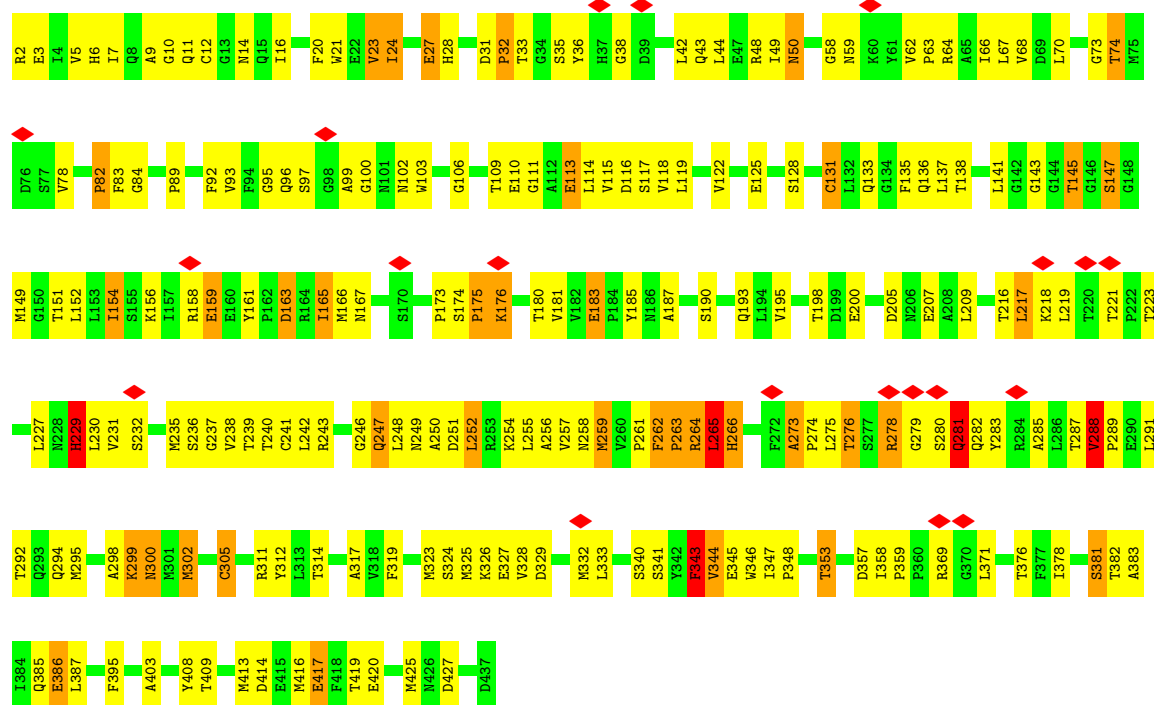
- Molecule 9 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).



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



• Molecule 3: Tubulin beta-2B chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21239	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.142	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0221	Depositor
Map size (Å)	244.79999, 212.67, 246.33	wwPDB
Map dimensions	160, 139, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.53, 1.53, 1.53	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TA1, ALF, ADP, GTP, MG, 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	C	0.64	1/2753 (0.0%)	1.06	17/3709 (0.5%)
2	A	0.49	1/3300 (0.0%)	0.90	5/4482 (0.1%)
3	B	0.45	0/3426	0.87	3/4642 (0.1%)
All	All	0.53	2/9479 (0.0%)	0.94	25/12833 (0.2%)

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
1	C	1	0
2	A	0	1
3	B	1	0
All	All	2	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	ARG	NE-CZ	6.84	1.40	1.33
1	C	412	GLU	C-N	5.15	1.41	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	412	GLU	CA-C-N	10.33	141.73	121.58
1	C	412	GLU	C-N-CA	10.33	141.73	121.58
1	C	165	LYS	CB-CG-CD	-9.74	88.91	111.30
2	A	2	ARG	NE-CZ-NH2	-8.55	111.50	119.20
1	C	413	ARG	CA-C-N	-7.21	109.06	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	413	ARG	C-N-CA	-7.21	109.06	120.60
1	C	108	SER	N-CA-C	-6.42	101.45	110.50
3	B	262	PHE	CA-C-N	6.22	127.62	119.84
3	B	262	PHE	C-N-CA	6.22	127.62	119.84
1	C	430	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	C	165	LYS	CG-CD-CE	-6.09	97.28	111.30
1	C	430	ASN	CA-CB-CG	6.04	118.64	112.60
2	A	428	LEU	N-CA-C	-5.87	106.45	113.97
1	C	88	CYS	CA-C-N	-5.84	115.94	123.19
1	C	88	CYS	C-N-CA	-5.84	115.94	123.19
1	C	99	ALA	O-C-N	5.81	126.56	121.39
1	C	473	GLY	N-CA-C	5.66	119.71	112.13
1	C	378	ARG	CD-NE-CZ	-5.63	116.51	124.40
3	B	229	HIS	CA-CB-CG	5.42	119.22	113.80
2	A	172	TYR	CA-C-N	5.38	126.56	119.84
2	A	172	TYR	C-N-CA	5.38	126.56	119.84
1	C	139	THR	N-CA-C	5.26	116.82	111.14
2	A	429	GLU	N-CA-C	-5.26	106.01	112.90
1	C	430	ASN	CB-CA-C	5.21	119.44	110.79
1	C	413	ARG	CA-C-O	5.14	125.69	119.11

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	472	THR	CA
3	B	280	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2701	0	2700	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3227	0	3143	178	0
3	B	3351	0	3229	144	0
4	C	27	0	12	23	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	C	5	0	0	0	0
7	A	32	0	12	7	0
8	B	28	0	12	8	0
9	B	62	0	51	7	0
All	All	9435	0	9159	495	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 27.

All (495) 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:A:2:ARG:CZ	2:A:133:GLN:HG2	1.66	1.24
2:A:11:GLN:HB3	7:A:500:GTP:O2B	1.44	1.18
1:C:164:GLY:HA2	4:C:601:ADP:O5'	1.52	1.09
3:B:12:CYS:SG	8:B:600:GDP:C4	2.45	1.09
1:C:164:GLY:HA3	4:C:601:ADP:H8	1.14	1.05
1:C:164:GLY:HA3	4:C:601:ADP:C8	1.94	1.03
2:A:2:ARG:NH2	2:A:133:GLN:HG2	1.73	1.02
2:A:11:GLN:CB	7:A:500:GTP:O2B	2.15	0.94
2:A:2:ARG:CD	2:A:133:GLN:HB2	1.98	0.93
2:A:2:ARG:CZ	2:A:133:GLN:CG	2.46	0.93
3:B:11:GLN:HB3	8:B:600:GDP:O2B	1.71	0.91
1:C:443:LEU:HG	1:C:506:LEU:HG	1.52	0.90
1:C:164:GLY:HA2	4:C:601:ADP:PA	2.11	0.90
3:B:70:LEU:H	3:B:145:THR:HG21	1.36	0.90
1:C:68:LEU:HD23	1:C:95:LEU:HD12	1.56	0.87
1:C:140:MET:HE3	1:C:178:ILE:HA	1.57	0.85
1:C:68:LEU:HD23	1:C:95:LEU:CD1	2.06	0.84
1:C:166:THR:N	4:C:601:ADP:O2A	2.12	0.83
3:B:20:PHE:HA	3:B:232:SER:HB3	1.58	0.83
1:C:378:ARG:HA	1:C:378:ARG:NE	1.94	0.82
1:C:378:ARG:HA	1:C:378:ARG:HE	1.45	0.82
2:A:11:GLN:HG2	2:A:15:GLN:HE21	1.45	0.82
1:C:164:GLY:CA	4:C:601:ADP:H8	1.93	0.81
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HG	1:C:404:SER:HB2	1.63	0.80
1:C:412:GLU:O	1:C:415:LYS:HE2	1.81	0.79
1:C:71:ARG:HG3	4:C:601:ADP:C5	2.17	0.79
1:C:314:ASP:HB2	1:C:325:ARG:HG3	1.63	0.79
3:B:27:GLU:OE2	9:B:601:TA1:C41	2.31	0.78
1:C:172:THR:HG23	1:C:175:ASP:H	1.48	0.78
1:C:95:LEU:HD21	1:C:125:ILE:HD13	1.64	0.78
1:C:94:THR:HG23	1:C:120:PHE:O	1.84	0.77
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.67	0.77
1:C:95:LEU:HG	1:C:125:ILE:HG21	1.65	0.77
1:C:101:LYS:HD2	1:C:113:VAL:HB	1.65	0.76
3:B:12:CYS:SG	8:B:600:GDP:C5	2.79	0.76
2:A:2:ARG:HH22	2:A:252:LEU:HG	1.50	0.76
1:C:300:VAL:HG13	1:C:387:ILE:HG22	1.65	0.76
2:A:2:ARG:HH22	2:A:252:LEU:CG	1.97	0.76
1:C:375:GLN:NE2	4:C:601:ADP:H3'	2.01	0.76
1:C:375:GLN:NE2	4:C:601:ADP:O1A	2.20	0.75
2:A:2:ARG:CZ	2:A:243:ARG:CZ	2.64	0.74
2:A:2:ARG:HH12	2:A:252:LEU:HD12	1.51	0.74
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.68	0.74
2:A:2:ARG:NH1	2:A:252:LEU:HD12	2.02	0.74
1:C:71:ARG:HG2	1:C:72:PRO:HD2	1.69	0.74
2:A:2:ARG:NH2	2:A:252:LEU:H	1.86	0.74
2:A:2:ARG:HB3	2:A:243:ARG:NH1	2.03	0.74
1:C:328:LEU:HD21	1:C:340:VAL:HG12	1.71	0.73
2:A:2:ARG:NE	2:A:243:ARG:HH12	1.87	0.73
3:B:11:GLN:CB	8:B:600:GDP:O2B	2.36	0.72
1:C:157:THR:CG2	1:C:165:LYS:HE3	2.18	0.72
2:A:66:VAL:HG12	2:A:91:GLN:HB3	1.72	0.72
1:C:136:PHE:HA	1:C:140:MET:HB2	1.71	0.72
3:B:264:ARG:O	3:B:265:LEU:HB3	1.89	0.71
1:C:183:LEU:HB3	1:C:351:VAL:HG13	1.71	0.71
2:A:2:ARG:HD3	2:A:133:GLN:HB2	1.71	0.71
2:A:112:LYS:O	2:A:115:ILE:HG22	1.91	0.70
1:C:378:ARG:O	1:C:429:ILE:HD11	1.91	0.70
1:C:107:LYS:HG2	2:A:427:ALA:HB2	1.74	0.70
2:A:2:ARG:HH22	2:A:252:LEU:CB	2.05	0.70
1:C:68:LEU:HD12	1:C:481:VAL:HB	1.74	0.69
1:C:86:CYS:HA	1:C:98:GLN:O	1.91	0.69
1:C:64:VAL:HG21	1:C:479:MET:HE3	1.75	0.69
1:C:157:THR:HG23	1:C:165:LYS:HE3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2:ARG:CZ	2:A:243:ARG:NH1	2.56	0.69
1:C:155:ILE:HG22	1:C:478:CYS:HB3	1.75	0.69
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.76	0.68
2:A:11:GLN:HG2	2:A:15:GLN:NE2	2.07	0.68
3:B:12:CYS:HB2	8:B:600:GDP:O1A	1.94	0.68
3:B:151:THR:HG23	3:B:193:GLN:HB2	1.76	0.67
2:A:2:ARG:NE	2:A:243:ARG:NH1	2.42	0.67
1:C:325:ARG:O	1:C:326:GLN:HB2	1.95	0.67
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.30	0.67
1:C:71:ARG:CG	4:C:601:ADP:C5	2.77	0.67
2:A:2:ARG:HH12	2:A:252:LEU:CD1	2.08	0.67
1:C:432:SER:HB3	1:C:463:LEU:HD12	1.76	0.67
2:A:2:ARG:CZ	2:A:133:GLN:CB	2.73	0.67
2:A:27:GLU:HB3	2:A:361:THR:HG21	1.76	0.66
1:C:132:GLN:HG2	1:C:177:GLY:HA2	1.78	0.66
1:C:302:ILE:HG13	1:C:348:VAL:HG22	1.76	0.66
1:C:70:ILE:HG22	1:C:483:VAL:HB	1.77	0.66
3:B:156:LYS:HE2	3:B:156:LYS:HA	1.78	0.66
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.78	0.65
2:A:70:LEU:HB2	2:A:99:ALA:HA	1.76	0.65
2:A:242:LEU:HD11	2:A:250:VAL:HB	1.78	0.65
2:A:222:PRO:HD2	3:B:326:LYS:HB3	1.79	0.65
3:B:258:ASN:O	3:B:314:THR:HG21	1.97	0.65
1:C:165:LYS:N	4:C:601:ADP:O1B	2.21	0.65
1:C:349:ARG:H	1:C:349:ARG:HD2	1.62	0.64
3:B:119:LEU:HA	3:B:122:VAL:HG22	1.78	0.64
1:C:378:ARG:HD2	1:C:425:GLU:HB3	1.80	0.64
9:B:601:TA1:H463	9:B:601:TA1:H261	1.80	0.64
2:A:2:ARG:NH2	2:A:252:LEU:HB2	2.12	0.64
2:A:2:ARG:NE	2:A:133:GLN:HG2	2.12	0.64
1:C:415:LYS:HD3	1:C:430:ASN:ND2	2.13	0.63
2:A:269:LEU:HD13	2:A:303:VAL:HG11	1.78	0.63
3:B:276:THR:HG22	3:B:281:GLN:HG3	1.80	0.63
2:A:201:ALA:O	2:A:268:PRO:HD2	1.98	0.63
1:C:73:PHE:HB3	1:C:78:LEU:HG	1.81	0.63
2:A:11:GLN:NE2	3:B:249:ASN:OD1	2.31	0.63
1:C:169:ILE:HG21	1:C:407:ASP:HB2	1.80	0.63
2:A:269:LEU:HD22	2:A:303:VAL:HG21	1.80	0.63
3:B:259:MET:HG2	3:B:314:THR:HB	1.81	0.63
2:A:106:GLY:O	2:A:111:GLY:HA3	1.97	0.62
1:C:432:SER:O	1:C:435:THR:HG22	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:255:PHE:HZ	2:A:318:LEU:HD11	1.64	0.62
3:B:9:ALA:HA	3:B:68:VAL:HG23	1.81	0.62
3:B:5:VAL:HG12	3:B:64:ARG:HG2	1.80	0.62
3:B:27:GLU:OE2	9:B:601:TA1:H411	1.99	0.62
2:A:256:GLN:O	2:A:260:VAL:HG22	2.00	0.62
3:B:250:ALA:HA	3:B:254:LYS:HE3	1.82	0.62
1:C:137:ASN:O	1:C:141:LYS:HG2	1.98	0.62
2:A:101:ASN:ND2	7:A:500:GTP:O3G	2.27	0.61
1:C:506:LEU:HD13	1:C:506:LEU:H	1.63	0.61
2:A:16:ILE:HD12	2:A:171:ILE:HD11	1.82	0.61
2:A:220:GLU:C	2:A:222:PRO:HD3	2.25	0.61
1:C:316:LEU:HG	1:C:357:LEU:HD11	1.83	0.61
3:B:48:ARG:HG2	3:B:243:ARG:HB3	1.81	0.61
1:C:95:LEU:CD2	1:C:125:ILE:HD13	2.31	0.61
1:C:101:LYS:HG3	1:C:487:ALA:HB1	1.83	0.61
2:A:149:PHE:O	2:A:152:LEU:HG	2.01	0.61
3:B:166:MET:O	3:B:198:THR:HG23	2.01	0.61
1:C:378:ARG:HD2	1:C:425:GLU:CB	2.31	0.61
2:A:154:MET:HE1	2:A:166:LYS:HB3	1.82	0.61
3:B:78:VAL:O	3:B:84:GLY:HA3	2.00	0.61
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.83	0.60
3:B:305:CYS:HB3	3:B:386:GLU:HB2	1.82	0.60
3:B:165:ILE:HD12	3:B:252:LEU:HB3	1.84	0.60
1:C:68:LEU:CD2	1:C:95:LEU:HD12	2.29	0.60
1:C:164:GLY:C	4:C:601:ADP:O2A	2.44	0.60
2:A:151:SER:CB	2:A:193:THR:HG21	2.31	0.60
1:C:157:THR:HG21	1:C:165:LYS:HB3	1.83	0.60
1:C:160:VAL:HG11	1:C:489:THR:HG21	1.82	0.60
3:B:12:CYS:SG	8:B:600:GDP:N9	2.74	0.60
2:A:174:ALA:HB1	2:A:207:GLU:HB2	1.84	0.60
1:C:141:LYS:O	1:C:145:LYS:HG2	2.01	0.60
3:B:312:TYR:HB2	3:B:343:PHE:HA	1.84	0.59
2:A:184:PRO:O	2:A:188:ILE:HG12	2.02	0.59
2:A:205:ASP:HB3	2:A:303:VAL:HA	1.85	0.59
3:B:328:VAL:O	3:B:332:MET:HG2	2.03	0.59
1:C:95:LEU:HB2	1:C:120:PHE:HB2	1.84	0.59
1:C:71:ARG:HG3	4:C:601:ADP:C8	2.37	0.59
2:A:406:HIS:CE1	3:B:263:PRO:HD3	2.38	0.59
1:C:64:VAL:HA	1:C:508:HIS:CE1	2.38	0.58
2:A:71:GLU:HG2	2:A:74:VAL:HG23	1.85	0.58
2:A:205:ASP:CB	2:A:303:VAL:HA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:VAL:HG11	1:C:185:LEU:HB3	1.86	0.58
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.86	0.58
3:B:273:ALA:CB	3:B:274:PRO:HD3	2.32	0.58
3:B:259:MET:HA	3:B:314:THR:HG21	1.85	0.58
1:C:95:LEU:HD21	1:C:125:ILE:CD1	2.34	0.57
3:B:6:HIS:HA	3:B:136:GLN:HB2	1.86	0.57
2:A:2:ARG:NE	2:A:133:GLN:CG	2.65	0.57
1:C:68:LEU:HD23	1:C:95:LEU:HD11	1.84	0.57
3:B:68:VAL:HB	3:B:149:MET:SD	2.45	0.57
1:C:152:ASN:HD22	1:C:474:ARG:HD2	1.70	0.57
1:C:306:GLU:HG2	1:C:315:LEU:HD21	1.87	0.57
2:A:11:GLN:HG3	2:A:74:VAL:HG21	1.87	0.57
3:B:7:ILE:HG12	3:B:66:ILE:HD12	1.87	0.57
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.86	0.57
2:A:2:ARG:CD	2:A:243:ARG:HH12	2.18	0.57
1:C:446:ASN:HA	1:C:449:ASN:OD1	2.05	0.56
1:C:126:PHE:HZ	1:C:138:LEU:HD11	1.69	0.56
1:C:415:LYS:HD3	1:C:430:ASN:HD22	1.68	0.56
2:A:11:GLN:OE1	7:A:500:GTP:O1A	2.23	0.56
1:C:355:TRP:HA	1:C:358:LEU:HD12	1.87	0.56
1:C:422:ARG:HA	1:C:425:GLU:OE1	2.06	0.56
2:A:317:LEU:HD23	2:A:377:MET:HB2	1.87	0.56
2:A:2:ARG:NH2	2:A:243:ARG:NH2	2.54	0.56
2:A:3:GLU:HG3	2:A:4:CYS:H	1.69	0.56
3:B:10:GLY:HA2	3:B:145:THR:HB	1.88	0.56
3:B:70:LEU:N	3:B:145:THR:HG21	2.16	0.56
3:B:103:TRP:HZ2	3:B:151:THR:HG21	1.71	0.56
1:C:71:ARG:HD2	1:C:72:PRO:O	2.06	0.56
2:A:320:ARG:O	2:A:373:ARG:HA	2.06	0.56
2:A:177:VAL:HG22	3:B:333:LEU:HD22	1.89	0.55
3:B:11:GLN:HA	3:B:74:THR:HG21	1.87	0.55
1:C:71:ARG:HG3	4:C:601:ADP:N7	2.21	0.55
2:A:436:GLY:C	2:A:438:ASP:H	2.14	0.55
3:B:299:LYS:O	3:B:300:ASN:HB3	2.07	0.55
2:A:312:TYR:O	2:A:344:VAL:HG23	2.06	0.55
3:B:16:ILE:HD11	3:B:231:VAL:HG11	1.88	0.55
1:C:165:LYS:HA	1:C:482:ASN:ND2	2.21	0.55
1:C:328:LEU:HD11	1:C:340:VAL:HB	1.88	0.55
3:B:229:HIS:NE2	9:B:601:TA1:H361	2.20	0.55
1:C:437:GLY:HA2	1:C:499:PHE:CE1	2.42	0.55
2:A:371:VAL:HG12	2:A:372:GLN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:151:THR:HG23	3:B:193:GLN:CB	2.36	0.55
1:C:143:MET:HB2	1:C:153:TRP:CE2	2.41	0.55
3:B:274:PRO:HG2	3:B:371:LEU:HD21	1.90	0.54
1:C:490:TYR:HA	1:C:493:THR:HG22	1.88	0.54
1:C:71:ARG:HG3	4:C:601:ADP:C4	2.41	0.54
1:C:180:PRO:HB3	1:C:355:TRP:HE1	1.72	0.54
2:A:381:THR:C	2:A:383:ALA:H	2.14	0.54
1:C:157:THR:CG2	1:C:165:LYS:HB3	2.38	0.54
3:B:255:LEU:HD11	3:B:378:ILE:HD12	1.90	0.54
2:A:2:ARG:CZ	2:A:243:ARG:NH2	2.71	0.53
2:A:223:THR:HB	2:A:225:THR:HG22	1.89	0.53
1:C:183:LEU:O	1:C:186:ILE:HG22	2.08	0.53
1:C:450:ARG:HD3	1:C:451:SER:H	1.72	0.53
3:B:110:GLU:O	3:B:113:GLU:HG3	2.07	0.53
3:B:114:LEU:O	3:B:118:VAL:HG23	2.09	0.53
1:C:94:THR:HG22	1:C:95:LEU:N	2.22	0.53
1:C:304:PHE:HE2	1:C:358:LEU:HA	1.74	0.53
3:B:154:ILE:HG22	3:B:166:MET:HE2	1.90	0.53
1:C:334:GLN:HA	3:B:416:MET:SD	2.49	0.53
3:B:2:ARG:HA	3:B:131:CYS:O	2.08	0.53
3:B:174:SER:HB3	3:B:207:GLU:HG2	1.91	0.53
3:B:180:THR:HG22	3:B:181:VAL:H	1.73	0.53
3:B:413:MET:HG2	3:B:414:ASP:H	1.75	0.52
3:B:67:LEU:HD12	3:B:92:PHE:CD1	2.44	0.52
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.91	0.52
2:A:2:ARG:HH21	2:A:252:LEU:H	1.57	0.52
2:A:2:ARG:NH2	2:A:252:LEU:CB	2.70	0.52
2:A:151:SER:HB3	2:A:193:THR:HG21	1.90	0.52
1:C:92:THR:O	1:C:125:ILE:HG13	2.09	0.52
1:C:169:ILE:HG23	1:C:179:LEU:HD13	1.91	0.52
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.91	0.52
2:A:335:ILE:O	2:A:338:LYS:HB2	2.10	0.52
1:C:70:ILE:HD11	1:C:128:PRO:HD3	1.92	0.52
1:C:302:ILE:HG13	1:C:348:VAL:CG2	2.39	0.52
3:B:175:PRO:HD2	3:B:207:GLU:CD	2.35	0.52
2:A:205:ASP:HB3	2:A:208:ALA:HB3	1.92	0.52
1:C:435:THR:HA	1:C:438:ARG:HG2	1.91	0.51
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.92	0.51
2:A:237:SER:HA	2:A:241:SER:OG	2.10	0.51
1:C:153:TRP:HE1	1:C:155:ILE:HG23	1.76	0.51
2:A:331:ALA:O	2:A:335:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:HB2	4:C:601:ADP:O2B	2.10	0.51
1:C:382:ILE:HG12	1:C:406:CYS:SG	2.50	0.51
2:A:218:ASP:O	2:A:219:ILE:HG23	2.11	0.51
3:B:11:GLN:OE1	8:B:600:GDP:O2A	2.28	0.51
3:B:281:GLN:O	3:B:283:TYR:N	2.44	0.51
2:A:2:ARG:CZ	2:A:133:GLN:HB2	2.40	0.51
2:A:205:ASP:O	2:A:209:ILE:HG13	2.10	0.51
2:A:423:GLU:O	2:A:426:ALA:HB3	2.11	0.51
1:C:313:TYR:HE2	1:C:364:ASN:HB3	1.75	0.51
2:A:114:ILE:HB	2:A:149:PHE:CE2	2.46	0.51
2:A:319:TYR:CD2	2:A:375:VAL:HG22	2.45	0.51
3:B:317:ALA:HB1	3:B:319:PHE:HE1	1.75	0.51
3:B:385:GLN:C	3:B:387:LEU:H	2.19	0.51
3:B:137:LEU:HD22	3:B:154:ILE:HG23	1.92	0.50
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.92	0.50
3:B:70:LEU:HD23	3:B:95:GLY:HA3	1.94	0.50
1:C:160:VAL:HG23	1:C:411:SER:OG	2.11	0.50
3:B:49:ILE:HG13	3:B:50:ASN:H	1.76	0.50
3:B:119:LEU:HD21	3:B:156:LYS:HB3	1.93	0.50
3:B:317:ALA:HB1	3:B:319:PHE:CE1	2.47	0.50
2:A:172:TYR:HE1	2:A:391:LEU:HD22	1.76	0.50
2:A:2:ARG:HD2	2:A:133:GLN:HB2	1.90	0.50
2:A:271:THR:HB	2:A:377:MET:O	2.11	0.50
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.92	0.50
3:B:21:TRP:HA	3:B:24:ILE:CG2	2.41	0.50
1:C:390:LEU:HD12	1:C:398:PRO:HG3	1.94	0.49
2:A:2:ARG:NE	2:A:133:GLN:HB2	2.27	0.49
2:A:26:LEU:HD21	2:A:364:PRO:HD3	1.93	0.49
2:A:301:GLN:HE22	2:A:306:ASP:HA	1.78	0.49
1:C:71:ARG:CG	4:C:601:ADP:C4	2.95	0.49
1:C:312:LEU:HD22	1:C:328:LEU:HB2	1.95	0.49
2:A:11:GLN:N	7:A:500:GTP:O2B	2.45	0.49
2:A:12:ALA:HB3	2:A:140:SER:OG	2.13	0.49
1:C:73:PHE:HE1	1:C:485:PRO:HB2	1.78	0.49
1:C:164:GLY:CA	4:C:601:ADP:PA	2.95	0.49
1:C:431:THR:OG1	2:A:410:GLY:HA2	2.13	0.49
2:A:194:THR:HG23	2:A:198:SER:OG	2.12	0.49
1:C:73:PHE:CE1	1:C:485:PRO:HB2	2.48	0.49
1:C:165:LYS:H	4:C:601:ADP:PB	2.33	0.49
2:A:312:TYR:HA	2:A:381:THR:HG22	1.95	0.49
1:C:160:VAL:HG11	1:C:489:THR:CG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:SER:C	1:C:453:GLN:HG3	2.38	0.48
2:A:248:LEU:HB3	2:A:355:ILE:H	1.77	0.48
3:B:44:LEU:HA	3:B:49:ILE:HG23	1.94	0.48
1:C:300:VAL:O	1:C:347:HIS:HA	2.14	0.48
1:C:94:THR:HG21	1:C:119:LYS:HE3	1.96	0.48
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.47	0.48
3:B:231:VAL:HA	3:B:302:MET:HE1	1.94	0.48
3:B:93:VAL:HG12	3:B:114:LEU:HD11	1.95	0.48
1:C:418:LYS:HD2	1:C:422:ARG:HB3	1.95	0.48
2:A:238:ILE:O	2:A:242:LEU:HB2	2.13	0.48
1:C:378:ARG:HH11	1:C:425:GLU:HB2	1.79	0.48
2:A:362:VAL:HG11	2:A:368:LEU:O	2.13	0.48
1:C:441:ALA:O	1:C:444:ARG:HG3	2.14	0.48
3:B:2:ARG:HD3	3:B:133:GLN:NE2	2.28	0.48
2:A:225:THR:O	2:A:229:ARG:HG3	2.13	0.48
1:C:456:ILE:HG12	1:C:458:PHE:CE2	2.49	0.48
2:A:402:ARG:O	2:A:405:VAL:HB	2.14	0.48
3:B:66:ILE:HD13	3:B:122:VAL:HG12	1.95	0.48
3:B:288:VAL:HA	3:B:291:LEU:HD13	1.96	0.48
1:C:378:ARG:CD	1:C:425:GLU:HB3	2.44	0.47
2:A:414:GLU:OE1	2:A:417:GLU:HG2	2.14	0.47
1:C:95:LEU:HD21	1:C:125:ILE:CG1	2.44	0.47
2:A:16:ILE:HD11	2:A:231:ILE:HG21	1.96	0.47
1:C:169:ILE:HG13	1:C:407:ASP:HB2	1.95	0.47
3:B:288:VAL:N	3:B:289:PRO:HD2	2.30	0.47
1:C:140:MET:CE	1:C:178:ILE:HA	2.37	0.47
3:B:32:PRO:HD3	3:B:83:PHE:CE2	2.50	0.47
1:C:111:ARG:NH2	1:C:116:ALA:HB3	2.29	0.47
1:C:167:TYR:CD1	4:C:601:ADP:O2'	2.56	0.47
3:B:115:VAL:HG21	3:B:152:LEU:CD2	2.45	0.47
3:B:141:LEU:HG	3:B:190:SER:OG	2.15	0.47
3:B:261:PRO:HD2	3:B:266:HIS:ND1	2.30	0.47
2:A:158:SER:HB2	2:A:197:HIS:HD2	1.79	0.47
3:B:89:PRO:HA	3:B:92:PHE:HD2	1.79	0.47
3:B:264:ARG:HD2	3:B:264:ARG:HA	1.51	0.47
1:C:68:LEU:O	1:C:125:ILE:HA	2.15	0.47
1:C:355:TRP:O	1:C:359:LYS:HG2	2.15	0.47
2:A:14:VAL:HG11	2:A:75:ILE:HD13	1.97	0.47
2:A:286:LEU:O	2:A:291:ILE:HG13	2.15	0.47
3:B:31:ASP:CG	3:B:32:PRO:HD2	2.40	0.47
1:C:136:PHE:HE1	1:C:185:LEU:HD23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ILE:HG13	1:C:391:GLN:HA	1.97	0.47
2:A:382:THR:HA	2:A:432:TYR:HD2	1.81	0.46
3:B:195:VAL:HA	3:B:265:LEU:HD23	1.97	0.46
2:A:86:LEU:O	2:A:86:LEU:HG	2.15	0.46
3:B:82:PRO:HB2	3:B:83:PHE:H	1.55	0.46
3:B:217:LEU:C	3:B:219:LEU:H	2.22	0.46
1:C:147:VAL:HG21	1:C:403:LEU:HD13	1.97	0.46
2:A:5:ILE:HG22	2:A:6:SER:H	1.80	0.46
2:A:137:VAL:HG21	2:A:154:MET:SD	2.56	0.46
3:B:324:SER:C	3:B:326:LYS:H	2.24	0.46
1:C:90:GLU:O	1:C:91:ASN:HB3	2.16	0.46
2:A:107:HIS:HA	2:A:152:LEU:HD23	1.98	0.46
2:A:224:TYR:HE2	3:B:248:LEU:HB2	1.81	0.46
1:C:136:PHE:CE1	1:C:185:LEU:HD23	2.50	0.46
1:C:388:LEU:HG	1:C:400:ILE:HG13	1.96	0.46
2:A:216:ASN:O	2:A:217:LEU:HB2	2.15	0.46
2:A:271:THR:HA	2:A:302:MET:HG3	1.97	0.46
1:C:71:ARG:HG2	4:C:601:ADP:C5	2.50	0.45
1:C:179:LEU:HB2	1:C:180:PRO:HD3	1.97	0.45
1:C:458:PHE:CE1	1:C:468:GLN:HA	2.51	0.45
2:A:2:ARG:HB3	2:A:243:ARG:HH12	1.75	0.45
2:A:2:ARG:HD3	2:A:133:GLN:CB	2.45	0.45
1:C:69:ARG:HH21	1:C:135:PHE:HD2	1.64	0.45
1:C:381:SER:HB2	1:C:407:ASP:HB3	1.99	0.45
2:A:276:ILE:HG23	2:A:369:ALA:CB	2.46	0.45
2:A:362:VAL:HG13	2:A:368:LEU:HB2	1.99	0.45
2:A:144:GLY:H	7:A:500:GTP:PG	2.40	0.45
3:B:312:TYR:HA	3:B:381:SER:HA	1.98	0.45
1:C:97:LEU:O	1:C:117:THR:HA	2.16	0.45
2:A:201:ALA:HB3	2:A:267:PHE:CD2	2.51	0.45
2:A:70:LEU:CB	2:A:99:ALA:HA	2.43	0.45
1:C:88:CYS:HB2	1:C:96:VAL:HG23	1.97	0.45
1:C:117:THR:HG22	1:C:118:HIS:N	2.31	0.45
1:C:130:VAL:HG21	1:C:134:ALA:HB2	1.99	0.45
1:C:449:ASN:CG	1:C:453:GLN:HG2	2.41	0.45
2:A:143:GLY:HA3	7:A:500:GTP:O1B	2.17	0.45
2:A:273:ALA:HB2	2:A:295:CYS:SG	2.57	0.45
2:A:2:ARG:NH1	2:A:133:GLN:CB	2.80	0.45
2:A:324:VAL:HB	2:A:327:ASP:HB2	1.99	0.45
2:A:341:ILE:HG12	2:A:341:ILE:O	2.16	0.45
2:A:381:THR:O	2:A:384:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:195:VAL:HA	3:B:265:LEU:CD2	2.46	0.45
3:B:232:SER:HA	3:B:235:MET:HG2	1.98	0.45
3:B:299:LYS:O	3:B:300:ASN:CB	2.64	0.45
2:A:2:ARG:NE	2:A:133:GLN:OE1	2.49	0.44
3:B:113:GLU:HG3	3:B:113:GLU:H	1.65	0.44
3:B:216:THR:HG22	3:B:275:LEU:O	2.17	0.44
3:B:230:LEU:HD13	9:B:601:TA1:H081	1.99	0.44
2:A:7:ILE:HG22	2:A:66:VAL:CG2	2.48	0.44
2:A:381:THR:C	2:A:383:ALA:N	2.76	0.44
3:B:156:LYS:HA	3:B:156:LYS:CE	2.46	0.44
3:B:256:ALA:C	3:B:258:ASN:H	2.26	0.44
3:B:161:TYR:C	3:B:163:ASP:H	2.26	0.44
3:B:259:MET:O	3:B:261:PRO:HD3	2.17	0.44
1:C:311:LEU:HD21	3:B:159:GLU:HG2	2.00	0.44
2:A:9:VAL:HG21	2:A:149:PHE:HB3	2.00	0.44
2:A:369:ALA:O	2:A:370:LYS:HB3	2.17	0.44
3:B:417:GLU:O	3:B:420:GLU:HB3	2.18	0.44
2:A:88:HIS:C	2:A:90:GLU:H	2.26	0.44
2:A:148:GLY:O	2:A:151:SER:HB2	2.18	0.44
3:B:3:GLU:HB3	3:B:64:ARG:NH2	2.33	0.44
1:C:107:LYS:CG	2:A:427:ALA:HB2	2.46	0.44
3:B:332:MET:HG3	3:B:353:THR:CG2	2.48	0.44
1:C:148:LEU:HD13	1:C:190:LEU:HA	1.99	0.44
1:C:375:GLN:HE22	4:C:601:ADP:H3'	1.78	0.44
2:A:10:GLY:HA2	2:A:145:THR:HB	1.98	0.44
3:B:49:ILE:HG13	3:B:50:ASN:N	2.32	0.44
3:B:175:PRO:HB2	3:B:176:LYS:H	1.60	0.44
1:C:66:VAL:HG12	1:C:479:MET:HB2	1.99	0.44
1:C:412:GLU:OE2	1:C:426:ALA:HB2	2.18	0.44
2:A:155:GLU:HG2	2:A:197:HIS:CE1	2.53	0.44
2:A:205:ASP:HB2	2:A:303:VAL:HA	1.99	0.44
2:A:234:ILE:HG21	2:A:302:MET:HE1	2.00	0.44
2:A:22:GLU:HG3	2:A:83:TYR:HE2	1.83	0.44
3:B:237:GLY:O	3:B:241:CYS:HB3	2.18	0.44
1:C:98:GLN:HA	1:C:116:ALA:O	2.17	0.43
2:A:5:ILE:HD12	2:A:135:PHE:CE2	2.53	0.43
2:A:319:TYR:HD2	2:A:375:VAL:HG22	1.83	0.43
1:C:90:GLU:HA	1:C:90:GLU:OE1	2.18	0.43
1:C:358:LEU:O	1:C:362:ARG:HG2	2.17	0.43
3:B:145:THR:HG22	3:B:149:MET:HE3	2.00	0.43
1:C:72:PRO:HB3	1:C:128:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HG	1:C:405:LEU:HD22	1.99	0.43
1:C:300:VAL:CG1	1:C:387:ILE:HG22	2.42	0.43
1:C:455:LEU:HD13	1:C:456:ILE:H	1.83	0.43
2:A:213:CYS:O	2:A:219:ILE:HG13	2.19	0.43
3:B:242:LEU:HB3	3:B:250:ALA:O	2.18	0.43
1:C:439:CYS:HA	1:C:457:PRO:HG2	2.00	0.43
1:C:470:PHE:CE1	1:C:477:SER:HB3	2.54	0.43
3:B:173:PRO:HG2	3:B:187:ALA:HB2	2.01	0.43
2:A:213:CYS:HB3	2:A:219:ILE:HD11	2.01	0.43
3:B:62:VAL:HA	3:B:63:PRO:HD2	1.85	0.43
1:C:163:SER:HB3	1:C:482:ASN:CB	2.48	0.43
2:A:69:ASP:HA	2:A:145:THR:HG21	2.01	0.43
1:C:170:GLN:HG2	1:C:171:GLY:O	2.19	0.43
1:C:177:GLY:C	1:C:180:PRO:HD2	2.43	0.43
2:A:259:LEU:HD11	2:A:378:LEU:HD12	2.00	0.43
3:B:185:TYR:HD2	3:B:408:TYR:CE1	2.36	0.43
1:C:165:LYS:HA	1:C:482:ASN:HD22	1.81	0.43
1:C:467:PHE:O	1:C:470:PHE:HB3	2.19	0.43
2:A:204:VAL:HG21	2:A:231:ILE:CD1	2.49	0.43
9:B:601:TA1:H463	9:B:601:TA1:C26	2.46	0.43
1:C:304:PHE:CE2	1:C:358:LEU:HD23	2.55	0.42
3:B:42:LEU:C	3:B:44:LEU:H	2.27	0.42
2:A:19:ALA:CB	2:A:228:ASN:HB3	2.49	0.42
1:C:157:THR:HG22	1:C:407:ASP:HA	2.01	0.42
2:A:2:ARG:CG	2:A:243:ARG:HH12	2.32	0.42
2:A:68:VAL:HG22	2:A:93:ILE:HB	2.02	0.42
3:B:383:ALA:C	3:B:385:GLN:H	2.27	0.42
1:C:450:ARG:HD3	1:C:451:SER:N	2.34	0.42
2:A:21:TRP:HE1	2:A:63:PRO:HB3	1.84	0.42
2:A:402:ARG:O	2:A:403:ALA:C	2.63	0.42
3:B:64:ARG:HG3	3:B:125:GLU:OE1	2.20	0.42
1:C:163:SER:HB3	1:C:482:ASN:HB3	2.00	0.42
1:C:444:ARG:O	1:C:447:GLN:HB3	2.20	0.42
2:A:5:ILE:HG22	2:A:6:SER:N	2.33	0.42
2:A:200:CYS:SG	2:A:268:PRO:HG3	2.60	0.42
3:B:44:LEU:O	3:B:49:ILE:HG12	2.20	0.42
3:B:100:GLY:C	3:B:102:ASN:H	2.28	0.42
3:B:246:GLY:HA2	3:B:357:ASP:HB2	2.01	0.42
3:B:345:GLU:C	3:B:347:ILE:H	2.27	0.42
1:C:304:PHE:HB3	1:C:315:LEU:HB2	2.02	0.42
1:C:456:ILE:HA	1:C:457:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:23:VAL:HG21	3:B:232:SER:HB2	2.01	0.42
3:B:257:VAL:O	3:B:257:VAL:HG12	2.19	0.42
1:C:399:LYS:HE3	1:C:399:LYS:HB2	1.87	0.42
1:C:474:ARG:H	1:C:474:ARG:HG3	1.57	0.42
2:A:21:TRP:O	2:A:24:TYR:HB2	2.20	0.42
2:A:253:THR:O	2:A:256:GLN:HG2	2.19	0.42
3:B:198:THR:HG22	3:B:200:GLU:H	1.84	0.42
1:C:61:SER:O	1:C:62:GLU:HG2	2.20	0.42
1:C:349:ARG:HD3	1:C:353:GLU:OE2	2.20	0.42
2:A:79:ARG:O	2:A:84:ARG:HG3	2.19	0.42
3:B:103:TRP:HD1	3:B:147:SER:HB2	1.85	0.42
3:B:278:ARG:HG3	9:B:601:TA1:O08	2.19	0.42
2:A:70:LEU:HD21	2:A:114:ILE:HG13	2.02	0.41
2:A:100:ALA:O	2:A:144:GLY:HA3	2.19	0.41
2:A:221:ARG:N	2:A:222:PRO:HD3	2.35	0.41
2:A:345:ASP:C	2:A:347:CYS:H	2.28	0.41
2:A:177:VAL:CG1	3:B:329:ASP:HB3	2.51	0.41
3:B:261:PRO:HD2	3:B:266:HIS:CE1	2.55	0.41
1:C:68:LEU:HB3	1:C:125:ILE:HG22	2.02	0.41
2:A:420:GLU:O	2:A:424:ASP:HB2	2.21	0.41
1:C:94:THR:CG2	1:C:95:LEU:N	2.82	0.41
1:C:333:ASP:C	3:B:416:MET:HG2	2.46	0.41
3:B:174:SER:HA	3:B:175:PRO:HD3	1.93	0.41
2:A:5:ILE:HD11	2:A:126:ALA:HA	2.03	0.41
2:A:25:CYS:HB3	2:A:30:ILE:O	2.20	0.41
2:A:320:ARG:HB2	2:A:358:GLU:O	2.20	0.41
1:C:307:ILE:CG2	1:C:380:HIS:HB2	2.51	0.41
2:A:2:ARG:CD	2:A:243:ARG:NH1	2.82	0.41
2:A:273:ALA:HB3	2:A:274:PRO:HD3	2.03	0.41
2:A:315:CYS:HB3	2:A:377:MET:SD	2.60	0.41
1:C:308:TYR:HB2	1:C:379:SER:HB3	2.02	0.41
3:B:288:VAL:HG11	3:B:327:GLU:O	2.21	0.41
1:C:169:ILE:HG23	1:C:179:LEU:CD1	2.50	0.41
1:C:402:GLU:O	1:C:402:GLU:HG3	2.21	0.41
2:A:13:GLY:HA2	2:A:16:ILE:HG22	2.02	0.41
2:A:221:ARG:HA	3:B:324:SER:CB	2.51	0.41
2:A:242:LEU:HG	2:A:250:VAL:O	2.20	0.41
1:C:71:ARG:HG2	4:C:601:ADP:C6	2.56	0.41
1:C:126:PHE:CZ	1:C:138:LEU:HD11	2.54	0.41
1:C:165:LYS:CD	1:C:408:LEU:O	2.69	0.41
1:C:165:LYS:CE	1:C:408:LEU:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:PRO:HA	1:C:319:PRO:HD3	1.93	0.41
2:A:2:ARG:HA	2:A:131:GLY:O	2.21	0.41
3:B:143:GLY:HA3	8:B:600:GDP:O3A	2.21	0.41
3:B:247:GLN:H	3:B:247:GLN:HG2	1.55	0.41
3:B:262:PHE:HA	3:B:263:PRO:HD2	1.65	0.41
2:A:283:HIS:O	2:A:284:GLU:C	2.64	0.41
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.97	0.41
2:A:114:ILE:HB	2:A:149:PHE:HE2	1.84	0.40
3:B:111:GLY:O	3:B:115:VAL:HG23	2.21	0.40
3:B:175:PRO:HD2	3:B:207:GLU:OE1	2.20	0.40
2:A:72:PRO:HA	2:A:94:THR:HG21	2.04	0.40
1:C:98:GLN:HE21	1:C:98:GLN:HB2	1.54	0.40
3:B:106:GLY:O	3:B:111:GLY:HA3	2.21	0.40
3:B:347:ILE:HA	3:B:348:PRO:HD2	1.88	0.40
1:C:156:TYR:HA	1:C:406:CYS:O	2.22	0.40
3:B:28:HIS:HA	3:B:43:GLN:HB3	2.02	0.40
2:A:153:LEU:HD12	2:A:153:LEU:HA	1.97	0.40
2:A:344:VAL:HG12	2:A:345:ASP:N	2.36	0.40
3:B:35:SER:HB2	3:B:36:TYR:H	1.66	0.40
3:B:115:VAL:O	3:B:118:VAL:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	C	331/501 (66%)	317 (96%)	11 (3%)	3 (1%)	14	49
2	A	408/412 (99%)	283 (69%)	76 (19%)	49 (12%)	0	4
3	B	424/426 (100%)	297 (70%)	82 (19%)	45 (11%)	0	6
All	All	1163/1339 (87%)	897 (77%)	169 (14%)	97 (8%)	1	9

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	GLN
2	A	97	GLU
2	A	109	THR
2	A	141	PHE
2	A	183	GLU
2	A	217	LEU
2	A	240	ALA
2	A	280	LYS
2	A	284	GLU
2	A	285	GLN
2	A	309	HIS
2	A	370	LYS
2	A	403	ALA
2	A	437	VAL
3	B	82	PRO
3	B	97	SER
3	B	175	PRO
3	B	176	LYS
3	B	239	THR
3	B	240	THR
3	B	252	LEU
3	B	263	PRO
3	B	278	ARG
3	B	280	SER
3	B	281	GLN
3	B	282	GLN
3	B	288	VAL
3	B	294	GLN
3	B	343	PHE
3	B	344	VAL
3	B	369	ARG
3	B	403	ALA
2	A	96	LYS
2	A	108	TYR
2	A	249	ASN
2	A	255	PHE
2	A	265	GLY
2	A	266	HIS
2	A	287	SER
2	A	300	ASN
2	A	314	ALA
2	A	346	TRP

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Mol	Chain	Res	Type
3	B	23	VAL
3	B	32	PRO
3	B	38	GLY
3	B	128	SER
3	B	183	GLU
3	B	218	LYS
3	B	238	VAL
3	B	265	LEU
3	B	266	HIS
3	B	279	GLY
3	B	300	ASN
1	C	376	SER
2	A	63	PRO
2	A	104	ALA
2	A	131	GLY
2	A	218	ASP
2	A	219	ILE
2	A	238	ILE
2	A	239	THR
2	A	289	ALA
2	A	330	ALA
2	A	342	GLN
2	A	387	ALA
3	B	24	ILE
3	B	96	GLN
3	B	273	ALA
3	B	295	MET
3	B	311	ARG
3	B	386	GLU
1	C	62	GLU
2	A	279	GLU
2	A	348	PRO
2	A	373	ARG
2	A	386	GLU
3	B	50	ASN
3	B	99	ALA
3	B	298	ALA
2	A	24	TYR
2	A	369	ALA
3	B	285	ALA
3	B	302	MET
3	B	325	MET

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Mol	Chain	Res	Type
3	B	346	TRP
2	A	103	TYR
2	A	148	GLY
2	A	245	ASP
2	A	263	PRO
2	A	273	ALA
2	A	288	VAL
3	B	73	GLY
3	B	395	PHE
3	B	58	GLY
2	A	173	PRO
2	A	303	VAL
2	A	307	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	C	301/447 (67%)	239 (79%)	62 (21%)	1	7
2	A	347/347 (100%)	303 (87%)	44 (13%)	4	17
3	B	367/367 (100%)	315 (86%)	52 (14%)	3	15
All	All	1015/1161 (87%)	857 (84%)	158 (16%)	4	13

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	61	SER
1	C	63	LYS
1	C	73	PHE
1	C	83	ASP
1	C	96	VAL
1	C	108	SER
1	C	110	GLU
1	C	113	VAL
1	C	124	GLN

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Mol	Chain	Res	Type
1	C	129	GLU
1	C	132	GLN
1	C	135	PHE
1	C	138	LEU
1	C	140	MET
1	C	141	LYS
1	C	142	GLU
1	C	146	ASP
1	C	155	ILE
1	C	165	LYS
1	C	168	THR
1	C	183	LEU
1	C	185	LEU
1	C	300	VAL
1	C	301	TRP
1	C	303	SER
1	C	304	PHE
1	C	306	GLU
1	C	311	LEU
1	C	314	ASP
1	C	323	HIS
1	C	327	THR
1	C	328	LEU
1	C	332	GLU
1	C	342	ASP
1	C	347	HIS
1	C	348	VAL
1	C	349	ARG
1	C	350	ASP
1	C	355	TRP
1	C	356	LYS
1	C	357	LEU
1	C	366	SER
1	C	377	SER
1	C	378	ARG
1	C	391	GLN
1	C	400	ILE
1	C	401	SER
1	C	418	LYS
1	C	424	LYS
1	C	434	HIS
1	C	436	LEU

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Mol	Chain	Res	Type
1	C	444	ARG
1	C	450	ARG
1	C	453	GLN
1	C	455	LEU
1	C	462	LYS
1	C	464	THR
1	C	465	ARG
1	C	474	ARG
1	C	489	THR
1	C	493	THR
1	C	506	LEU
2	A	2	ARG
2	A	25	CYS
2	A	28	HIS
2	A	76	ASP
2	A	77	GLU
2	A	82	THR
2	A	101	ASN
2	A	127	ASP
2	A	132	LEU
2	A	136	SER
2	A	140	SER
2	A	141	PHE
2	A	145	THR
2	A	150	THR
2	A	155	GLU
2	A	170	SER
2	A	178	SER
2	A	183	GLU
2	A	191	THR
2	A	219	ILE
2	A	223	THR
2	A	234	ILE
2	A	236	SER
2	A	239	THR
2	A	276	ILE
2	A	277	SER
2	A	287	SER
2	A	305	CYS
2	A	315	CYS
2	A	323	VAL
2	A	334	THR

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Mol	Chain	Res	Type
2	A	340	THR
2	A	341	ILE
2	A	352	LYS
2	A	368	LEU
2	A	377	MET
2	A	378	LEU
2	A	382	THR
2	A	384	ILE
2	A	405	VAL
2	A	413	MET
2	A	414	GLU
2	A	433	GLU
2	A	439	SER
3	B	14	ASN
3	B	27	GLU
3	B	33	THR
3	B	59	ASN
3	B	74	THR
3	B	109	THR
3	B	113	GLU
3	B	116	ASP
3	B	117	SER
3	B	131	CYS
3	B	135	PHE
3	B	138	THR
3	B	145	THR
3	B	147	SER
3	B	154	ILE
3	B	158	ARG
3	B	159	GLU
3	B	163	ASP
3	B	165	ILE
3	B	167	ASN
3	B	205	ASP
3	B	217	LEU
3	B	221	THR
3	B	223	THR
3	B	229	HIS
3	B	236	SER
3	B	247	GLN
3	B	251	ASP
3	B	259	MET

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Mol	Chain	Res	Type
3	B	264	ARG
3	B	265	LEU
3	B	276	THR
3	B	281	GLN
3	B	287	THR
3	B	288	VAL
3	B	292	THR
3	B	299	LYS
3	B	305	CYS
3	B	323	MET
3	B	340	SER
3	B	341	SER
3	B	343	PHE
3	B	344	VAL
3	B	353	THR
3	B	376	THR
3	B	381	SER
3	B	382	THR
3	B	409	THR
3	B	417	GLU
3	B	419	THR
3	B	425	MET
3	B	427	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	84	GLN
1	C	98	GLN
1	C	118	HIS
1	C	124	GLN
1	C	188	ASN
1	C	326	GLN
1	C	344	ASN
1	C	375	GLN
1	C	430	ASN
1	C	434	HIS
1	C	454	ASN
1	C	482	ASN
2	A	8	HIS
2	A	11	GLN
2	A	15	GLN

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Mol	Chain	Res	Type
2	A	107	HIS
2	A	197	HIS
2	A	329	ASN
2	A	393	HIS
3	B	192	HIS
3	B	193	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GDP	B	600	-	29,30,30	2.86	11 (37%)	45,47,47	3.48	16 (35%)
7	GTP	A	500	5	33,34,34	1.93	4 (12%)	50,54,54	0.94	4 (8%)
6	ALF	C	603	-	4,4,4	1.41	0	-		
9	TA1	B	601	-	68,68,68	2.20	27 (39%)	105,105,105	1.49	12 (11%)
4	ADP	C	601	5	28,29,29	0.38	0	43,45,45	0.78	1 (2%)

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
7	GTP	A	500	5	-	3/22/38/38	0/3/3/3
9	TA1	B	601	-	-	9/41/127/127	0/7/7/7
8	GDP	B	600	-	-	4/16/32/32	0/3/3/3
4	ADP	C	601	5	-	1/16/32/32	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	600	GDP	PA-O3A	7.58	1.67	1.59
9	B	601	TA1	C06-C05	6.48	1.50	1.38
7	A	500	GTP	PA-O3A	-6.03	1.53	1.59
8	B	600	GDP	O6-C6	5.96	1.34	1.23
8	B	600	GDP	C8-N9	5.89	1.50	1.37
7	A	500	GTP	PB-O3A	-5.73	1.53	1.59
9	B	601	TA1	C08-C07	-5.65	1.25	1.38
7	A	500	GTP	PB-O3B	5.51	1.65	1.59
9	B	601	TA1	C18-C10	5.34	1.69	1.57
9	B	601	TA1	C05-C04	4.81	1.46	1.39
8	B	600	GDP	C2-N1	4.75	1.49	1.37
9	B	601	TA1	C45-C24	4.31	1.61	1.54
8	B	600	GDP	PB-O2B	-3.92	1.40	1.54
9	B	601	TA1	C36-C31	3.76	1.45	1.39
9	B	601	TA1	O02-C03	3.51	1.41	1.34
9	B	601	TA1	C25-C24	3.38	1.39	1.34
8	B	600	GDP	O4'-C1'	3.38	1.49	1.42
9	B	601	TA1	C46-C45	3.22	1.60	1.53
9	B	601	TA1	C43-C01	3.18	1.60	1.54
9	B	601	TA1	C11-C10	3.13	1.61	1.54
8	B	600	GDP	C8-N7	3.01	1.41	1.32
8	B	600	GDP	C5-N7	-2.84	1.33	1.39
9	B	601	TA1	C43-C26	2.77	1.58	1.52
8	B	600	GDP	C5-C4	2.65	1.46	1.38
9	B	601	TA1	C26-C25	2.62	1.56	1.51
9	B	601	TA1	C01-C45	2.55	1.66	1.56
9	B	601	TA1	C18-C20	2.52	1.62	1.55
9	B	601	TA1	C04-C03	-2.49	1.44	1.50
8	B	600	GDP	PB-O3B	2.44	1.63	1.54
8	B	600	GDP	C2-N3	-2.44	1.27	1.33
9	B	601	TA1	C16-C15	2.31	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	TA1	C41-C42	2.28	1.42	1.38
9	B	601	TA1	C08-C09	2.21	1.42	1.38
9	B	601	TA1	C37-C29	2.19	1.54	1.52
9	B	601	TA1	C33-C32	2.18	1.42	1.38
9	B	601	TA1	O09-C21	2.18	1.49	1.44
9	B	601	TA1	C10-C02	2.11	1.62	1.57
9	B	601	TA1	C07-C06	2.08	1.42	1.38
9	B	601	TA1	C39-C38	2.02	1.42	1.38
9	B	601	TA1	C34-C33	2.02	1.42	1.38
7	A	500	GTP	PB-O2B	-2.00	1.46	1.55
9	B	601	TA1	O02-C02	2.00	1.48	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	600	GDP	N9-C8-N7	-10.78	93.42	113.40
8	B	600	GDP	C8-N7-C5	9.24	120.72	104.26
8	B	600	GDP	C6-C5-N7	8.60	145.94	130.29
8	B	600	GDP	N2-C2-N3	6.28	131.92	119.67
8	B	600	GDP	C6-C5-C4	-6.20	109.51	118.83
8	B	600	GDP	C8-N9-C4	5.88	117.05	106.03
9	B	601	TA1	C06-C05-C04	-5.78	114.68	120.36
9	B	601	TA1	C07-C08-C09	5.70	127.27	120.24
8	B	600	GDP	C5-C6-N1	4.50	124.72	113.25
8	B	600	GDP	N2-C2-N1	-4.23	107.83	116.76
8	B	600	GDP	C2-N3-C4	4.10	119.36	112.30
9	B	601	TA1	C05-C04-C03	-4.02	111.54	120.40
8	B	600	GDP	O6-C6-C5	-3.95	116.10	126.53
8	B	600	GDP	C4-C5-N7	-3.86	104.56	110.67
8	B	600	GDP	C2-N1-C6	-3.80	118.21	125.11
9	B	601	TA1	C09-C04-C03	3.59	128.31	120.40
8	B	600	GDP	C2'-C3'-C4'	3.43	109.23	102.61
9	B	601	TA1	C17-C18-C20	3.23	109.82	102.58
9	B	601	TA1	O04-C11-C14	-2.98	101.82	108.13
9	B	601	TA1	C45-C01-C02	2.93	115.15	111.93
4	C	601	ADP	O3B-PB-O3A	2.70	113.69	104.64
8	B	600	GDP	C1'-N9-C8	-2.67	119.14	126.73
9	B	601	TA1	O01-C01-C43	2.50	113.42	107.04
7	A	500	GTP	O3A-PB-O1B	-2.44	103.36	110.70
9	B	601	TA1	C08-C09-C04	-2.32	118.08	120.36
8	B	600	GDP	O2'-C2'-C3'	2.30	119.20	111.82
9	B	601	TA1	C10-C18-C17	-2.24	102.30	106.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	601	TA1	C14-C11-C15	-2.23	83.08	85.38
9	B	601	TA1	O06-C15-C11	2.19	92.97	90.58
7	A	500	GTP	O2B-PB-O3A	2.19	113.18	107.27
7	A	500	GTP	O5'-C5'-C4'	2.10	116.13	108.99
8	B	600	GDP	C4'-O4'-C1'	2.06	114.01	109.47
7	A	500	GTP	O3G-PG-O3B	2.02	111.42	104.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	600	GDP	PA-O3A-PB-O2B
8	B	600	GDP	C5'-O5'-PA-O3A
8	B	600	GDP	C5'-O5'-PA-O1A
9	B	601	TA1	O02-C03-C04-C05
9	B	601	TA1	O02-C03-C04-C09
9	B	601	TA1	O03-C03-C04-C09
9	B	601	TA1	O03-C03-C04-C05
9	B	601	TA1	N01-C30-C31-C36
9	B	601	TA1	O14-C30-C31-C36
9	B	601	TA1	N01-C30-C31-C32
9	B	601	TA1	O14-C30-C31-C32
7	A	500	GTP	C3'-C4'-C5'-O5'
7	A	500	GTP	O4'-C4'-C5'-O5'
8	B	600	GDP	PA-O3A-PB-O3B
7	A	500	GTP	PG-O3B-PB-O1B
9	B	601	TA1	C15-C11-O04-C12
4	C	601	ADP	PB-O3A-PA-O2A

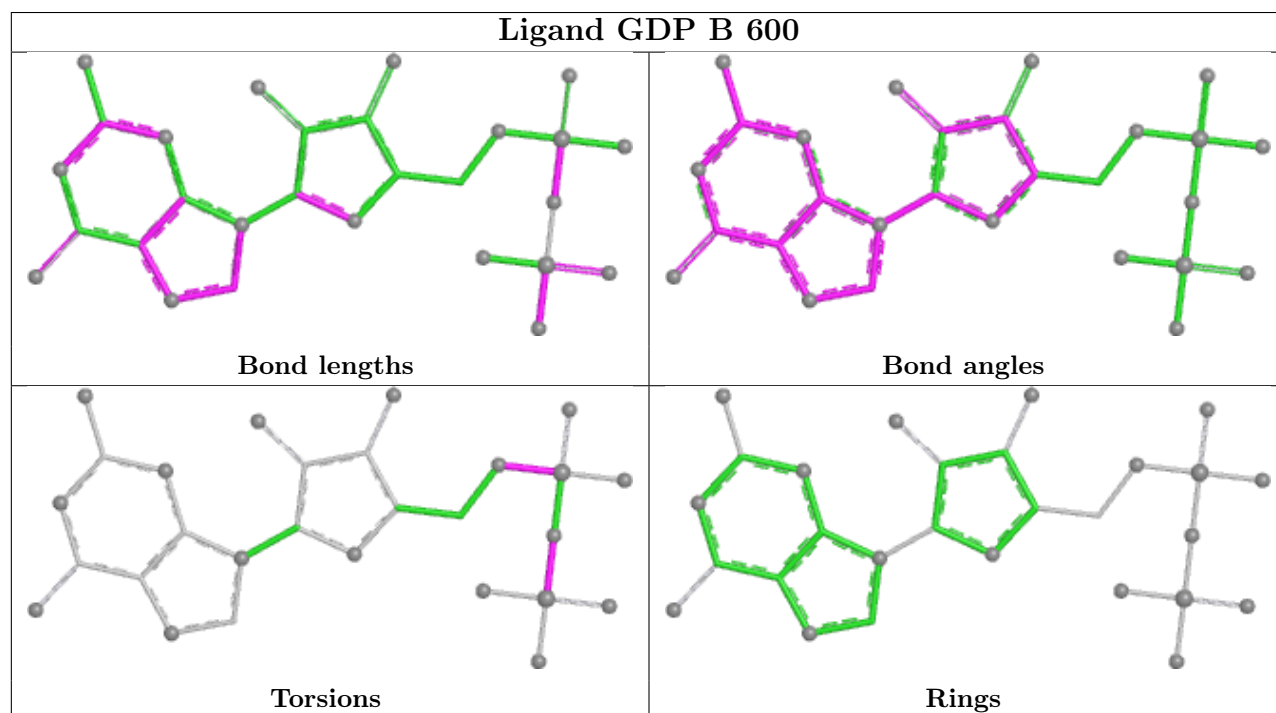
There are no ring outliers.

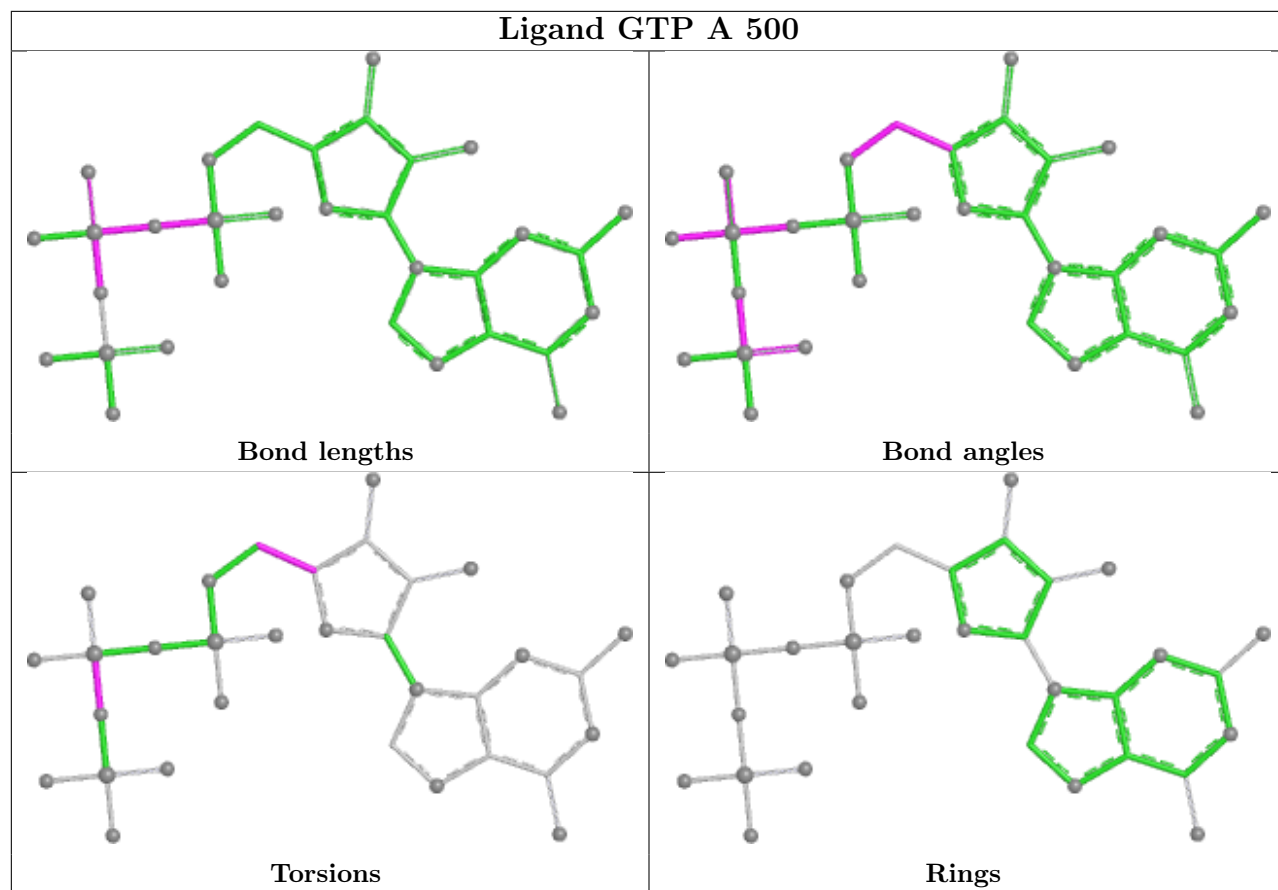
4 monomers are involved in 45 short contacts:

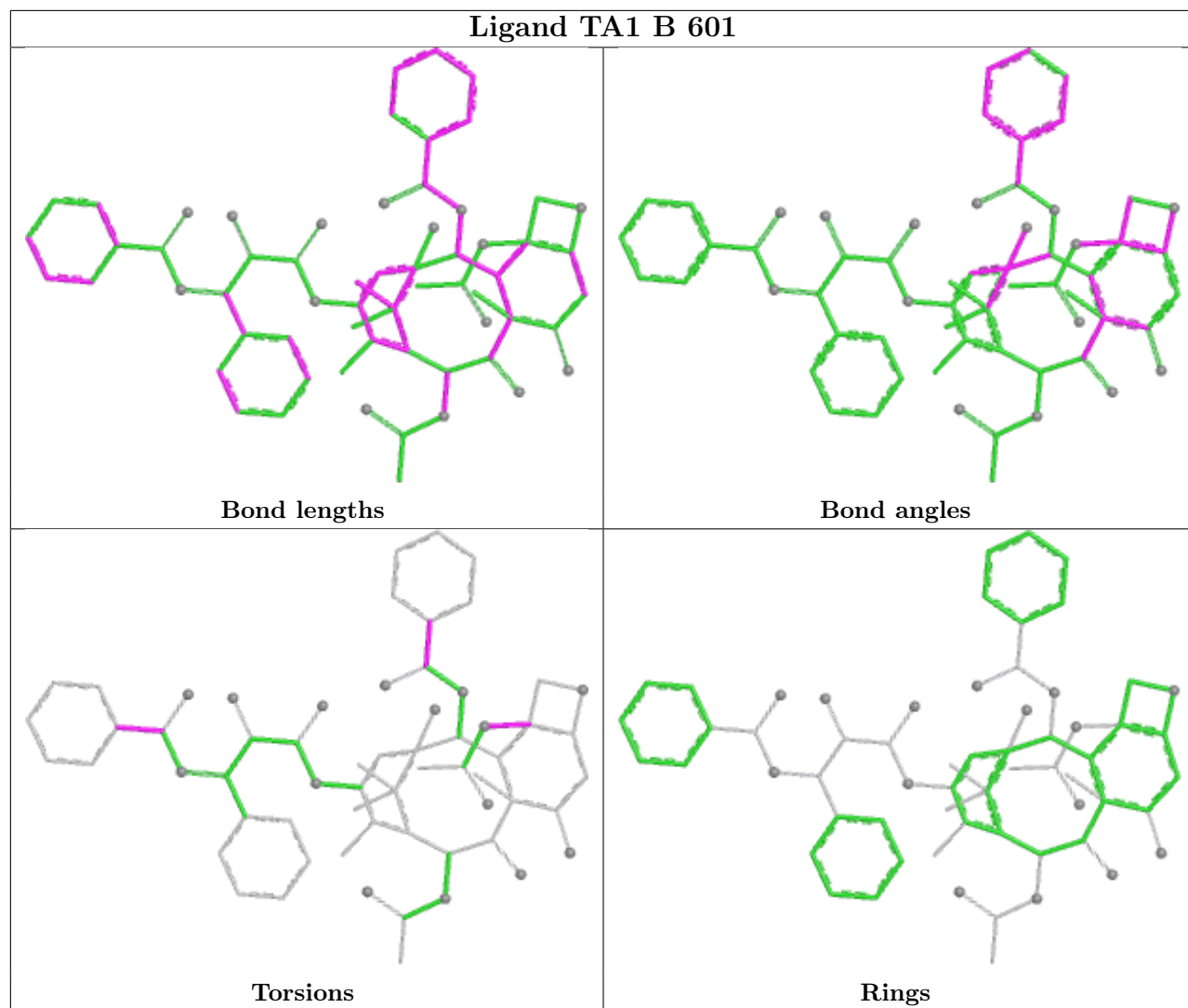
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	600	GDP	8	0
7	A	500	GTP	7	0
9	B	601	TA1	7	0
4	C	601	ADP	23	0

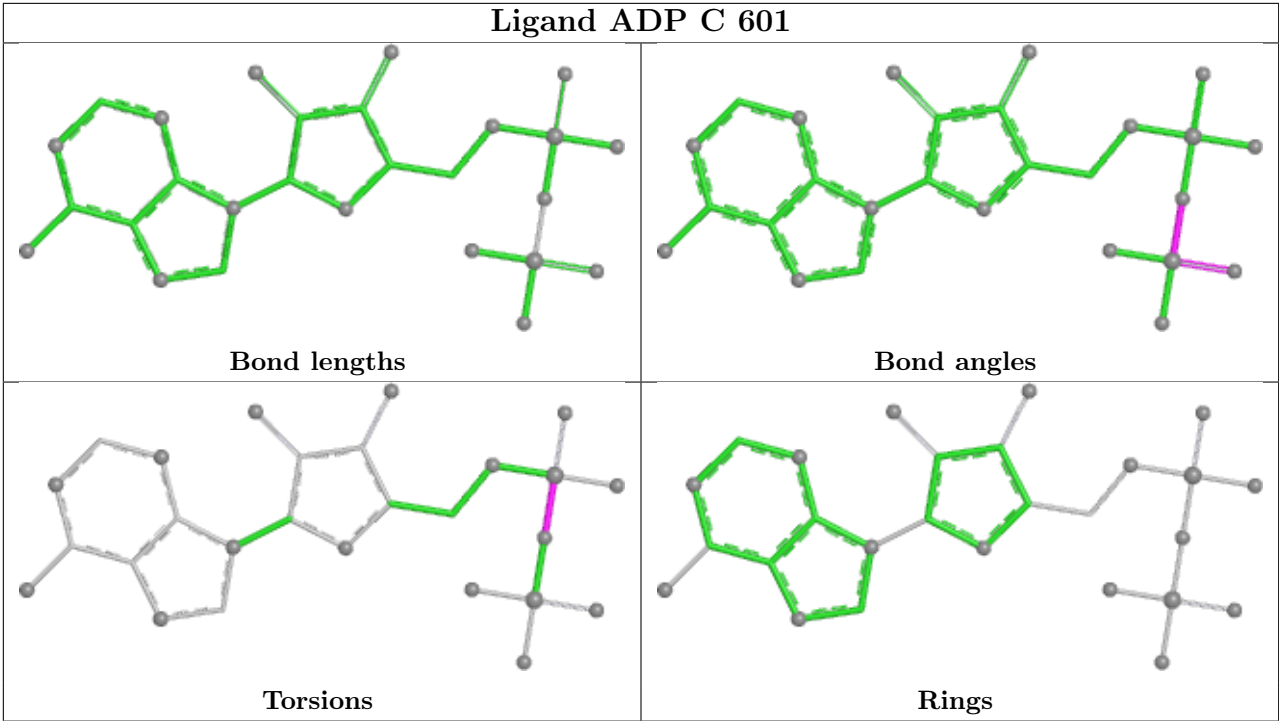
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	34:GLY	C	61:HIS	N	3.53

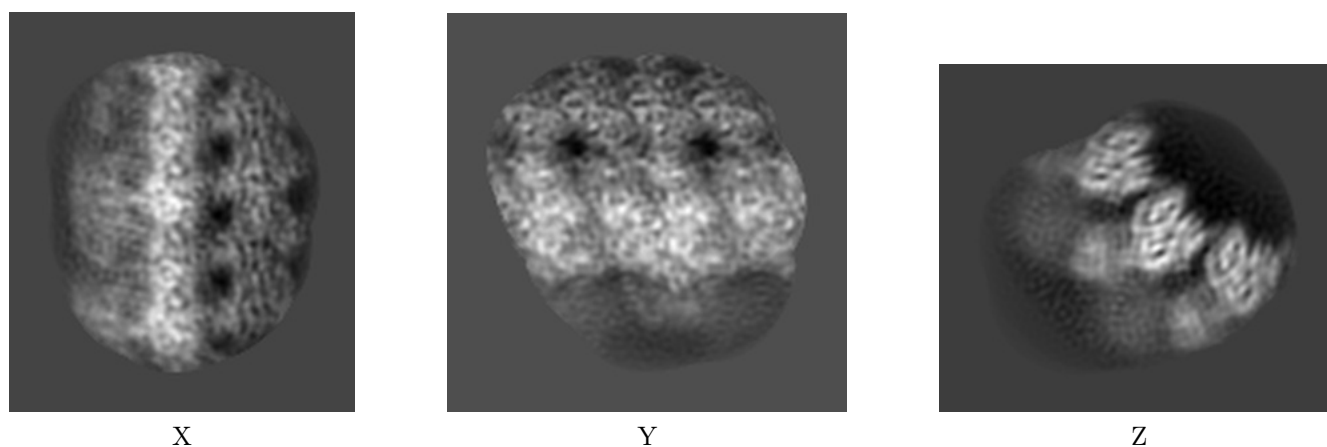
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3622. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

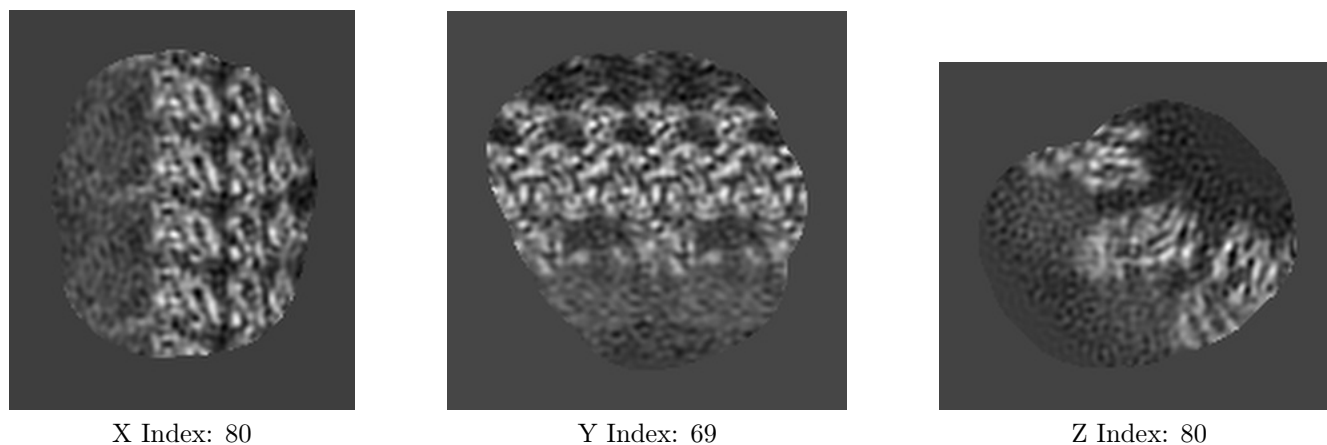
6.1.1 Primary map



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

6.2 Central slices [i](#)

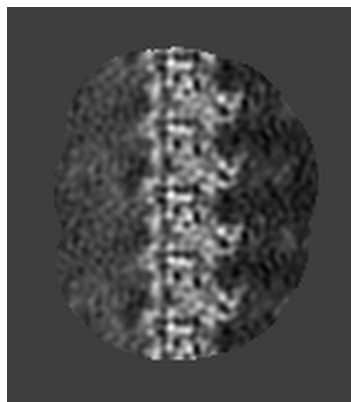
6.2.1 Primary map



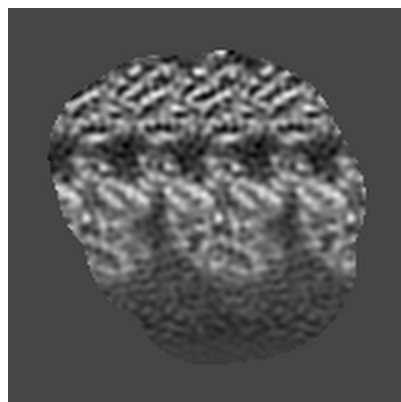
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

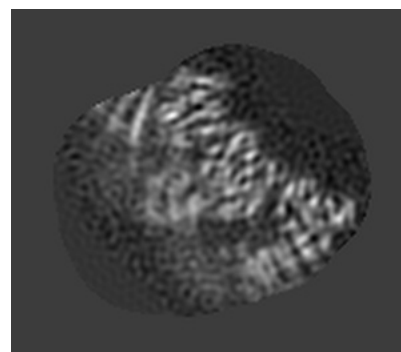
6.3.1 Primary map



X Index: 87



Y Index: 59

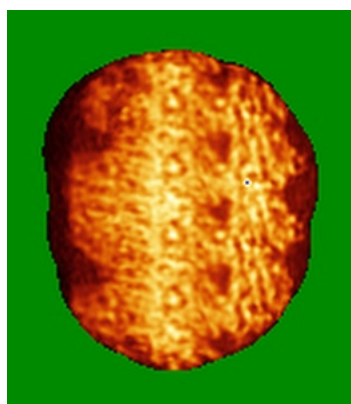


Z Index: 91

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

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

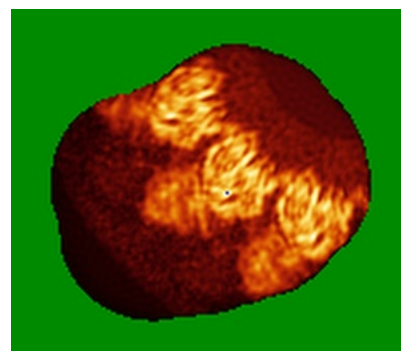
6.4.1 Primary map



X



Y

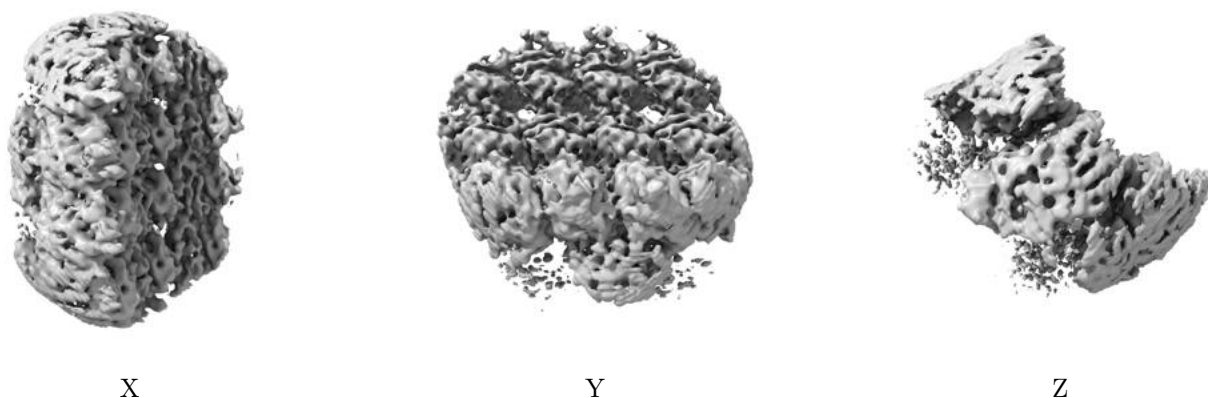


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0221. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

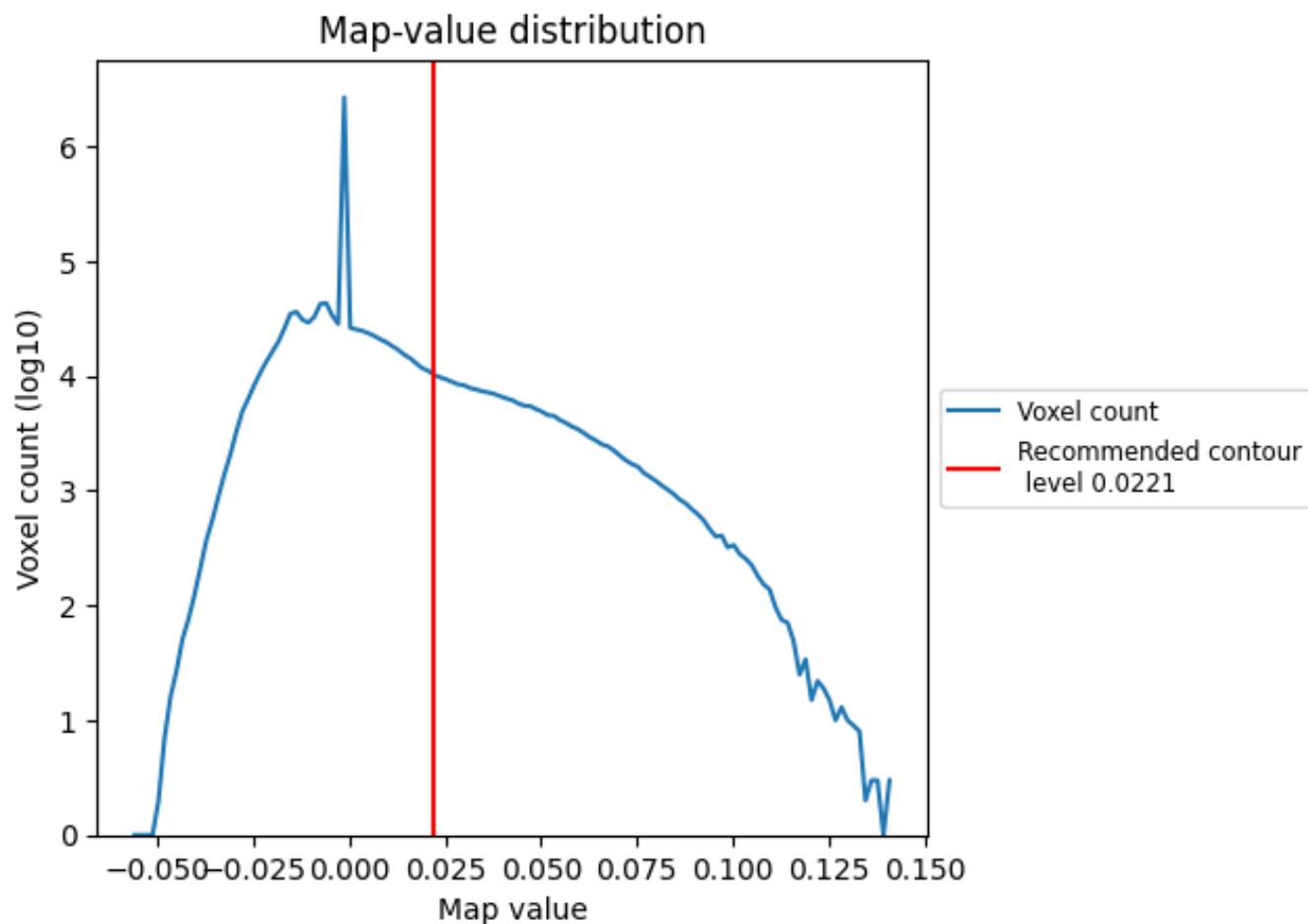
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

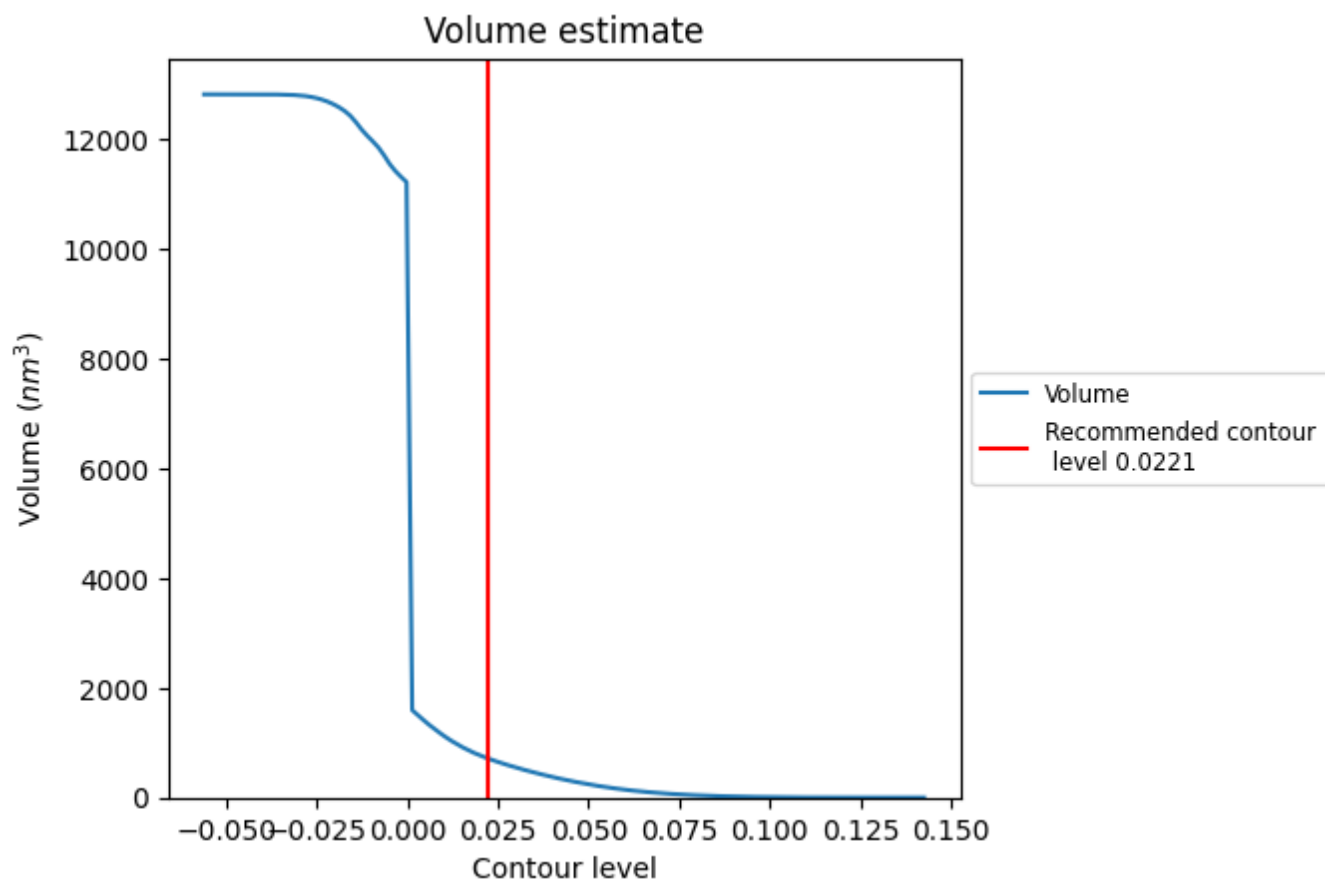
This section contains the results of statistical analysis of the map.

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 718 nm³; this corresponds to an approximate mass of 648 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

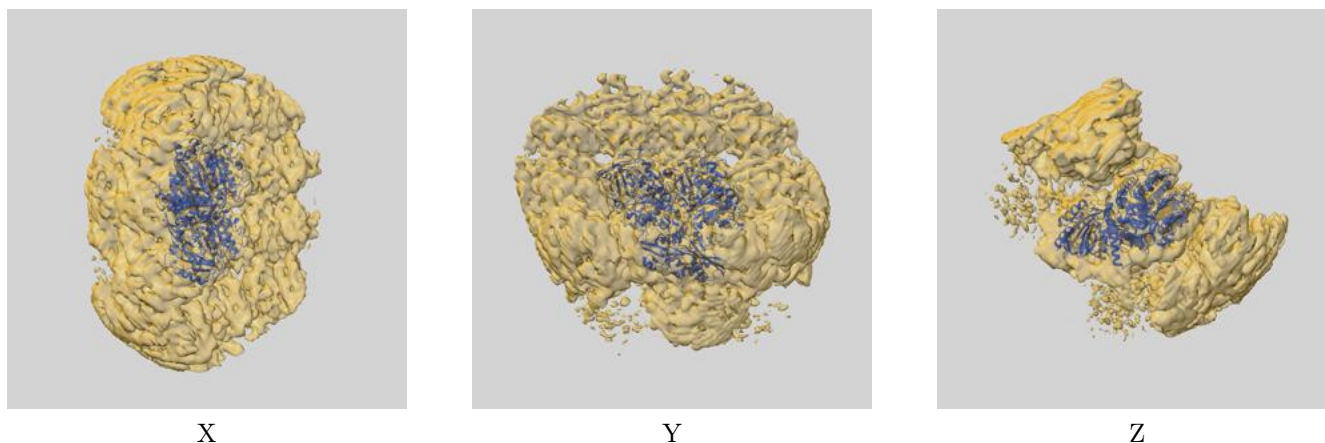
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

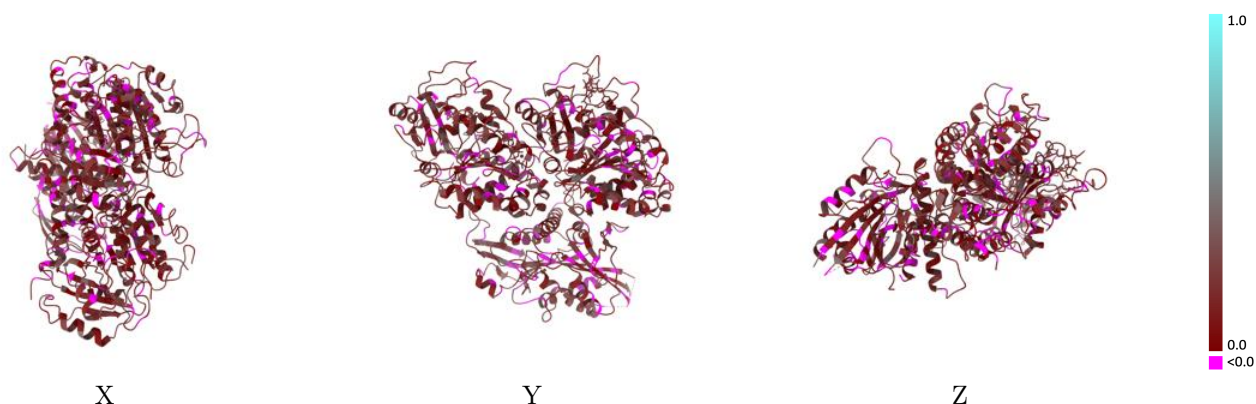
This section contains information regarding the fit between EMDB map EMD-3622 and PDB model 5ND4. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



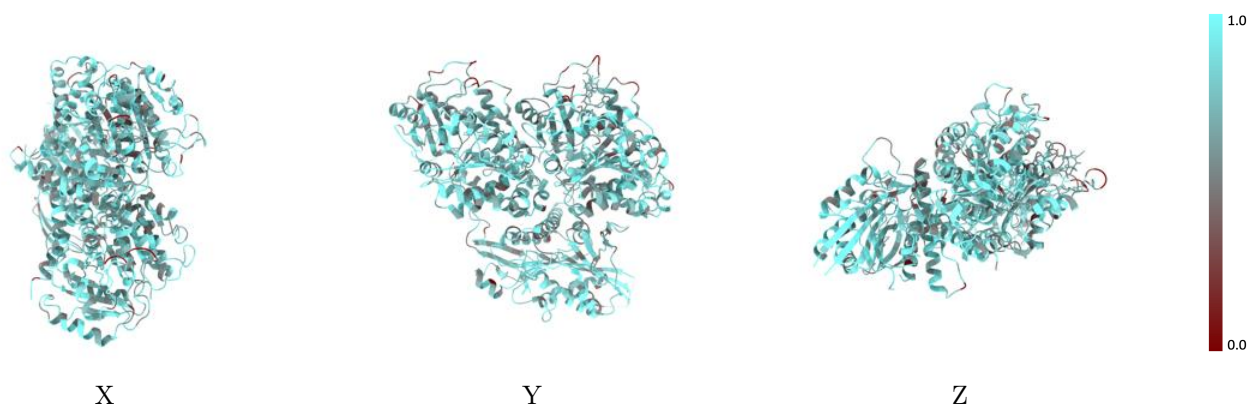
The images above show the 3D surface view of the map at the recommended contour level 0.0221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



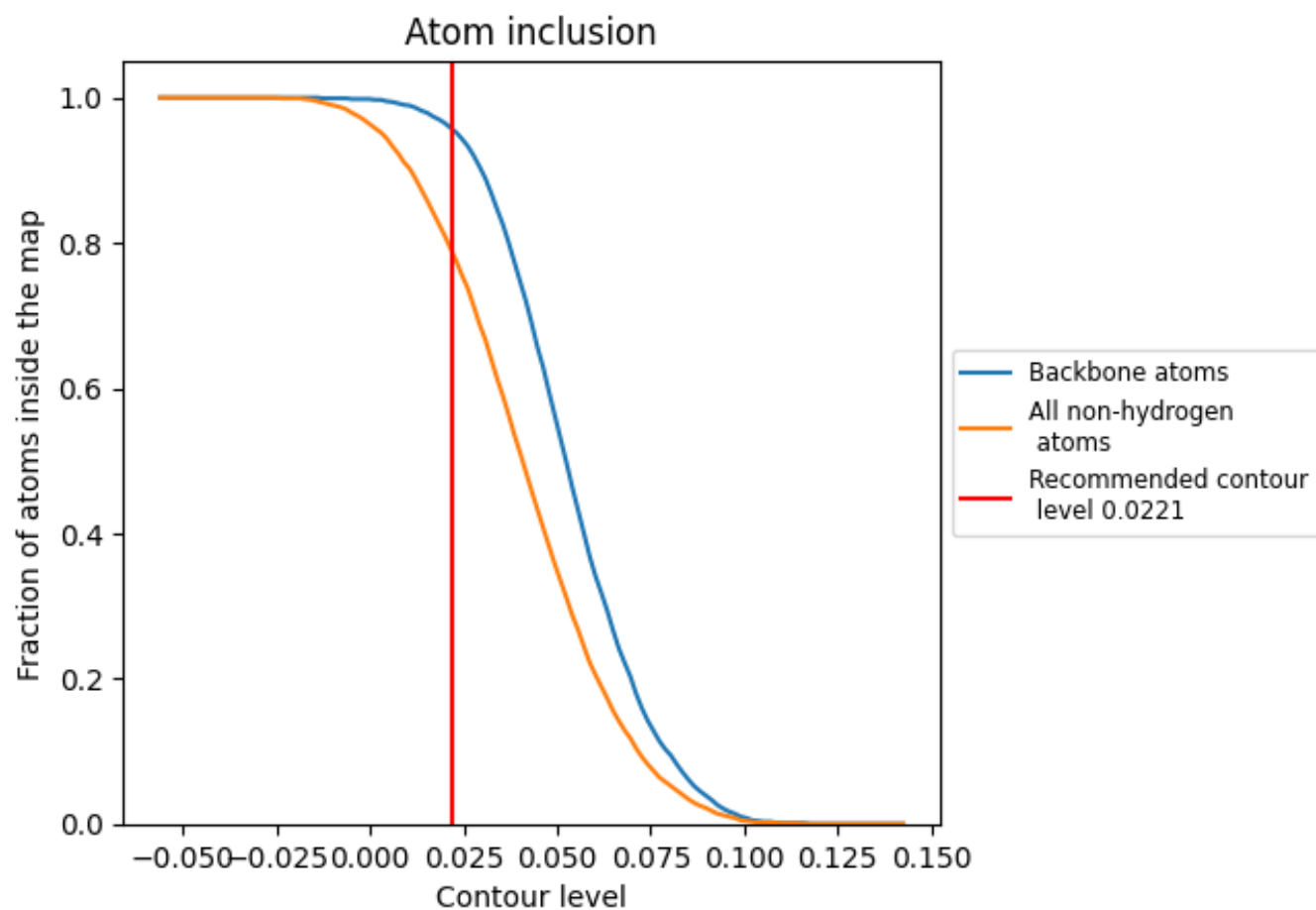
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0221).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 79% 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 (0.0221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.1480
A	0.7880	0.1600
B	0.7690	0.1490
C	0.8050	0.1310

