



Full wwPDB EM Validation Report ⓘ

Jul 27, 2026 – 08:26 PM JST

PDB ID : 9WCW / pdb_00009wcw
EMDB ID : EMD-65877
Title : AMP-PNP bound E.coli CnoX-GroEL complex, state I
Authors : Kim, J.; Roh, S.H.
Deposited on : 2025-08-18
Resolution : 2.73 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

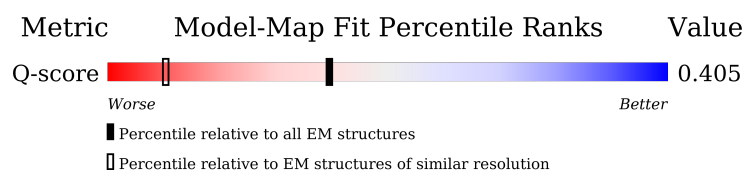
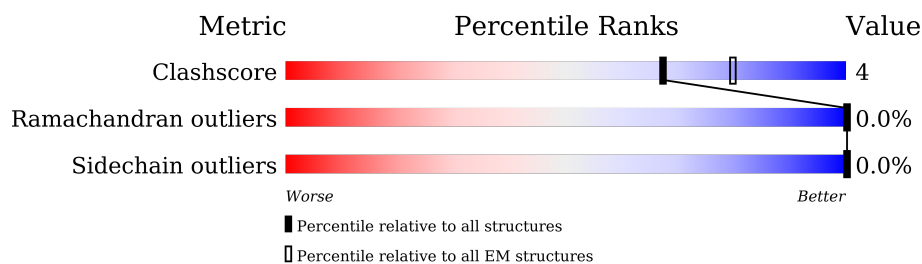
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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.



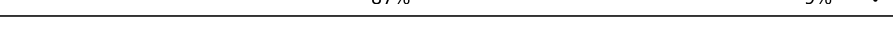
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

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	284	
1	B	284	
1	C	284	
1	D	284	

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Mol	Chain	Length	Quality of chain
1	E	284	 30% 69%
1	F	284	 30% 69%
1	M	284	 30% 69%
1	O	284	 30% 69%
1	Q	284	 30% 69%
1	S	284	 30% 69%
1	U	284	 30% 69%
1	W	284	 30% 69%
1	Y	284	 30% 69%
1	a	284	 30% 69%
2	G	548	 84% 11%
2	I	548	 85% 10%
2	J	548	 86% 10%
2	K	548	 86% 10%
2	L	548	 85% 11%
2	N	548	 83% 12%
2	P	548	 87% 8%
2	R	548	 86% 9%
2	T	548	 89% 7%
2	V	548	 88% 8%
2	X	548	 87% 8%
2	Z	548	 88% 8%
2	b	548	 87% 9%
2	c	548	 87% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 64078 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 Chaperedoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	88	Total	C	N	O	0	0
			689	430	123	136		
1	B	88	Total	C	N	O	0	0
			689	430	123	136		
1	C	88	Total	C	N	O	0	0
			689	430	123	136		
1	D	88	Total	C	N	O	0	0
			689	430	123	136		
1	E	88	Total	C	N	O	0	0
			689	430	123	136		
1	F	88	Total	C	N	O	0	0
			689	430	123	136		
1	M	88	Total	C	N	O	0	0
			689	430	123	136		
1	O	88	Total	C	N	O	0	0
			689	430	123	136		
1	Q	88	Total	C	N	O	0	0
			689	430	123	136		
1	S	88	Total	C	N	O	0	0
			689	430	123	136		
1	U	88	Total	C	N	O	0	0
			689	430	123	136		
1	W	88	Total	C	N	O	0	0
			689	430	123	136		
1	Y	88	Total	C	N	O	0	0
			689	430	123	136		
1	a	88	Total	C	N	O	0	0
			689	430	123	136		

- Molecule 2 is a protein called Chaperonin GroEL.

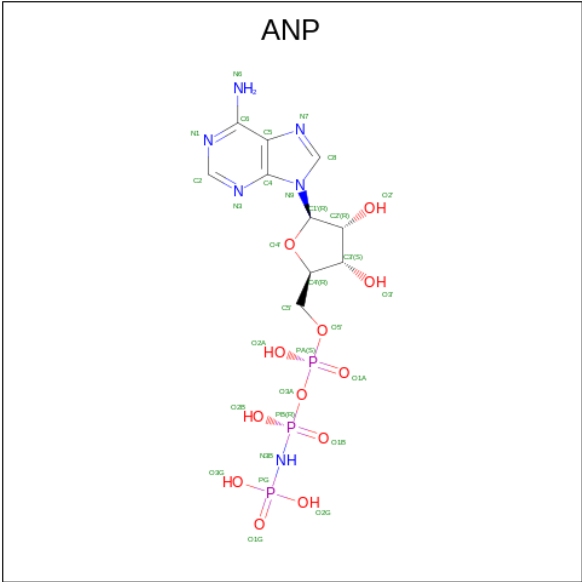
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	J	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	K	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	L	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	N	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	P	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	R	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	T	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	V	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	X	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	Z	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	b	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		
2	c	524	Total	C	N	O	S	0	0
			3855	2397	665	773	20		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	J	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	L	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	N	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	P	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	R	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	T	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	V	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	X	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	Z	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	b	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	c	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total 1	Mg 1	0
4	I	1	Total 1	Mg 1	0
4	J	1	Total 1	Mg 1	0
4	K	1	Total 1	Mg 1	0
4	L	1	Total 1	Mg 1	0
4	N	1	Total 1	Mg 1	0
4	P	1	Total 1	Mg 1	0
4	R	1	Total 1	Mg 1	0
4	T	1	Total 1	Mg 1	0
4	V	1	Total 1	Mg 1	0
4	X	1	Total 1	Mg 1	0
4	Z	1	Total 1	Mg 1	0
4	b	1	Total 1	Mg 1	0
4	c	1	Total 1	Mg 1	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total 1	K 1	0
5	I	1	Total 1	K 1	0
5	J	1	Total 1	K 1	0
5	K	1	Total 1	K 1	0
5	L	1	Total 1	K 1	0

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Mol	Chain	Residues	Atoms		AltConf
5	N	1	Total 1	K 1	0
5	P	1	Total 1	K 1	0
5	R	1	Total 1	K 1	0
5	T	1	Total 1	K 1	0
5	V	1	Total 1	K 1	0
5	X	1	Total 1	K 1	0
5	Z	1	Total 1	K 1	0
5	b	1	Total 1	K 1	0
5	c	1	Total 1	K 1	0

THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	Q253	K256	Y284
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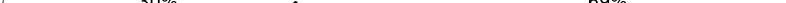
- Molecule 1: Chaperedoxin

Chain D:  30% . 69%

LEU ASP CYS ASP ALA ALA GLU GLN MET TLE TLE ALA ALA ALA GLN PHE GLY LEU LEU ARG ARG TLE TLE PRO PRO THR VAL TYR LEU LEU PHE GLN ASN GLY GLN GLN PRO PRO VAL VAL ASP GLY PHE PHE GLN GLY GLY PRO GLN GLN PRO GLU GLU ALA ALA TLE TLE ARG ALA LEU LEU LEU LEU ASP LYS VAL VAL PRO PRO ARG GLU GLU GLU GLU LEU LEU LYS ALA ALA GLN GLN

THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	+	Q253	+	K256	+	Y284
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- Molecule 1: Chaperedoxin

Chain E:  30% 69%

LEU ASP CYS ASP ALA GLU GLN MET TLE ALA ALA ALA GLN PHE LEU GLY LEU ARG ALA ALA TLE PRO THR VAL VAL TYR LEU LEU PHE GLN GLN ASN GLY GLY GLN GLN PRO PRO VAL VAL ASP GLY PHE GLN GLN GLN GLY PRO GLN PRO PRO GLU GLU ALA ALA TLE ARG ALA ALA LEU LEU LEU LEU ASP LYS VAL VAL LEU LEU PRO PRO ARG ARG GLY GLY GLY GLN GLN

THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	Q253	K256	Y284
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- Molecule 1: Chaperedoxin

Chain F: 30% . 69%

LEU ASP CYS ASP ALA GLN MET TLE ALA ALA ALA PHE LEU LEU ARG ALA TLE PRO THR VAL TYR LEU PHE GLN GLY GLY GLN PRO VAL ASP GLY PHE GLN PRO GLN GLU GLU GLU TLE ARG ALA LEU LEU LEU ASP VAL LYS LEU LEU LYS ARG GLU GLU GLU GLN

THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	Q253	K256	Y280	Y284
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- Molecule 1: Chaperedoxin

THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	Q253	K256	Y284
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------

Chain U: 30% . 69%

THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	Q253	K256	Y284
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Chain W: 30% . 69%

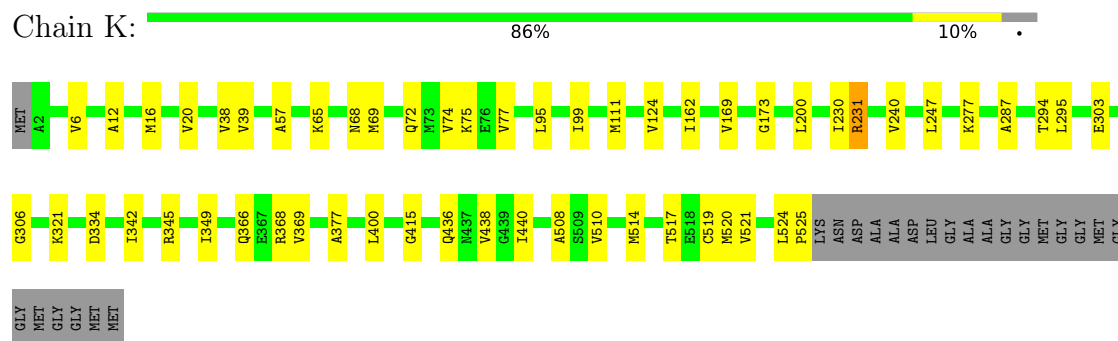
THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	Q253	K256	Y280	Y284
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------

Chain Y: 30% 69%

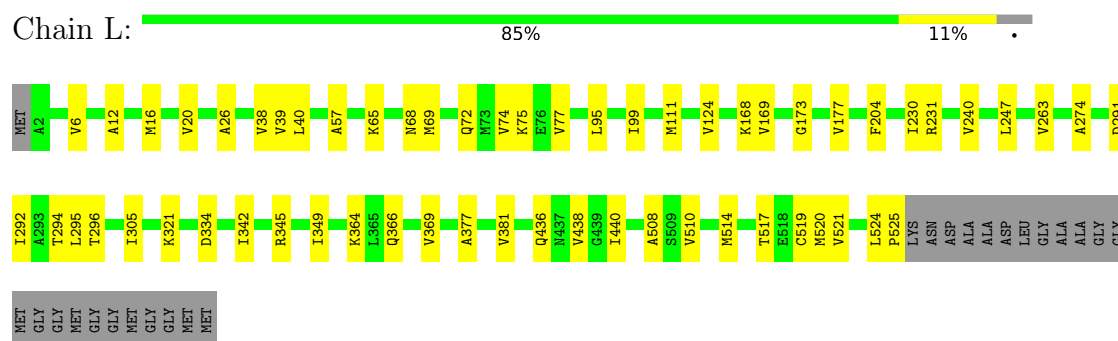
THR	ARG	TYR	GLN	GLY	LEU	VAL	ALA	GLN	ILE	GLU	LEU	LEU	LYS	GLN	ALA	A197	Q253	T254	R255	K256	Y284
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WORLDWIDE
PDB
PROTEIN DATA BANK

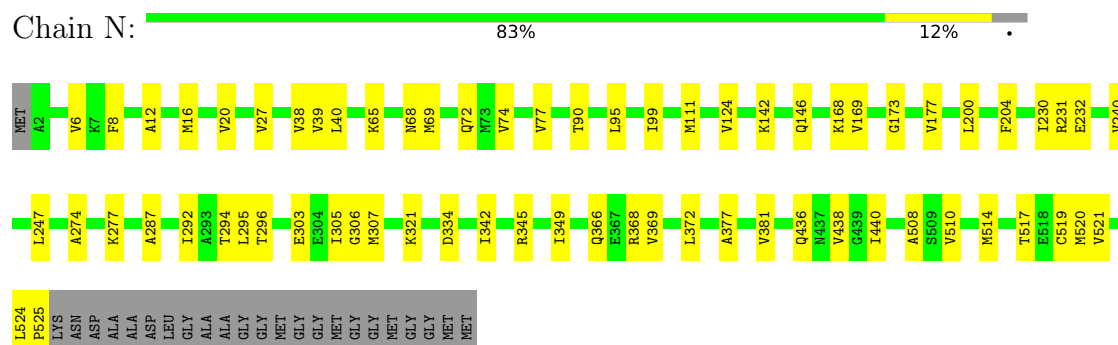
• Molecule 2: Chaperonin GroEL



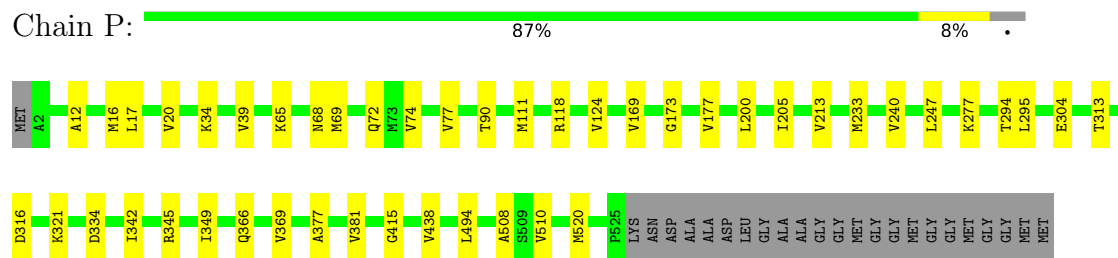
• Molecule 2: Chaperonin GroEL



• Molecule 2: Chaperonin GroEL



• Molecule 2: Chaperonin GroEL



• Molecule 2: Chaperonin GroEL

[illegible]

I349	A2	MET
Q366	A12	
V369	M16	
A377	L17	
G415	V20	
V438	K34	
A508	V39	
M520	K65	
P525	N68	
LYS	M69	
ASN	Q72	
ASP	M73	
ALA	V74	
ALA		
ASP	M111	
LEU	R118	
GLY	V124	
ALA		
ALA	V169	
GLY		
GLY	G173	
GLY	MET	
GLY	L200	
GLY	L205	
MET	V213	
GLY	MET	
GLY	M233	
MET	V240	
	L247	
	K277	
	T294	
	L295	
	I305	
	K321	
	D334	
	I342	
	R345	

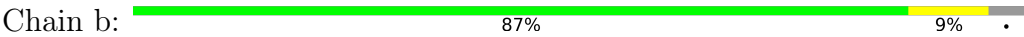
[illegible]

D316	A2	A12	M16	V20	K34	V39	K65	M68	Q72	V73	V74	V77	T90	L95	T98	M111	R118	V124	V169	GLY	G173	L200	I205	GLY	V213	V240	L247	K277	T284	L295	I305	T313
K321	D334	I342	R345	I349	Q366	V369	A377	Q436	M437	V438	G439	I440	A508	S509	V510	M520	P525	LYS	ASN	ASP	ALA	ASP	LEU	GLY	ALA	GLY	GLY	MET	GLY	GLY	MET	

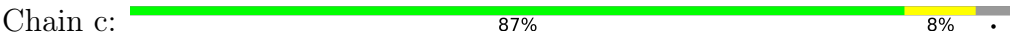
Met
A2
A12
M16
L17
V20
K34
V39
K65
N68
H69
Q72
M73
V74
M111
R118
V124
V169
G173
L200
I205
V213
M233
V240
L247
K277
T294
E303
E304
G305
I306
M307
T313
D316
V321



• Molecule 2: Chaperonin GroEL



• Molecule 2: Chaperonin GroEL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	214141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.019	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/697	0.30	0/942
1	B	0.13	0/697	0.30	0/942
1	C	0.13	0/697	0.29	0/942
1	D	0.13	0/697	0.29	0/942
1	E	0.13	0/697	0.30	0/942
1	F	0.13	0/697	0.29	0/942
1	M	0.13	0/697	0.29	0/942
1	O	0.13	0/697	0.29	0/942
1	Q	0.13	0/697	0.29	0/942
1	S	0.13	0/697	0.29	0/942
1	U	0.13	0/697	0.29	0/942
1	W	0.13	0/697	0.29	0/942
1	Y	0.13	0/697	0.29	0/942
1	a	0.13	0/697	0.29	0/942
2	G	0.25	1/3883 (0.0%)	0.43	0/5243
2	I	0.22	0/3883	0.44	0/5243
2	J	0.22	0/3883	0.43	0/5243
2	K	0.24	0/3883	0.43	0/5243
2	L	0.23	0/3883	0.44	0/5243
2	N	0.23	0/3883	0.44	0/5243
2	P	0.25	1/3883 (0.0%)	0.40	0/5243
2	R	0.22	0/3883	0.40	0/5243
2	T	0.24	0/3883	0.40	0/5243
2	V	0.25	1/3883 (0.0%)	0.39	0/5243
2	X	0.23	0/3883	0.39	0/5243
2	Z	0.22	0/3883	0.39	0/5243
2	b	0.22	0/3883	0.40	0/5243
2	c	0.22	0/3883	0.40	0/5243
All	All	0.22	3/64120 (0.0%)	0.40	0/86590

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	304	GLU	C-N	-7.28	1.25	1.33
2	P	304	GLU	C-N	-7.26	1.25	1.33
2	G	380	LYS	C-N	6.33	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	689	0	686	2	0
1	B	689	0	686	1	0
1	C	689	0	686	1	0
1	D	689	0	686	1	0
1	E	689	0	686	1	0
1	F	689	0	686	2	0
1	M	689	0	686	1	0
1	O	689	0	686	1	0
1	Q	689	0	686	2	0
1	S	689	0	686	1	0
1	U	689	0	686	1	0
1	W	689	0	686	2	0
1	Y	689	0	686	2	0
1	a	689	0	686	1	0
2	G	3855	0	3976	46	0
2	I	3855	0	3976	44	0
2	J	3855	0	3976	40	0
2	K	3855	0	3976	38	0
2	L	3855	0	3976	42	0
2	N	3855	0	3976	50	0
2	P	3855	0	3976	31	0
2	R	3855	0	3976	38	0
2	T	3855	0	3976	25	0
2	V	3855	0	3976	30	0
2	X	3855	0	3976	33	0
2	Z	3855	0	3976	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3855	0	3976	38	0
2	c	3855	0	3976	31	0
3	G	31	0	13	1	0
3	I	31	0	13	0	0
3	J	31	0	13	1	0
3	K	31	0	13	1	0
3	L	31	0	13	0	0
3	N	31	0	13	0	0
3	P	31	0	13	3	0
3	R	31	0	13	2	0
3	T	31	0	13	2	0
3	V	31	0	13	1	0
3	X	31	0	13	1	0
3	Z	31	0	13	1	0
3	b	31	0	13	2	0
3	c	31	0	13	1	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	N	1	0	0	0	0
4	P	1	0	0	0	0
4	R	1	0	0	0	0
4	T	1	0	0	0	0
4	V	1	0	0	0	0
4	X	1	0	0	0	0
4	Z	1	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
5	R	1	0	0	0	0
5	T	1	0	0	0	0
5	V	1	0	0	0	0
5	X	1	0	0	0	0
5	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	b	1	0	0	0	0
5	c	1	0	0	0	0
All	All	64078	0	65450	489	0

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

All (489) 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:Z:240:VAL:HG11	2:Z:247:LEU:HB2	1.61	0.82
2:c:240:VAL:HG11	2:c:247:LEU:HB2	1.62	0.82
2:P:240:VAL:HG11	2:P:247:LEU:HB2	1.61	0.82
2:b:240:VAL:HG11	2:b:247:LEU:HB2	1.62	0.81
2:X:294:THR:HG22	2:X:342:ILE:HD13	1.61	0.81
2:V:240:VAL:HG11	2:V:247:LEU:HB2	1.62	0.79
2:T:240:VAL:HG11	2:T:247:LEU:HB2	1.62	0.79
2:X:240:VAL:HG11	2:X:247:LEU:HB2	1.62	0.79
2:R:240:VAL:HG11	2:R:247:LEU:HB2	1.62	0.78
2:X:118:ARG:HH22	2:Z:34:LYS:HE2	1.48	0.78
2:P:34:LYS:HE2	2:c:118:ARG:HH22	1.49	0.77
2:V:118:ARG:HH22	2:X:34:LYS:HE2	1.48	0.77
2:R:118:ARG:HH22	2:T:34:LYS:HE2	1.48	0.77
2:T:118:ARG:HH22	2:V:34:LYS:HE2	1.49	0.76
2:P:118:ARG:HH22	2:R:34:LYS:HE2	1.49	0.76
2:Z:118:ARG:HH22	2:c:34:LYS:HE2	1.50	0.75
2:J:39:VAL:HG21	2:K:16:MET:HE1	1.71	0.72
2:G:38:VAL:HG22	2:b:519:CYS:HB3	1.71	0.71
2:G:39:VAL:HG21	2:b:16:MET:HE1	1.71	0.71
2:I:240:VAL:HG11	2:I:247:LEU:HB2	1.74	0.69
2:G:90:THR:H	3:G:600:ANP:HNB1	1.40	0.69
2:L:39:VAL:HG21	2:N:16:MET:HE1	1.74	0.68
2:I:39:VAL:HG21	2:J:16:MET:HE1	1.76	0.68
2:J:240:VAL:HG11	2:J:247:LEU:HB2	1.76	0.68
2:L:294:THR:HG22	2:L:342:ILE:HD13	1.76	0.68
2:K:240:VAL:HG11	2:K:247:LEU:HB2	1.76	0.68
2:P:169:VAL:HG21	2:P:377:ALA:HB2	1.76	0.68
2:L:240:VAL:HG11	2:L:247:LEU:HB2	1.75	0.68
2:G:16:MET:HE1	2:N:39:VAL:HG21	1.76	0.67
2:Z:169:VAL:HG21	2:Z:377:ALA:HB2	1.77	0.67
2:L:169:VAL:HG21	2:L:377:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:169:VAL:HG21	2:N:377:ALA:HB2	1.77	0.67
2:c:169:VAL:HG21	2:c:377:ALA:HB2	1.77	0.67
2:X:169:VAL:HG21	2:X:377:ALA:HB2	1.76	0.67
2:G:169:VAL:HG21	2:G:377:ALA:HB2	1.77	0.67
2:I:169:VAL:HG21	2:I:377:ALA:HB2	1.76	0.66
2:I:294:THR:HG22	2:I:342:ILE:HD13	1.77	0.66
2:G:240:VAL:HG11	2:G:247:LEU:HB2	1.76	0.66
2:N:240:VAL:HG11	2:N:247:LEU:HB2	1.76	0.66
2:J:169:VAL:HG21	2:J:377:ALA:HB2	1.76	0.66
2:T:169:VAL:HG21	2:T:377:ALA:HB2	1.76	0.66
2:b:169:VAL:HG21	2:b:377:ALA:HB2	1.77	0.66
2:R:169:VAL:HG21	2:R:377:ALA:HB2	1.77	0.66
2:K:169:VAL:HG21	2:K:377:ALA:HB2	1.77	0.65
2:J:294:THR:HG22	2:J:342:ILE:HD13	1.78	0.65
2:P:294:THR:HG22	2:P:342:ILE:HD13	1.79	0.65
2:N:294:THR:HG22	2:N:342:ILE:HD13	1.77	0.65
2:G:6:VAL:HG12	2:G:521:VAL:HG22	1.78	0.65
2:V:169:VAL:HG21	2:V:377:ALA:HB2	1.77	0.65
2:K:294:THR:HG22	2:K:342:ILE:HD13	1.79	0.65
2:J:6:VAL:HG12	2:J:521:VAL:HG22	1.79	0.65
2:L:6:VAL:HG12	2:L:521:VAL:HG22	1.80	0.64
2:N:6:VAL:HG12	2:N:521:VAL:HG22	1.80	0.64
2:G:295:LEU:HD23	2:G:342:ILE:HD12	1.79	0.64
2:K:6:VAL:HG12	2:K:521:VAL:HG22	1.80	0.64
2:I:6:VAL:HG12	2:I:521:VAL:HG22	1.78	0.64
2:V:294:THR:HG22	2:V:342:ILE:HD13	1.81	0.63
2:K:39:VAL:HG21	2:L:16:MET:HE1	1.80	0.63
2:N:303:GLU:O	2:N:306:GLY:N	2.30	0.63
2:R:294:THR:HG22	2:R:342:ILE:HD13	1.80	0.62
2:K:303:GLU:O	2:K:306:GLY:N	2.33	0.62
2:Z:294:THR:HG22	2:Z:342:ILE:HD13	1.82	0.61
2:I:303:GLU:O	2:I:306:GLY:N	2.30	0.61
2:J:39:VAL:HG21	2:K:16:MET:CE	2.29	0.61
2:T:294:THR:HG22	2:T:342:ILE:HD13	1.82	0.61
1:W:280:TYR:HD2	2:X:305:ILE:HG13	1.66	0.61
2:J:303:GLU:O	2:J:306:GLY:N	2.33	0.60
2:I:231:ARG:HD2	2:I:232:GLU:N	2.16	0.60
2:L:39:VAL:HG21	2:N:16:MET:CE	2.32	0.59
1:Q:280:TYR:HD2	2:R:305:ILE:HG13	1.66	0.59
2:X:169:VAL:HG12	2:X:173:GLY:HA3	1.84	0.59
2:V:169:VAL:HG12	2:V:173:GLY:HA3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:169:VAL:HG12	2:Z:173:GLY:HA3	1.85	0.59
2:R:90:THR:H	3:R:603:ANP:HNB1	1.49	0.58
2:T:169:VAL:HG12	2:T:173:GLY:HA3	1.84	0.58
2:R:169:VAL:HG12	2:R:173:GLY:HA3	1.85	0.58
2:b:169:VAL:HG12	2:b:173:GLY:HA3	1.85	0.58
2:c:169:VAL:HG12	2:c:173:GLY:HA3	1.85	0.58
2:G:39:VAL:HG21	2:b:16:MET:CE	2.34	0.57
2:J:90:THR:H	3:J:603:ANP:HNB1	1.52	0.57
2:c:177:VAL:HG23	2:c:381:VAL:HG23	1.87	0.57
2:b:177:VAL:HG23	2:b:381:VAL:HG23	1.87	0.57
2:V:90:THR:H	3:V:602:ANP:HNB1	1.51	0.57
2:P:169:VAL:HG12	2:P:173:GLY:HA3	1.86	0.57
2:J:169:VAL:HG12	2:J:173:GLY:HA3	1.87	0.56
2:X:90:THR:H	3:X:602:ANP:HNB1	1.52	0.56
2:I:169:VAL:HG12	2:I:173:GLY:HA3	1.87	0.56
2:K:169:VAL:HG12	2:K:173:GLY:HA3	1.88	0.56
2:L:291:ASP:OD1	2:L:345:ARG:NH2	2.27	0.56
2:P:345:ARG:O	2:P:349:ILE:HG13	2.06	0.56
2:Z:366:GLN:HA	2:Z:369:VAL:HG22	1.88	0.56
2:P:177:VAL:HG23	2:P:381:VAL:HG23	1.88	0.55
2:N:169:VAL:HG12	2:N:173:GLY:HA3	1.87	0.55
2:G:169:VAL:HG12	2:G:173:GLY:HA3	1.87	0.55
2:c:366:GLN:HA	2:c:369:VAL:HG22	1.89	0.55
2:J:38:VAL:HG22	2:K:519:CYS:HB3	1.89	0.55
2:J:68:ASN:O	2:J:72:GLN:HG2	2.07	0.55
2:V:345:ARG:O	2:V:349:ILE:HG13	2.06	0.55
2:b:200:LEU:HD21	2:b:277:LYS:HG3	1.89	0.55
2:c:111:MET:SD	2:c:438:VAL:HG11	2.47	0.55
2:c:294:THR:HG22	2:c:342:ILE:HD13	1.88	0.55
2:G:16:MET:CE	2:N:39:VAL:HG21	2.37	0.54
2:G:366:GLN:HA	2:G:369:VAL:HG22	1.89	0.54
2:I:38:VAL:HG22	2:J:519:CYS:HB3	1.89	0.54
2:I:39:VAL:HG21	2:J:16:MET:CE	2.36	0.54
2:N:68:ASN:O	2:N:72:GLN:HG2	2.06	0.54
1:A:280:TYR:HD2	2:G:305:ILE:HG13	1.72	0.54
2:G:68:ASN:O	2:G:72:GLN:HG2	2.07	0.54
2:V:366:GLN:HA	2:V:369:VAL:HG22	1.88	0.54
2:P:366:GLN:HA	2:P:369:VAL:HG22	1.88	0.54
2:T:366:GLN:HA	2:T:369:VAL:HG22	1.88	0.54
2:X:111:MET:SD	2:X:438:VAL:HG11	2.47	0.54
2:b:111:MET:SD	2:b:438:VAL:HG11	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:TYR:HD2	2:L:305:ILE:HG13	1.72	0.54
2:X:366:GLN:HA	2:X:369:VAL:HG22	1.88	0.54
2:K:39:VAL:HG21	2:L:16:MET:CE	2.38	0.54
2:b:366:GLN:HA	2:b:369:VAL:HG22	1.89	0.54
2:G:111:MET:SD	2:G:438:VAL:HG11	2.48	0.54
2:L:169:VAL:HG12	2:L:173:GLY:HA3	1.90	0.54
2:P:111:MET:SD	2:P:438:VAL:HG11	2.48	0.54
2:b:294:THR:HG22	2:b:342:ILE:HD13	1.88	0.54
1:E:253:GLN:HA	1:E:256:LYS:HE3	1.89	0.54
1:C:253:GLN:HA	1:C:256:LYS:HE3	1.89	0.54
2:J:111:MET:SD	2:J:438:VAL:HG11	2.48	0.54
2:V:111:MET:SD	2:V:438:VAL:HG11	2.48	0.54
2:K:111:MET:SD	2:K:438:VAL:HG11	2.48	0.53
2:L:38:VAL:HG22	2:N:519:CYS:HB3	1.89	0.53
2:L:68:ASN:O	2:L:72:GLN:HG2	2.08	0.53
2:R:366:GLN:HA	2:R:369:VAL:HG22	1.88	0.53
1:F:253:GLN:HA	1:F:256:LYS:HE3	1.90	0.53
2:I:68:ASN:O	2:I:72:GLN:HG2	2.07	0.53
2:N:111:MET:SD	2:N:438:VAL:HG11	2.49	0.53
2:R:200:LEU:HD21	2:R:277:LYS:HG3	1.90	0.53
2:Z:111:MET:SD	2:Z:438:VAL:HG11	2.48	0.53
2:G:519:CYS:HB3	2:N:38:VAL:HG22	1.89	0.53
2:K:68:ASN:O	2:K:72:GLN:HG2	2.08	0.53
2:L:111:MET:SD	2:L:438:VAL:HG11	2.48	0.53
2:R:345:ARG:O	2:R:349:ILE:HG13	2.08	0.53
2:V:200:LEU:HD21	2:V:277:LYS:HG3	1.90	0.53
2:c:200:LEU:HD21	2:c:277:LYS:HG3	1.89	0.53
2:N:366:GLN:HA	2:N:369:VAL:HG22	1.91	0.53
1:D:253:GLN:HA	1:D:256:LYS:HE3	1.89	0.53
2:G:40:LEU:HD23	2:b:521:VAL:HB	1.89	0.53
2:R:68:ASN:O	2:R:72:GLN:HG2	2.09	0.53
2:Z:205:ILE:HA	2:Z:213:VAL:HG22	1.91	0.53
2:L:366:GLN:HA	2:L:369:VAL:HG22	1.91	0.53
1:M:253:GLN:HA	1:M:256:LYS:HE3	1.90	0.53
2:I:111:MET:SD	2:I:438:VAL:HG11	2.49	0.53
2:P:68:ASN:O	2:P:72:GLN:HG2	2.09	0.53
1:B:253:GLN:HA	1:B:256:LYS:HE3	1.90	0.53
2:R:295:LEU:HD23	2:R:342:ILE:HD12	1.91	0.53
2:R:321:LYS:HB3	2:R:334:ASP:HB3	1.91	0.53
2:T:200:LEU:HD21	2:T:277:LYS:HG3	1.91	0.53
2:P:321:LYS:HB3	2:P:334:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:305:ILE:HG22	2:X:305:ILE:O	2.08	0.52
2:G:205:ILE:HA	2:G:213:VAL:HG22	1.91	0.52
2:b:321:LYS:HB3	2:b:334:ASP:HB3	1.92	0.52
2:V:295:LEU:HD23	2:V:342:ILE:HD12	1.91	0.52
2:T:111:MET:SD	2:T:438:VAL:HG11	2.50	0.52
2:R:111:MET:SD	2:R:438:VAL:HG11	2.50	0.52
2:T:321:LYS:HB3	2:T:334:ASP:HB3	1.92	0.52
2:X:200:LEU:HD21	2:X:277:LYS:HG3	1.92	0.52
2:c:321:LYS:HB3	2:c:334:ASP:HB3	1.92	0.52
2:T:68:ASN:O	2:T:72:GLN:HG2	2.09	0.52
2:Z:321:LYS:HB3	2:Z:334:ASP:HB3	1.92	0.52
2:V:12:ALA:HB1	2:V:520:MET:SD	2.50	0.52
2:X:321:LYS:HB3	2:X:334:ASP:HB3	1.92	0.52
2:Z:68:ASN:O	2:Z:72:GLN:HG2	2.09	0.52
2:b:65:LYS:O	2:b:69:MET:HG3	2.10	0.52
2:P:200:LEU:HD21	2:P:277:LYS:HG3	1.91	0.52
2:X:68:ASN:O	2:X:72:GLN:HG2	2.10	0.52
2:Z:200:LEU:HD21	2:Z:277:LYS:HG3	1.92	0.52
2:K:366:GLN:HA	2:K:369:VAL:HG22	1.91	0.52
2:L:295:LEU:HD23	2:L:342:ILE:HD12	1.91	0.52
2:R:205:ILE:HA	2:R:213:VAL:HG22	1.93	0.51
2:V:68:ASN:O	2:V:72:GLN:HG2	2.10	0.51
2:V:321:LYS:HB3	2:V:334:ASP:HB3	1.92	0.51
2:I:366:GLN:HA	2:I:369:VAL:HG22	1.91	0.51
2:J:295:LEU:HD23	2:J:342:ILE:HD12	1.92	0.51
2:G:321:LYS:HB3	2:G:334:ASP:HB3	1.93	0.51
2:Z:12:ALA:HB1	2:Z:520:MET:SD	2.50	0.51
2:c:68:ASN:O	2:c:72:GLN:HG2	2.10	0.51
2:J:366:GLN:HA	2:J:369:VAL:HG22	1.91	0.51
2:K:295:LEU:HD23	2:K:342:ILE:HD12	1.92	0.51
2:K:321:LYS:HB3	2:K:334:ASP:HB3	1.93	0.51
1:A:253:GLN:HA	1:A:256:LYS:HE3	1.90	0.51
2:J:524:LEU:HD12	2:J:525:PRO:HD2	1.93	0.51
2:X:12:ALA:HB1	2:X:520:MET:SD	2.50	0.51
2:c:205:ILE:HA	2:c:213:VAL:HG22	1.93	0.51
2:P:65:LYS:O	2:P:69:MET:HG3	2.11	0.51
2:T:205:ILE:HA	2:T:213:VAL:HG22	1.93	0.51
2:Z:65:LYS:O	2:Z:69:MET:HG3	2.10	0.51
2:Z:303:GLU:O	2:Z:306:GLY:N	2.44	0.51
2:b:205:ILE:HA	2:b:213:VAL:HG22	1.93	0.51
2:c:65:LYS:O	2:c:69:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:349:ILE:O	2:G:353:ILE:HG13	2.11	0.51
2:X:65:LYS:O	2:X:69:MET:HG3	2.10	0.51
2:b:68:ASN:O	2:b:72:GLN:HG2	2.10	0.50
2:I:295:LEU:HD23	2:I:342:ILE:HD12	1.93	0.50
2:I:524:LEU:HD12	2:I:525:PRO:HD2	1.93	0.50
2:L:321:LYS:HB3	2:L:334:ASP:HB3	1.94	0.50
2:N:321:LYS:HB3	2:N:334:ASP:HB3	1.94	0.50
2:R:177:VAL:HG23	2:R:381:VAL:HG23	1.92	0.50
2:R:305:ILE:O	2:R:305:ILE:HG22	2.10	0.50
1:W:253:GLN:HA	1:W:256:LYS:HE3	1.93	0.50
2:b:12:ALA:HB1	2:b:520:MET:SD	2.51	0.50
2:G:345:ARG:O	2:G:349:ILE:HG13	2.11	0.50
2:P:12:ALA:HB1	2:P:520:MET:SD	2.51	0.50
2:R:12:ALA:HB1	2:R:520:MET:SD	2.51	0.50
2:c:303:GLU:O	2:c:306:GLY:N	2.45	0.50
2:T:295:LEU:HD23	2:T:342:ILE:HD12	1.93	0.50
2:T:345:ARG:O	2:T:349:ILE:HG13	2.12	0.50
2:c:12:ALA:HB1	2:c:520:MET:SD	2.51	0.50
2:L:524:LEU:HD12	2:L:525:PRO:HD2	1.94	0.50
2:T:12:ALA:HB1	2:T:520:MET:SD	2.52	0.50
2:V:65:LYS:O	2:V:69:MET:HG3	2.11	0.50
2:K:12:ALA:HB1	2:K:520:MET:SD	2.52	0.50
2:L:345:ARG:O	2:L:349:ILE:HG13	2.12	0.50
2:N:12:ALA:HB1	2:N:520:MET:SD	2.52	0.50
2:P:295:LEU:HD23	2:P:342:ILE:HD12	1.94	0.50
2:R:65:LYS:O	2:R:69:MET:HG3	2.12	0.50
1:U:253:GLN:HA	1:U:256:LYS:HE3	1.93	0.50
2:I:69:MET:CE	2:b:39:VAL:HG12	2.42	0.50
2:I:321:LYS:HB3	2:I:334:ASP:HB3	1.94	0.50
2:P:205:ILE:HA	2:P:213:VAL:HG22	1.94	0.50
2:V:205:ILE:HA	2:V:213:VAL:HG22	1.93	0.50
2:b:303:GLU:O	2:b:306:GLY:N	2.45	0.50
2:c:185:ASP:OD1	2:c:382:GLY:N	2.40	0.50
1:O:253:GLN:HA	1:O:256:LYS:HE3	1.93	0.49
2:T:65:LYS:O	2:T:69:MET:HG3	2.12	0.49
2:J:321:LYS:HB3	2:J:334:ASP:HB3	1.94	0.49
2:L:12:ALA:HB1	2:L:520:MET:SD	2.52	0.49
1:Q:253:GLN:HA	1:Q:256:LYS:HE3	1.94	0.49
1:Y:253:GLN:HA	1:Y:256:LYS:HE3	1.93	0.49
2:I:12:ALA:HB1	2:I:520:MET:SD	2.53	0.49
2:N:231:ARG:HB3	2:N:231:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:177:VAL:CG2	2:c:381:VAL:HG23	2.42	0.49
2:J:12:ALA:HB1	2:J:520:MET:SD	2.52	0.49
2:Z:415:GLY:HA2	3:Z:603:ANP:H1'	1.94	0.49
2:K:524:LEU:HD12	2:K:525:PRO:HD2	1.95	0.49
2:N:295:LEU:HD23	2:N:342:ILE:HD12	1.93	0.49
1:S:253:GLN:HA	1:S:256:LYS:HE3	1.93	0.49
2:b:177:VAL:CG2	2:b:381:VAL:HG23	2.42	0.49
2:G:12:ALA:HB1	2:G:520:MET:SD	2.53	0.49
2:K:38:VAL:HG22	2:L:519:CYS:HB3	1.94	0.48
1:a:253:GLN:HA	1:a:256:LYS:HE3	1.93	0.48
2:N:95:LEU:O	2:N:99:ILE:HG13	2.13	0.48
2:N:524:LEU:HD12	2:N:525:PRO:HD2	1.94	0.48
2:G:39:VAL:HG12	2:b:69:MET:CE	2.43	0.48
2:G:294:THR:HG22	2:G:342:ILE:HD13	1.96	0.48
2:X:205:ILE:HA	2:X:213:VAL:HG22	1.95	0.48
2:P:16:MET:HE1	2:R:39:VAL:HG21	1.96	0.48
2:X:16:MET:HE1	2:Z:39:VAL:HG21	1.95	0.48
2:G:291:ASP:OD1	2:G:345:ARG:NE	2.42	0.48
2:G:57:ALA:O	2:G:75:LYS:HD2	2.13	0.48
2:P:39:VAL:HG21	2:c:16:MET:HE1	1.96	0.48
2:P:177:VAL:CG2	2:P:381:VAL:HG23	2.44	0.48
2:I:303:GLU:C	2:I:306:GLY:H	2.22	0.48
2:I:345:ARG:O	2:I:349:ILE:HG13	2.14	0.47
2:K:95:LEU:O	2:K:99:ILE:HG13	2.14	0.47
2:I:77:VAL:HG21	2:I:510:VAL:HB	1.96	0.47
2:K:345:ARG:O	2:K:349:ILE:HG13	2.15	0.47
2:G:230:ILE:O	2:G:231:ARG:C	2.57	0.47
2:G:524:LEU:HD12	2:G:525:PRO:HD2	1.96	0.47
2:L:95:LEU:O	2:L:99:ILE:HG13	2.14	0.47
2:L:177:VAL:HG23	2:L:381:VAL:HG23	1.97	0.47
2:N:177:VAL:CG2	2:N:381:VAL:HG23	2.45	0.47
2:N:177:VAL:HG23	2:N:381:VAL:HG23	1.95	0.47
2:R:16:MET:HE1	2:T:39:VAL:HG21	1.96	0.47
2:I:69:MET:HE2	2:b:39:VAL:HG12	1.97	0.47
2:T:415:GLY:HA2	3:T:603:ANP:H1'	1.97	0.47
2:X:345:ARG:O	2:X:349:ILE:HG13	2.15	0.47
2:Z:345:ARG:O	2:Z:349:ILE:HG13	2.15	0.47
2:J:77:VAL:HG21	2:J:510:VAL:HB	1.96	0.47
2:J:303:GLU:C	2:J:306:GLY:H	2.23	0.47
2:G:77:VAL:HG21	2:G:510:VAL:HB	1.96	0.47
2:J:95:LEU:O	2:J:99:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:77:VAL:HG21	2:N:510:VAL:HB	1.96	0.47
2:b:185:ASP:OD1	2:b:382:GLY:N	2.40	0.47
2:I:95:LEU:O	2:I:99:ILE:HG13	2.14	0.46
2:K:230:ILE:O	2:K:231:ARG:C	2.57	0.46
2:c:345:ARG:O	2:c:349:ILE:HG13	2.15	0.46
2:I:521:VAL:HB	2:b:40:LEU:HD23	1.97	0.46
2:L:77:VAL:HG21	2:L:510:VAL:HB	1.96	0.46
2:G:95:LEU:O	2:G:99:ILE:HG13	2.14	0.46
2:Z:16:MET:HE1	2:c:39:VAL:HG21	1.97	0.46
2:L:57:ALA:O	2:L:75:LYS:HD2	2.15	0.46
2:K:77:VAL:HG21	2:K:510:VAL:HB	1.96	0.46
2:V:16:MET:HE1	2:X:39:VAL:HG21	1.96	0.46
2:K:20:VAL:HG23	2:K:74:VAL:HG21	1.98	0.46
2:b:345:ARG:O	2:b:349:ILE:HG13	2.15	0.46
2:I:65:LYS:O	2:I:69:MET:HG3	2.16	0.46
2:J:65:LYS:O	2:J:69:MET:HG3	2.16	0.46
2:J:230:ILE:O	2:J:231:ARG:C	2.56	0.46
2:L:177:VAL:CG2	2:L:381:VAL:HG23	2.45	0.46
2:N:345:ARG:O	2:N:349:ILE:HG13	2.16	0.46
2:R:177:VAL:CG2	2:R:381:VAL:HG23	2.46	0.46
2:b:169:VAL:CG2	2:b:377:ALA:HB2	2.46	0.46
2:L:204:PHE:CD2	2:L:274:ALA:HA	2.51	0.45
2:G:16:MET:O	2:G:20:VAL:HG12	2.16	0.45
2:J:20:VAL:CG2	2:J:74:VAL:HG21	2.46	0.45
2:K:65:LYS:O	2:K:69:MET:HG3	2.17	0.45
2:J:16:MET:O	2:J:20:VAL:HG12	2.15	0.45
2:L:65:LYS:O	2:L:69:MET:HG3	2.16	0.45
2:R:169:VAL:CG2	2:R:377:ALA:HB2	2.46	0.45
2:T:16:MET:HE1	2:V:39:VAL:HG21	1.97	0.45
2:T:169:VAL:CG2	2:T:377:ALA:HB2	2.45	0.45
2:G:20:VAL:CG2	2:G:74:VAL:HG21	2.46	0.45
2:N:20:VAL:CG2	2:N:74:VAL:HG21	2.46	0.45
2:N:231:ARG:HH22	2:N:232:GLU:HG2	1.81	0.45
2:I:20:VAL:CG2	2:I:74:VAL:HG21	2.46	0.45
2:K:303:GLU:C	2:K:306:GLY:H	2.22	0.45
2:K:514:MET:O	2:K:517:THR:HG22	2.17	0.45
2:N:65:LYS:O	2:N:69:MET:HG3	2.15	0.45
2:N:231:ARG:NH2	2:N:232:GLU:HG2	2.31	0.45
2:G:26:ALA:HA	2:b:8:PHE:HE1	1.82	0.45
2:N:305:ILE:O	2:N:305:ILE:HG22	2.17	0.45
2:R:185:ASP:OD1	2:R:382:GLY:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:65:LYS:O	2:G:69:MET:HG3	2.17	0.45
2:G:169:VAL:CG2	2:G:377:ALA:HB2	2.47	0.45
2:N:20:VAL:HG23	2:N:74:VAL:HG21	1.98	0.45
2:J:345:ARG:O	2:J:349:ILE:HG13	2.17	0.44
2:X:313:THR:N	2:X:316:ASP:OD2	2.44	0.44
2:c:124:VAL:HG21	2:c:508:ALA:HB2	1.99	0.44
2:G:20:VAL:HG23	2:G:74:VAL:HG21	1.98	0.44
2:I:16:MET:O	2:I:20:VAL:HG12	2.16	0.44
2:I:57:ALA:O	2:I:75:LYS:HD2	2.17	0.44
2:J:200:LEU:HD21	2:J:277:LYS:HG3	1.99	0.44
2:K:231:ARG:HB3	2:K:231:ARG:NH1	2.32	0.44
2:L:20:VAL:HG23	2:L:74:VAL:HG21	1.99	0.44
2:J:514:MET:O	2:J:517:THR:HG22	2.18	0.44
2:K:20:VAL:CG2	2:K:74:VAL:HG21	2.47	0.44
2:P:124:VAL:HG21	2:P:508:ALA:HB2	2.00	0.44
2:N:16:MET:O	2:N:20:VAL:HG12	2.17	0.44
2:P:90:THR:H	3:P:603:ANP:HNB1	1.64	0.44
2:J:20:VAL:HG23	2:J:74:VAL:HG21	1.99	0.44
2:L:20:VAL:CG2	2:L:74:VAL:HG21	2.47	0.44
2:I:230:ILE:O	2:I:231:ARG:C	2.58	0.44
2:c:233:MET:HE3	2:c:233:MET:HB3	1.94	0.44
2:G:514:MET:O	2:G:517:THR:HG22	2.18	0.44
2:V:169:VAL:CG2	2:V:377:ALA:HB2	2.46	0.44
2:Z:124:VAL:HG21	2:Z:508:ALA:HB2	1.99	0.44
2:X:124:VAL:HG21	2:X:508:ALA:HB2	1.99	0.43
2:I:20:VAL:HG23	2:I:74:VAL:HG21	1.99	0.43
2:I:306:GLY:O	2:I:307:MET:C	2.61	0.43
2:K:16:MET:O	2:K:20:VAL:HG12	2.18	0.43
2:L:169:VAL:CG2	2:L:377:ALA:HB2	2.47	0.43
2:N:169:VAL:CG2	2:N:377:ALA:HB2	2.48	0.43
2:X:169:VAL:CG2	2:X:377:ALA:HB2	2.45	0.43
2:K:415:GLY:H	3:K:600:ANP:HO2'	1.60	0.43
2:L:436:GLN:O	2:L:440:ILE:HG13	2.18	0.43
2:G:292:ILE:O	2:G:296:THR:HG22	2.19	0.43
2:L:16:MET:O	2:L:20:VAL:HG12	2.18	0.43
2:I:436:GLN:O	2:I:440:ILE:HG13	2.19	0.43
2:K:436:GLN:O	2:K:440:ILE:HG13	2.18	0.43
1:Y:255:ARG:NH2	2:Z:304:GLU:OE1	2.51	0.43
2:Z:304:GLU:C	2:Z:306:GLY:N	2.77	0.43
2:L:514:MET:O	2:L:517:THR:HG22	2.19	0.43
2:N:204:PHE:CD2	2:N:274:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:514:MET:O	2:N:517:THR:HG22	2.19	0.43
2:R:304:GLU:O	2:R:305:ILE:HD13	2.19	0.43
2:G:168:LYS:HE2	2:G:168:LYS:HB2	1.88	0.43
2:G:513:LEU:HD23	2:G:513:LEU:HA	1.88	0.43
2:L:204:PHE:HE1	2:L:263:VAL:HA	1.84	0.43
2:P:313:THR:N	2:P:316:ASP:OD2	2.45	0.43
2:T:20:VAL:HG23	2:T:74:VAL:HG21	2.01	0.43
2:V:295:LEU:HD23	2:V:295:LEU:HA	1.88	0.43
2:b:124:VAL:HG21	2:b:508:ALA:HB2	1.99	0.43
2:c:313:THR:N	2:c:316:ASP:OD2	2.44	0.42
2:I:305:ILE:O	2:I:305:ILE:HG22	2.19	0.42
2:I:514:MET:O	2:I:517:THR:HG22	2.19	0.42
2:L:230:ILE:O	2:L:231:ARG:C	2.59	0.42
2:V:124:VAL:HG21	2:V:508:ALA:HB2	2.01	0.42
2:T:124:VAL:HG21	2:T:508:ALA:HB2	2.00	0.42
2:X:294:THR:CG2	2:X:342:ILE:HD13	2.42	0.42
2:K:200:LEU:HD21	2:K:277:LYS:HG3	2.01	0.42
2:R:313:THR:N	2:R:316:ASP:OD2	2.45	0.42
2:I:204:PHE:HE1	2:I:263:VAL:HA	1.84	0.42
2:J:57:ALA:O	2:J:75:LYS:HD2	2.19	0.42
2:P:415:GLY:H	3:P:603:ANP:HO2'	1.63	0.42
2:K:169:VAL:CG2	2:K:377:ALA:HB2	2.48	0.42
2:L:40:LEU:HD23	2:N:521:VAL:HB	2.02	0.42
2:T:17:LEU:HA	2:T:20:VAL:HG12	2.02	0.42
2:Z:169:VAL:CG2	2:Z:377:ALA:HB2	2.46	0.42
2:Z:306:GLY:O	2:Z:307:MET:C	2.62	0.42
2:J:436:GLN:O	2:J:440:ILE:HG13	2.20	0.42
2:N:230:ILE:O	2:N:231:ARG:C	2.58	0.42
2:N:292:ILE:O	2:N:296:THR:HG22	2.20	0.42
2:R:124:VAL:HG21	2:R:508:ALA:HB2	2.01	0.42
3:T:603:ANP:O1B	3:T:603:ANP:O3G	2.37	0.42
2:X:77:VAL:HG21	2:X:510:VAL:HB	2.02	0.42
2:I:295:LEU:HD23	2:I:295:LEU:HA	1.86	0.42
2:G:436:GLN:O	2:G:440:ILE:HG13	2.19	0.41
2:N:306:GLY:O	2:N:307:MET:C	2.61	0.41
2:Z:233:MET:HE3	2:Z:233:MET:HB3	1.94	0.41
2:b:233:MET:HE3	2:b:233:MET:HB3	1.94	0.41
2:b:372:LEU:HD23	2:b:372:LEU:HA	1.93	0.41
2:P:77:VAL:HG11	2:P:510:VAL:HB	2.02	0.41
2:P:169:VAL:CG2	2:P:377:ALA:HB2	2.45	0.41
2:K:287:ALA:HB1	2:K:368:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:66:PHE:HD1	2:R:520:MET:HE2	1.84	0.41
2:R:372:LEU:HD23	2:R:372:LEU:HA	1.93	0.41
2:V:20:VAL:HG23	2:V:74:VAL:HG21	2.02	0.41
2:X:16:MET:O	2:X:20:VAL:HG12	2.20	0.41
2:Z:493:ILE:C	2:Z:494:LEU:HD12	2.46	0.41
2:G:200:LEU:HD21	2:G:277:LYS:HG3	2.02	0.41
2:L:168:LYS:HB2	2:L:168:LYS:HE2	1.87	0.41
2:T:20:VAL:CG2	2:T:74:VAL:HG21	2.51	0.41
2:b:415:GLY:H	3:b:603:ANP:HO2'	1.65	0.41
2:N:168:LYS:HE2	2:N:168:LYS:HB2	1.87	0.41
2:R:16:MET:HE3	2:R:520:MET:SD	2.61	0.41
2:c:20:VAL:CG2	2:c:74:VAL:HG21	2.51	0.41
2:J:169:VAL:CG2	2:J:377:ALA:HB2	2.47	0.41
2:K:57:ALA:O	2:K:75:LYS:HD2	2.20	0.41
2:L:292:ILE:O	2:L:296:THR:HG22	2.21	0.41
2:N:436:GLN:O	2:N:440:ILE:HG13	2.20	0.41
2:P:494:LEU:C	2:P:494:LEU:HD12	2.45	0.41
2:R:20:VAL:HG23	2:R:74:VAL:HG21	2.03	0.41
2:R:233:MET:HE3	2:R:233:MET:HB3	1.94	0.41
2:V:20:VAL:CG2	2:V:74:VAL:HG21	2.50	0.41
2:V:313:THR:N	2:V:316:ASP:OD2	2.45	0.41
2:I:200:LEU:HD21	2:I:277:LYS:HG3	2.03	0.41
2:K:124:VAL:HG21	2:K:508:ALA:CB	2.51	0.41
2:N:27:VAL:HG12	2:N:90:THR:HG23	2.01	0.41
2:V:16:MET:HE3	2:V:520:MET:SD	2.61	0.41
2:b:16:MET:O	2:b:20:VAL:HG12	2.20	0.41
2:b:90:THR:H	3:b:603:ANP:HNB1	1.68	0.41
2:c:169:VAL:CG2	2:c:377:ALA:HB2	2.46	0.41
2:N:372:LEU:HD23	2:N:372:LEU:HA	1.95	0.41
2:P:415:GLY:HA2	3:P:603:ANP:H1'	2.03	0.41
2:X:295:LEU:HA	2:X:342:ILE:HD11	2.01	0.41
2:Z:20:VAL:HG23	2:Z:74:VAL:HG21	2.01	0.41
2:b:20:VAL:CG2	2:b:74:VAL:HG21	2.51	0.41
2:G:521:VAL:HB	2:N:40:LEU:HD23	2.03	0.41
2:I:40:LEU:HD23	2:J:521:VAL:HB	2.02	0.41
2:J:102:GLU:HB2	2:J:442:VAL:HG13	2.02	0.41
2:J:342:ILE:H	2:J:342:ILE:HG12	1.70	0.41
2:K:162:ILE:HD12	2:K:400:LEU:HD13	2.03	0.41
2:N:124:VAL:HG21	2:N:508:ALA:CB	2.51	0.41
2:N:287:ALA:HB1	2:N:368:ARG:CZ	2.51	0.41
2:P:17:LEU:HA	2:P:20:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:233:MET:HE3	2:P:233:MET:HB3	1.93	0.41
2:R:17:LEU:HA	2:R:20:VAL:HG12	2.03	0.41
2:R:415:GLY:HA2	3:R:603:ANP:H1'	2.02	0.41
2:V:102:GLU:HB2	2:V:442:VAL:HG13	2.03	0.41
2:X:17:LEU:HA	2:X:20:VAL:HG12	2.03	0.41
2:Z:20:VAL:CG2	2:Z:74:VAL:HG21	2.51	0.41
2:Z:313:THR:N	2:Z:316:ASP:OD2	2.44	0.41
2:I:292:ILE:O	2:I:296:THR:HG22	2.21	0.41
2:J:231:ARG:O	2:J:232:GLU:C	2.64	0.41
2:R:77:VAL:HG21	2:R:510:VAL:HB	2.02	0.41
2:V:17:LEU:HA	2:V:20:VAL:HG12	2.03	0.41
2:V:66:PHE:HD1	2:V:520:MET:HE2	1.85	0.41
2:c:16:MET:HE3	2:c:520:MET:SD	2.61	0.41
2:J:303:GLU:O	2:J:306:GLY:HA2	2.22	0.40
2:T:233:MET:HE3	2:T:233:MET:HB3	1.94	0.40
2:X:20:VAL:HG23	2:X:74:VAL:HG21	2.01	0.40
2:c:16:MET:O	2:c:20:VAL:HG12	2.20	0.40
2:c:90:THR:H	3:c:603:ANP:HNB1	1.68	0.40
2:G:124:VAL:HG21	2:G:508:ALA:CB	2.51	0.40
2:G:202:PRO:O	2:G:205:ILE:HG12	2.20	0.40
2:I:169:VAL:CG2	2:I:377:ALA:HB2	2.47	0.40
2:I:229:ASN:HB2	2:I:231:ARG:HE	1.86	0.40
2:L:26:ALA:HA	2:N:8:PHE:HE1	1.86	0.40
2:X:16:MET:HE3	2:X:520:MET:SD	2.61	0.40
2:X:20:VAL:CG2	2:X:74:VAL:HG21	2.50	0.40
2:b:16:MET:HE3	2:b:520:MET:SD	2.62	0.40
2:I:364:LYS:HD3	2:I:364:LYS:HA	1.85	0.40
2:N:142:LYS:O	2:N:146:GLN:HG3	2.22	0.40
2:V:16:MET:O	2:V:20:VAL:HG12	2.21	0.40
2:c:95:LEU:O	2:c:99:ILE:HG13	2.21	0.40
2:G:233:MET:HE3	2:G:233:MET:HB3	2.01	0.40
2:P:20:VAL:HG23	2:P:74:VAL:HG21	2.03	0.40
2:R:77:VAL:HG11	2:R:510:VAL:HB	2.04	0.40
2:R:494:LEU:C	2:R:494:LEU:HD12	2.46	0.40
2:Z:17:LEU:HA	2:Z:20:VAL:HG12	2.03	0.40
2:b:102:GLU:HB2	2:b:442:VAL:HG13	2.03	0.40
2:I:69:MET:HE2	2:b:39:VAL:CG1	2.51	0.40
2:I:342:ILE:H	2:I:342:ILE:HG12	1.71	0.40
2:J:494:LEU:O	2:J:494:LEU:HD12	2.21	0.40
2:L:124:VAL:HG21	2:L:508:ALA:CB	2.52	0.40
2:L:364:LYS:HA	2:L:364:LYS:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:200:LEU:HD21	2:N:277:LYS:HG3	2.03	0.40
2:N:287:ALA:HB1	2:N:368:ARG:NH2	2.37	0.40
2:X:95:LEU:O	2:X:99:ILE:HG13	2.21	0.40
2:X:436:GLN:O	2:X:440:ILE:HG13	2.22	0.40
2:Z:16:MET:O	2:Z:20:VAL:HG12	2.21	0.40
2:b:17:LEU:HA	2:b:20:VAL:HG12	2.03	0.40
2:c:20:VAL:HG23	2:c:74:VAL:HG21	2.03	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	A	86/284 (30%)	86 (100%)	0	0	100	100
1	B	86/284 (30%)	86 (100%)	0	0	100	100
1	C	86/284 (30%)	86 (100%)	0	0	100	100
1	D	86/284 (30%)	86 (100%)	0	0	100	100
1	E	86/284 (30%)	86 (100%)	0	0	100	100
1	F	86/284 (30%)	86 (100%)	0	0	100	100
1	M	86/284 (30%)	86 (100%)	0	0	100	100
1	O	86/284 (30%)	86 (100%)	0	0	100	100
1	Q	86/284 (30%)	86 (100%)	0	0	100	100
1	S	86/284 (30%)	86 (100%)	0	0	100	100
1	U	86/284 (30%)	86 (100%)	0	0	100	100
1	W	86/284 (30%)	86 (100%)	0	0	100	100
1	Y	86/284 (30%)	86 (100%)	0	0	100	100
1	a	86/284 (30%)	86 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	522/548 (95%)	520 (100%)	2 (0%)	0	100	100
2	I	522/548 (95%)	520 (100%)	2 (0%)	0	100	100
2	J	522/548 (95%)	518 (99%)	4 (1%)	0	100	100
2	K	522/548 (95%)	520 (100%)	2 (0%)	0	100	100
2	L	522/548 (95%)	519 (99%)	3 (1%)	0	100	100
2	N	522/548 (95%)	518 (99%)	4 (1%)	0	100	100
2	P	522/548 (95%)	519 (99%)	3 (1%)	0	100	100
2	R	522/548 (95%)	519 (99%)	3 (1%)	0	100	100
2	T	522/548 (95%)	517 (99%)	4 (1%)	1 (0%)	43	62
2	V	522/548 (95%)	519 (99%)	3 (1%)	0	100	100
2	X	522/548 (95%)	518 (99%)	4 (1%)	0	100	100
2	Z	522/548 (95%)	515 (99%)	6 (1%)	1 (0%)	43	62
2	b	522/548 (95%)	517 (99%)	4 (1%)	1 (0%)	43	62
2	c	522/548 (95%)	517 (99%)	4 (1%)	1 (0%)	43	62
All	All	8512/11648 (73%)	8460 (99%)	48 (1%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	307	MET
2	b	307	MET
2	c	307	MET
2	T	305	ILE

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	69/238 (29%)	69 (100%)	0	100	100
1	B	69/238 (29%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	69/238 (29%)	69 (100%)	0	100	100
1	D	69/238 (29%)	69 (100%)	0	100	100
1	E	69/238 (29%)	69 (100%)	0	100	100
1	F	69/238 (29%)	69 (100%)	0	100	100
1	M	69/238 (29%)	69 (100%)	0	100	100
1	O	69/238 (29%)	69 (100%)	0	100	100
1	Q	69/238 (29%)	69 (100%)	0	100	100
1	S	69/238 (29%)	69 (100%)	0	100	100
1	U	69/238 (29%)	69 (100%)	0	100	100
1	W	69/238 (29%)	69 (100%)	0	100	100
1	Y	69/238 (29%)	69 (100%)	0	100	100
1	a	69/238 (29%)	69 (100%)	0	100	100
2	G	404/415 (97%)	404 (100%)	0	100	100
2	I	404/415 (97%)	404 (100%)	0	100	100
2	J	404/415 (97%)	404 (100%)	0	100	100
2	K	404/415 (97%)	403 (100%)	1 (0%)	87	94
2	L	404/415 (97%)	404 (100%)	0	100	100
2	N	404/415 (97%)	404 (100%)	0	100	100
2	P	404/415 (97%)	404 (100%)	0	100	100
2	R	404/415 (97%)	404 (100%)	0	100	100
2	T	404/415 (97%)	404 (100%)	0	100	100
2	V	404/415 (97%)	404 (100%)	0	100	100
2	X	404/415 (97%)	404 (100%)	0	100	100
2	Z	404/415 (97%)	404 (100%)	0	100	100
2	b	404/415 (97%)	404 (100%)	0	100	100
2	c	404/415 (97%)	404 (100%)	0	100	100
All	All	6622/9142 (72%)	6621 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	B	206	GLN
1	C	203	GLN
1	C	206	GLN
1	D	206	GLN
1	D	278	GLN
1	E	206	GLN
1	E	278	GLN
1	F	206	GLN
2	G	10	ASN
2	G	72	GLN
2	G	290	GLN
2	I	72	GLN
2	I	290	GLN
2	J	72	GLN
2	J	290	GLN
2	K	72	GLN
2	K	290	GLN
2	L	72	GLN
2	L	290	GLN
1	M	206	GLN
1	M	278	GLN
2	N	72	GLN
2	N	290	GLN
1	O	206	GLN
2	P	37	ASN
2	P	72	GLN
2	P	82	ASN
2	P	290	GLN
1	Q	203	GLN
1	Q	206	GLN
2	R	37	ASN
2	R	72	GLN
2	R	82	ASN
2	R	290	GLN
1	S	203	GLN
1	S	206	GLN
2	T	37	ASN
2	T	72	GLN
2	T	82	ASN
2	T	290	GLN

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Mol	Chain	Res	Type
1	U	203	GLN
1	U	206	GLN
2	V	37	ASN
2	V	72	GLN
2	V	82	ASN
2	V	290	GLN
1	W	203	GLN
1	W	206	GLN
2	X	37	ASN
2	X	72	GLN
2	X	82	ASN
2	X	290	GLN
1	Y	206	GLN
2	Z	37	ASN
2	Z	72	GLN
2	Z	82	ASN
2	Z	290	GLN
1	a	206	GLN
2	b	72	GLN
2	b	82	ASN
2	b	290	GLN
2	c	37	ASN
2	c	72	GLN
2	c	82	ASN
2	c	290	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 28 are monoatomic - leaving 14 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
3	ANP	R	603	4	32,33,33	0.99	5 (15%)	44,52,52	0.75	2 (4%)
3	ANP	J	603	4,5	32,33,33	0.98	4 (12%)	44,52,52	0.84	2 (4%)
3	ANP	L	603	4,5	32,33,33	1.00	4 (12%)	44,52,52	0.85	2 (4%)
3	ANP	c	603	4,5	32,33,33	0.99	5 (15%)	44,52,52	0.84	2 (4%)
3	ANP	Z	603	4	32,33,33	0.91	4 (12%)	44,52,52	0.86	2 (4%)
3	ANP	P	603	4,5	32,33,33	1.00	5 (15%)	44,52,52	0.84	2 (4%)
3	ANP	V	602	4	32,33,33	0.99	5 (15%)	44,52,52	0.75	2 (4%)
3	ANP	X	602	4,5	32,33,33	1.01	4 (12%)	44,52,52	0.81	2 (4%)
3	ANP	I	603	4,5	32,33,33	0.96	4 (12%)	44,52,52	0.82	2 (4%)
3	ANP	N	601	4,5	32,33,33	0.97	3 (9%)	44,52,52	0.81	2 (4%)
3	ANP	b	603	4,5	32,33,33	0.98	5 (15%)	44,52,52	0.84	2 (4%)
3	ANP	T	603	4	32,33,33	0.90	4 (12%)	44,52,52	0.83	2 (4%)
3	ANP	G	600	4,5	32,33,33	0.96	4 (12%)	44,52,52	0.85	1 (2%)
3	ANP	K	600	4,5	32,33,33	0.97	4 (12%)	44,52,52	0.82	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	R	603	4	-	6/18/38/38	0/3/3/3
3	ANP	J	603	4,5	-	6/18/38/38	0/3/3/3
3	ANP	L	603	4,5	-	8/18/38/38	0/3/3/3
3	ANP	c	603	4,5	-	7/18/38/38	0/3/3/3
3	ANP	Z	603	4	-	5/18/38/38	0/3/3/3
3	ANP	P	603	4,5	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	V	602	4	-	6/18/38/38	0/3/3/3
3	ANP	X	602	4,5	-	7/18/38/38	0/3/3/3
3	ANP	I	603	4,5	-	9/18/38/38	0/3/3/3
3	ANP	N	601	4,5	-	10/18/38/38	0/3/3/3
3	ANP	b	603	4,5	-	7/18/38/38	0/3/3/3
3	ANP	T	603	4	-	4/18/38/38	0/3/3/3
3	ANP	G	600	4,5	-	5/18/38/38	0/3/3/3
3	ANP	K	600	4,5	-	9/18/38/38	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	602	ANP	PB-O3A	-2.87	1.55	1.59
3	L	603	ANP	PB-O3A	-2.87	1.55	1.59
3	J	603	ANP	PB-O3A	-2.86	1.55	1.59
3	b	603	ANP	PG-N3B	2.81	1.70	1.63
3	R	603	ANP	PG-N3B	2.80	1.70	1.63
3	L	603	ANP	PG-N3B	2.79	1.70	1.63
3	V	602	ANP	PG-N3B	2.79	1.70	1.63
3	c	603	ANP	PG-N3B	2.79	1.70	1.63
3	P	603	ANP	PB-O3A	-2.79	1.55	1.59
3	I	603	ANP	PB-O3A	-2.77	1.55	1.59
3	P	603	ANP	PG-N3B	2.77	1.70	1.63
3	X	602	ANP	PG-N3B	2.76	1.70	1.63
3	J	603	ANP	PG-N3B	2.74	1.70	1.63
3	N	601	ANP	PG-N3B	2.73	1.70	1.63
3	V	602	ANP	PB-O3A	-2.73	1.55	1.59
3	K	600	ANP	PB-O3A	-2.72	1.55	1.59
3	G	600	ANP	PB-O3A	-2.71	1.55	1.59
3	R	603	ANP	PB-O3A	-2.69	1.55	1.59
3	c	603	ANP	PB-O3A	-2.66	1.55	1.59
3	N	601	ANP	PB-O3A	-2.65	1.55	1.59
3	b	603	ANP	PB-O3A	-2.65	1.55	1.59
3	Z	603	ANP	PB-O3A	-2.63	1.55	1.59
3	G	600	ANP	PG-N3B	2.62	1.70	1.63
3	K	600	ANP	PG-N3B	2.58	1.70	1.63
3	I	603	ANP	PG-N3B	2.55	1.70	1.63
3	L	603	ANP	PG-O1G	2.53	1.50	1.46
3	K	600	ANP	PG-O1G	2.50	1.50	1.46
3	c	603	ANP	PG-O1G	2.47	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	602	ANP	PG-O1G	2.44	1.50	1.46
3	T	603	ANP	PB-O3A	-2.44	1.56	1.59
3	R	603	ANP	PG-O1G	2.44	1.50	1.46
3	I	603	ANP	PG-O1G	2.43	1.50	1.46
3	G	600	ANP	PG-O1G	2.42	1.50	1.46
3	b	603	ANP	PG-O1G	2.42	1.50	1.46
3	P	603	ANP	PG-O1G	2.40	1.50	1.46
3	V	602	ANP	PG-O1G	2.40	1.50	1.46
3	N	601	ANP	PG-O1G	2.39	1.49	1.46
3	J	603	ANP	PG-O1G	2.37	1.49	1.46
3	T	603	ANP	PG-O1G	2.33	1.49	1.46
3	T	603	ANP	PG-N3B	2.33	1.69	1.63
3	Z	603	ANP	PG-N3B	2.29	1.69	1.63
3	Z	603	ANP	PG-O1G	2.28	1.49	1.46
3	X	602	ANP	PB-O1B	2.19	1.49	1.46
3	V	602	ANP	PB-O1B	2.16	1.49	1.46
3	P	603	ANP	PB-O1B	2.16	1.49	1.46
3	I	603	ANP	PB-O1B	2.10	1.49	1.46
3	b	603	ANP	PB-O1B	2.10	1.49	1.46
3	Z	603	ANP	PB-O1B	2.07	1.49	1.46
3	V	602	ANP	PB-N3B	2.06	1.68	1.63
3	J	603	ANP	PB-O1B	2.06	1.49	1.46
3	R	603	ANP	PB-O1B	2.06	1.49	1.46
3	c	603	ANP	PB-N3B	2.06	1.68	1.63
3	T	603	ANP	PB-O1B	2.05	1.49	1.46
3	G	600	ANP	PB-O1B	2.05	1.49	1.46
3	K	600	ANP	PB-O1B	2.03	1.49	1.46
3	c	603	ANP	PB-O1B	2.03	1.49	1.46
3	R	603	ANP	PB-N3B	2.03	1.68	1.63
3	b	603	ANP	PB-N3B	2.03	1.68	1.63
3	L	603	ANP	PB-O1B	2.01	1.49	1.46
3	P	603	ANP	PB-N3B	2.00	1.68	1.63

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	600	ANP	PB-O3A-PA	-4.31	117.44	132.62
3	P	603	ANP	PB-O3A-PA	-4.31	117.45	132.62
3	b	603	ANP	PB-O3A-PA	-4.17	117.94	132.62
3	c	603	ANP	PB-O3A-PA	-4.17	117.94	132.62
3	X	602	ANP	PB-O3A-PA	-4.08	118.24	132.62
3	J	603	ANP	PB-O3A-PA	-3.99	118.58	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	603	ANP	PB-O3A-PA	-3.96	118.66	132.62
3	Z	603	ANP	PB-O3A-PA	-3.85	119.04	132.62
3	K	600	ANP	PB-O3A-PA	-3.69	119.62	132.62
3	I	603	ANP	PB-O3A-PA	-3.66	119.74	132.62
3	T	603	ANP	PB-O3A-PA	-3.59	119.98	132.62
3	N	601	ANP	PB-O3A-PA	-3.57	120.04	132.62
3	V	602	ANP	PB-O3A-PA	-3.42	120.56	132.62
3	R	603	ANP	PB-O3A-PA	-3.29	121.05	132.62
3	N	601	ANP	O2G-PG-O1G	-2.25	107.80	113.45
3	K	600	ANP	O2G-PG-O1G	-2.22	107.87	113.45
3	I	603	ANP	O2G-PG-O1G	-2.20	107.91	113.45
3	R	603	ANP	O2G-PG-O1G	-2.12	108.13	113.45
3	c	603	ANP	O2G-PG-O1G	-2.11	108.14	113.45
3	Z	603	ANP	O1B-PB-N3B	-2.09	108.69	111.77
3	b	603	ANP	O2G-PG-O1G	-2.09	108.19	113.45
3	P	603	ANP	O2G-PG-O1G	-2.08	108.22	113.45
3	V	602	ANP	O2G-PG-O1G	-2.08	108.23	113.45
3	T	603	ANP	O1B-PB-N3B	-2.08	108.71	111.77
3	X	602	ANP	O2G-PG-O1G	-2.04	108.34	113.45
3	L	603	ANP	O2G-PG-O1G	-2.02	108.36	113.45
3	J	603	ANP	O2G-PG-O1G	-2.00	108.42	113.45

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	600	ANP	PG-N3B-PB-O1B
3	G	600	ANP	C5'-O5'-PA-O1A
3	G	600	ANP	C5'-O5'-PA-O2A
3	I	603	ANP	PB-N3B-PG-O1G
3	I	603	ANP	PG-N3B-PB-O1B
3	I	603	ANP	PG-N3B-PB-O3A
3	I	603	ANP	PB-O3A-PA-O5'
3	I	603	ANP	C5'-O5'-PA-O2A
3	I	603	ANP	C3'-C4'-C5'-O5'
3	J	603	ANP	PG-N3B-PB-O1B
3	J	603	ANP	C5'-O5'-PA-O1A
3	J	603	ANP	C5'-O5'-PA-O2A
3	K	600	ANP	PB-N3B-PG-O1G
3	K	600	ANP	PG-N3B-PB-O1B
3	K	600	ANP	PG-N3B-PB-O3A
3	K	600	ANP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
3	K	600	ANP	C5'-O5'-PA-O2A
3	K	600	ANP	C3'-C4'-C5'-O5'
3	L	603	ANP	PG-N3B-PB-O1B
3	L	603	ANP	PA-O3A-PB-O1B
3	L	603	ANP	PA-O3A-PB-O2B
3	L	603	ANP	C5'-O5'-PA-O1A
3	L	603	ANP	C5'-O5'-PA-O2A
3	N	601	ANP	PB-N3B-PG-O1G
3	N	601	ANP	PG-N3B-PB-O1B
3	N	601	ANP	PG-N3B-PB-O3A
3	N	601	ANP	PA-O3A-PB-O1B
3	N	601	ANP	C5'-O5'-PA-O1A
3	N	601	ANP	C5'-O5'-PA-O2A
3	N	601	ANP	C3'-C4'-C5'-O5'
3	P	603	ANP	PG-N3B-PB-O1B
3	P	603	ANP	C5'-O5'-PA-O2A
3	P	603	ANP	C3'-C4'-C5'-O5'
3	R	603	ANP	PG-N3B-PB-O1B
3	R	603	ANP	PB-O3A-PA-O5'
3	R	603	ANP	O4'-C4'-C5'-O5'
3	T	603	ANP	PB-N3B-PG-O1G
3	T	603	ANP	PG-N3B-PB-O1B
3	T	603	ANP	PA-O3A-PB-O2B
3	V	602	ANP	PG-N3B-PB-O1B
3	X	602	ANP	PG-N3B-PB-O1B
3	X	602	ANP	PB-O3A-PA-O5'
3	X	602	ANP	C5'-O5'-PA-O2A
3	X	602	ANP	C3'-C4'-C5'-O5'
3	Z	603	ANP	PB-N3B-PG-O1G
3	Z	603	ANP	PG-N3B-PB-O1B
3	Z	603	ANP	PG-N3B-PB-O3A
3	Z	603	ANP	PA-O3A-PB-O2B
3	b	603	ANP	PG-N3B-PB-O1B
3	b	603	ANP	C5'-O5'-PA-O2A
3	b	603	ANP	C3'-C4'-C5'-O5'
3	c	603	ANP	PG-N3B-PB-O1B
3	c	603	ANP	C5'-O5'-PA-O2A
3	c	603	ANP	C3'-C4'-C5'-O5'
3	I	603	ANP	O4'-C4'-C5'-O5'
3	K	600	ANP	O4'-C4'-C5'-O5'
3	L	603	ANP	C3'-C4'-C5'-O5'
3	R	603	ANP	C3'-C4'-C5'-O5'

Continued on next page...

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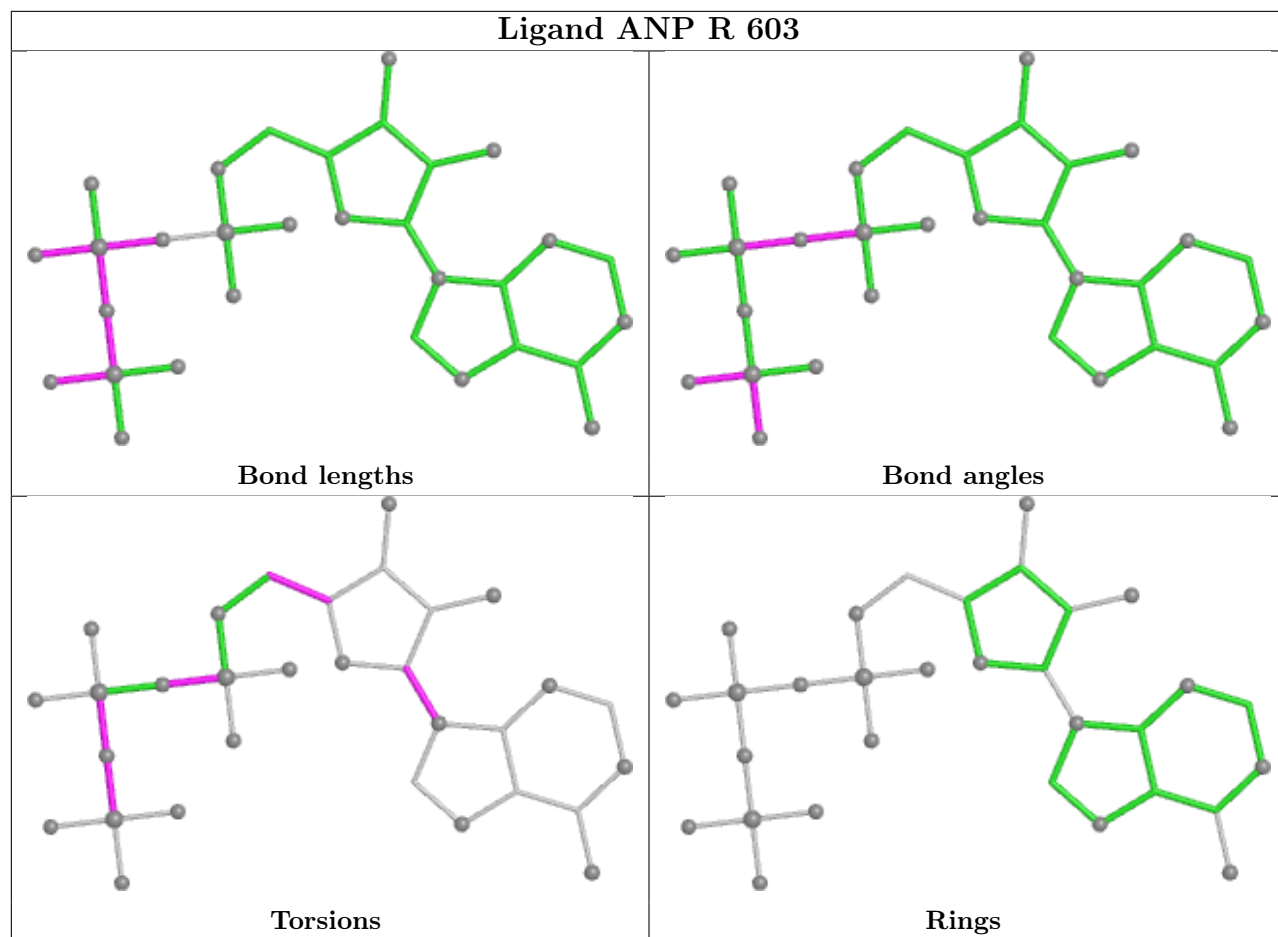
Mol	Chain	Res	Type	Atoms
3	J	603	ANP	C3'-C4'-C5'-O5'
3	G	600	ANP	C3'-C4'-C5'-O5'
3	P	603	ANP	O4'-C4'-C5'-O5'
3	N	601	ANP	O4'-C4'-C5'-O5'
3	X	602	ANP	O4'-C4'-C5'-O5'
3	b	603	ANP	O4'-C4'-C5'-O5'
3	c	603	ANP	O4'-C4'-C5'-O5'
3	P	603	ANP	PB-O3A-PA-O5'
3	V	602	ANP	PB-O3A-PA-O5'
3	b	603	ANP	PB-O3A-PA-O5'
3	c	603	ANP	PB-O3A-PA-O5'
3	V	602	ANP	O4'-C4'-C5'-O5'
3	I	603	ANP	C5'-O5'-PA-O3A
3	K	600	ANP	C5'-O5'-PA-O3A
3	L	603	ANP	C5'-O5'-PA-O3A
3	P	603	ANP	C5'-O5'-PA-O3A
3	X	602	ANP	C5'-O5'-PA-O3A
3	b	603	ANP	C5'-O5'-PA-O3A
3	c	603	ANP	C5'-O5'-PA-O3A
3	V	602	ANP	C2'-C1'-N9-C8
3	I	603	ANP	C5'-O5'-PA-O1A
3	K	600	ANP	C5'-O5'-PA-O1A
3	P	603	ANP	C5'-O5'-PA-O1A
3	X	602	ANP	C5'-O5'-PA-O1A
3	b	603	ANP	C5'-O5'-PA-O1A
3	c	603	ANP	C5'-O5'-PA-O1A
3	L	603	ANP	O4'-C4'-C5'-O5'
3	Z	603	ANP	C3'-C4'-C5'-O5'
3	J	603	ANP	O4'-C4'-C5'-O5'
3	N	601	ANP	PA-O3A-PB-O2B
3	V	602	ANP	C3'-C4'-C5'-O5'
3	R	603	ANP	C2'-C1'-N9-C8
3	G	600	ANP	C5'-O5'-PA-O3A
3	J	603	ANP	C5'-O5'-PA-O3A
3	N	601	ANP	C5'-O5'-PA-O3A
3	V	602	ANP	O4'-C1'-N9-C8
3	R	603	ANP	PB-N3B-PG-O1G
3	T	603	ANP	PG-N3B-PB-O3A

There are no ring outliers.

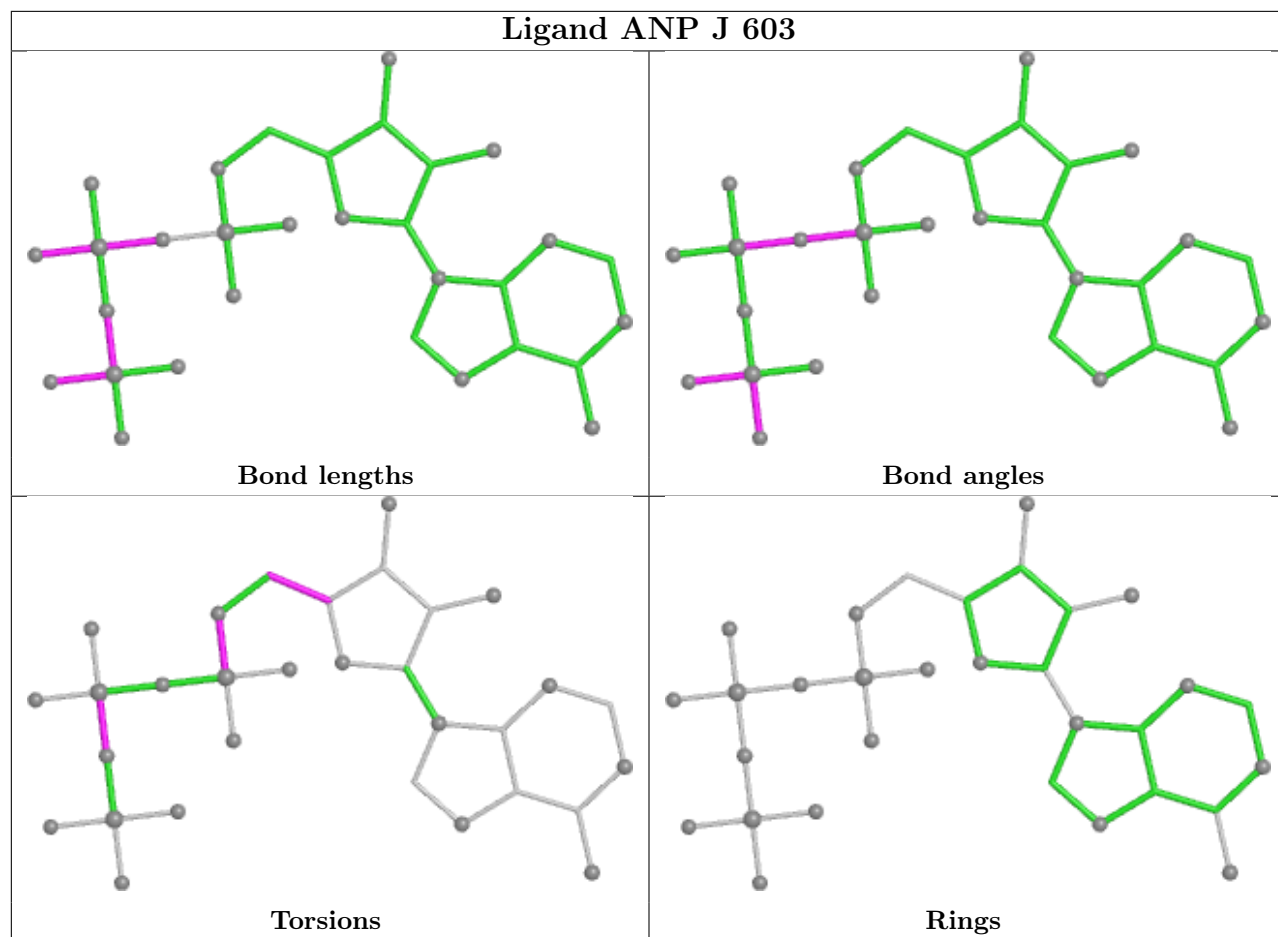
11 monomers are involved in 16 short contacts:

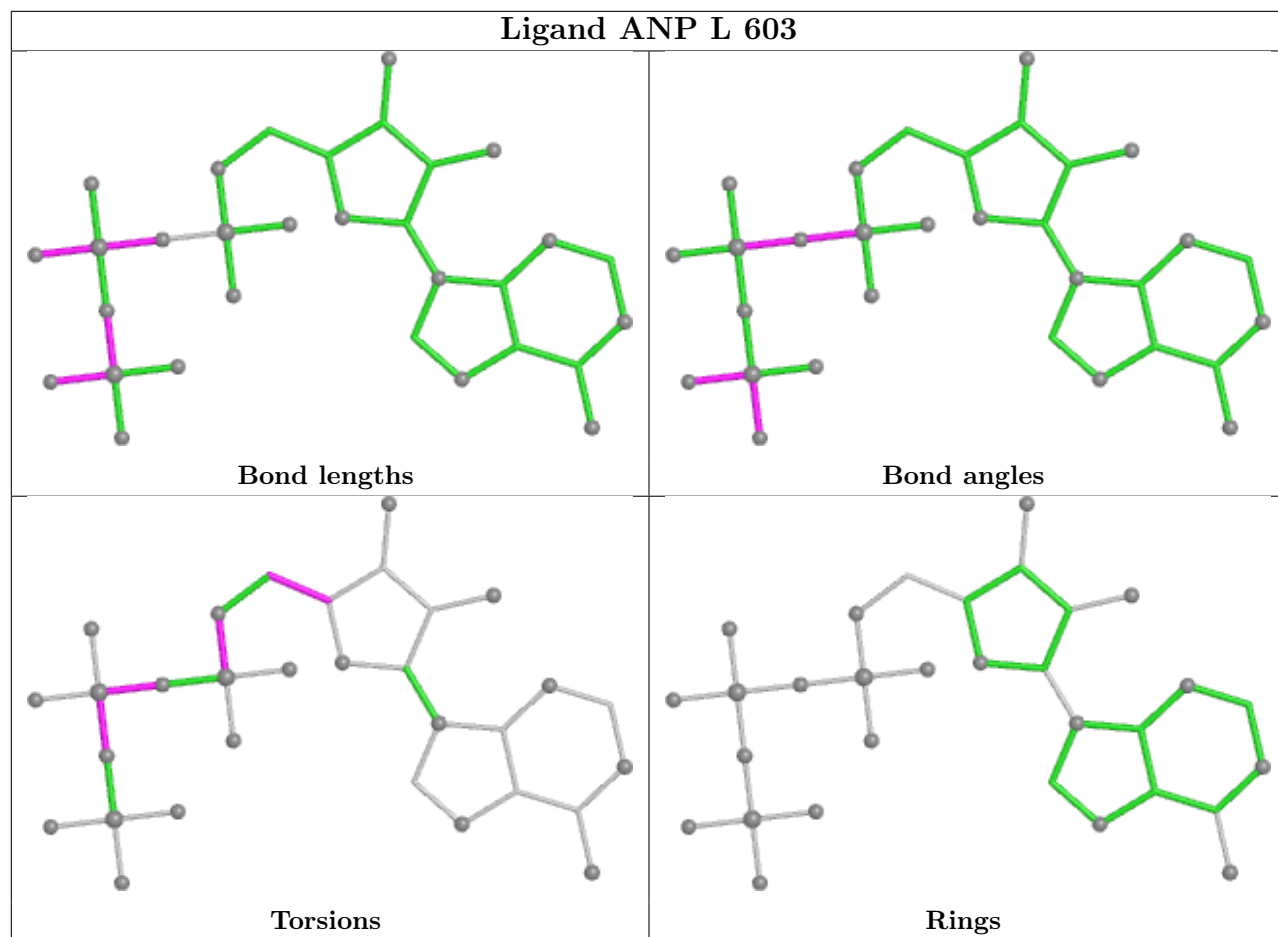
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	603	ANP	2	0
3	J	603	ANP	1	0
3	c	603	ANP	1	0
3	Z	603	ANP	1	0
3	P	603	ANP	3	0
3	V	602	ANP	1	0
3	X	602	ANP	1	0
3	b	603	ANP	2	0
3	T	603	ANP	2	0
3	G	600	ANP	1	0
3	K	600	ANP	1	0

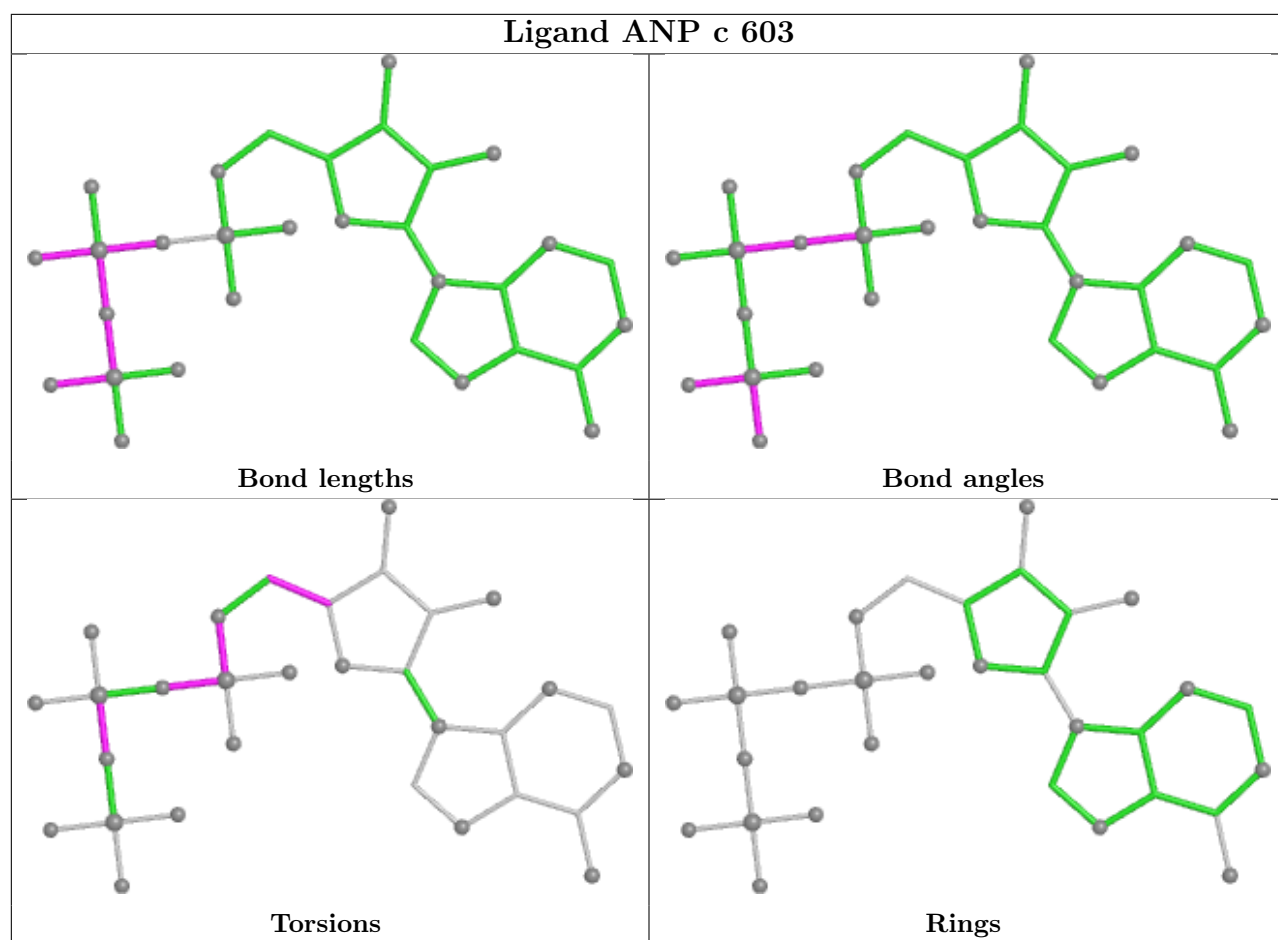
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

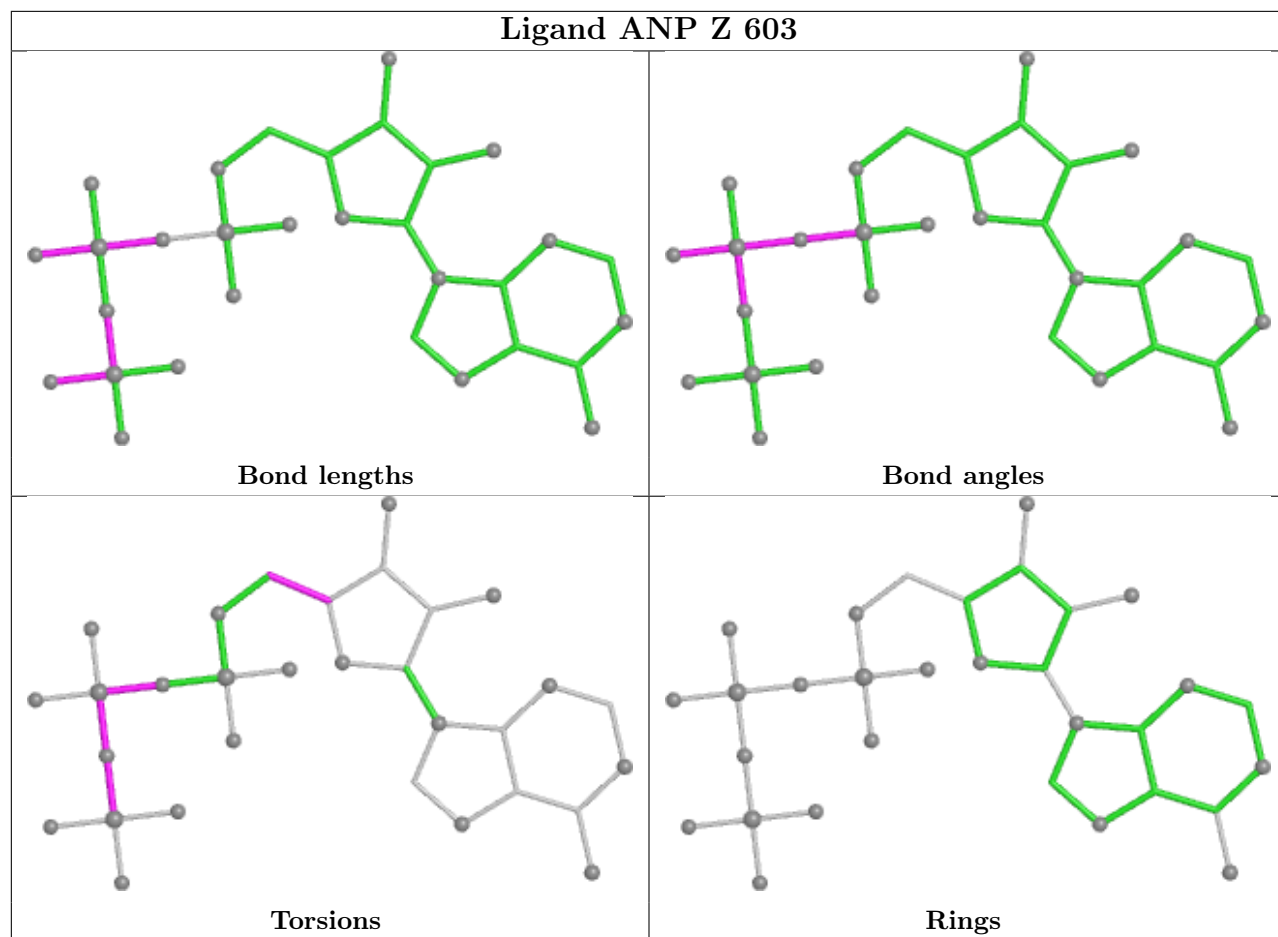


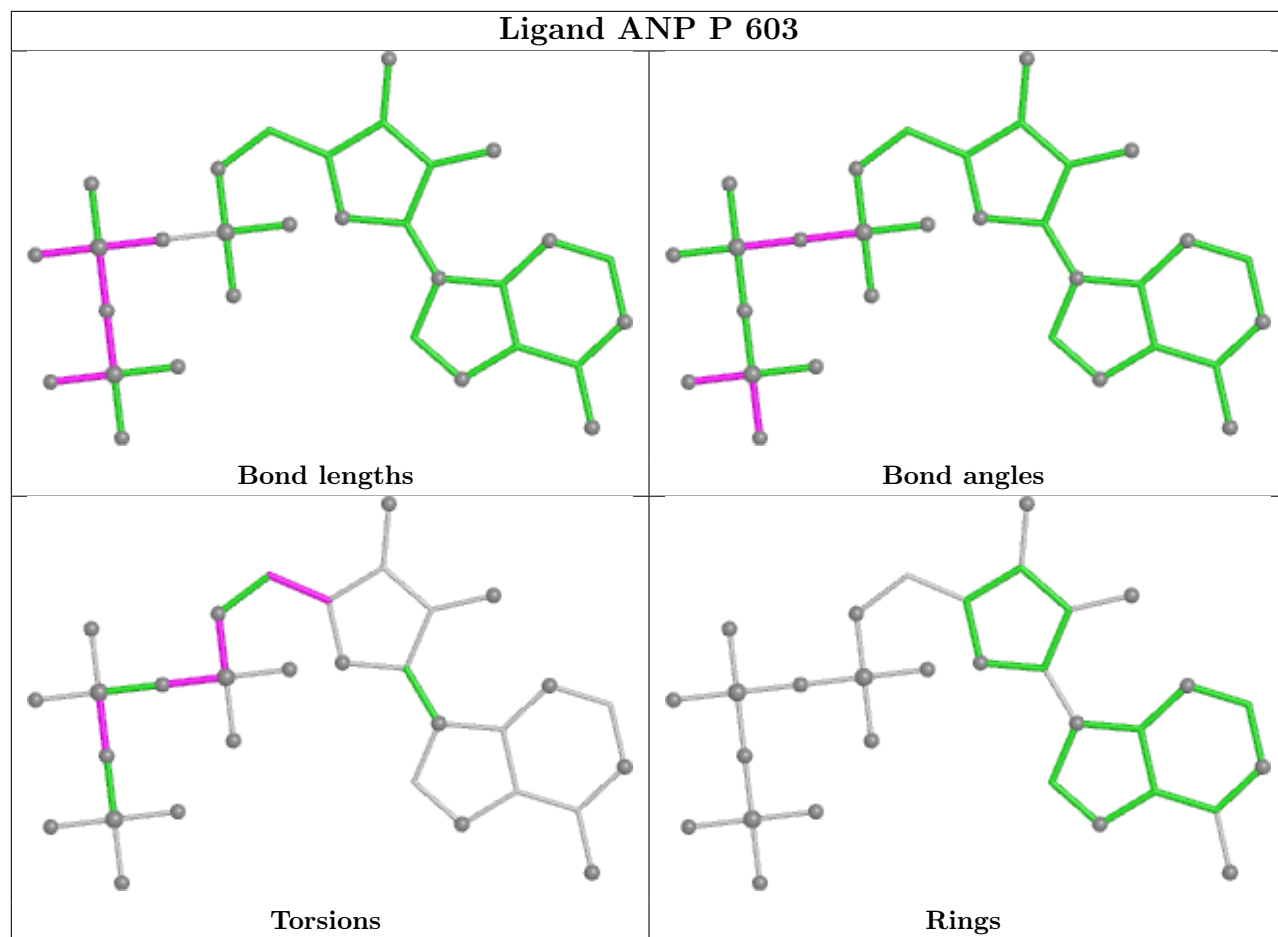
Ligand ANP J 603







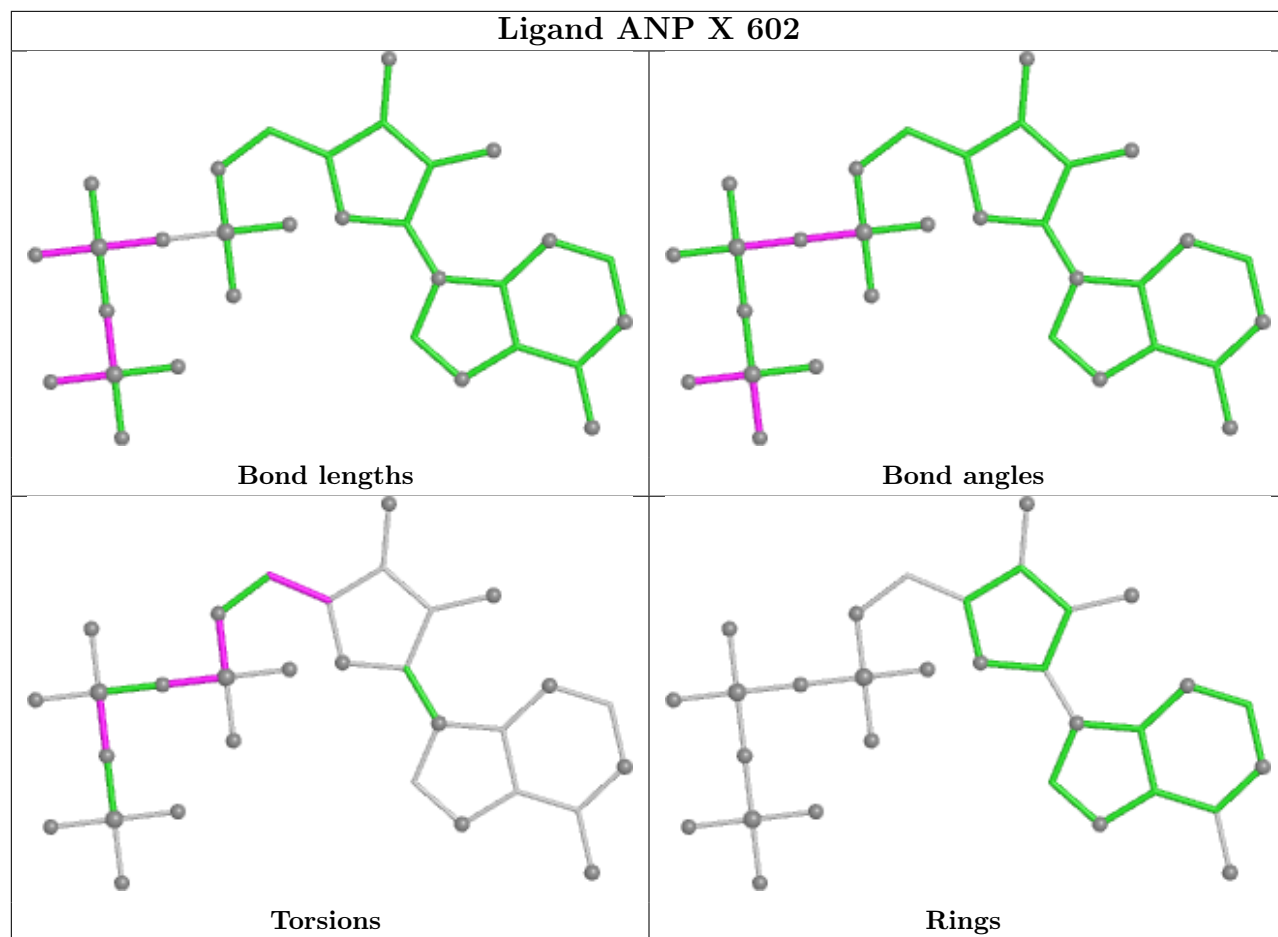




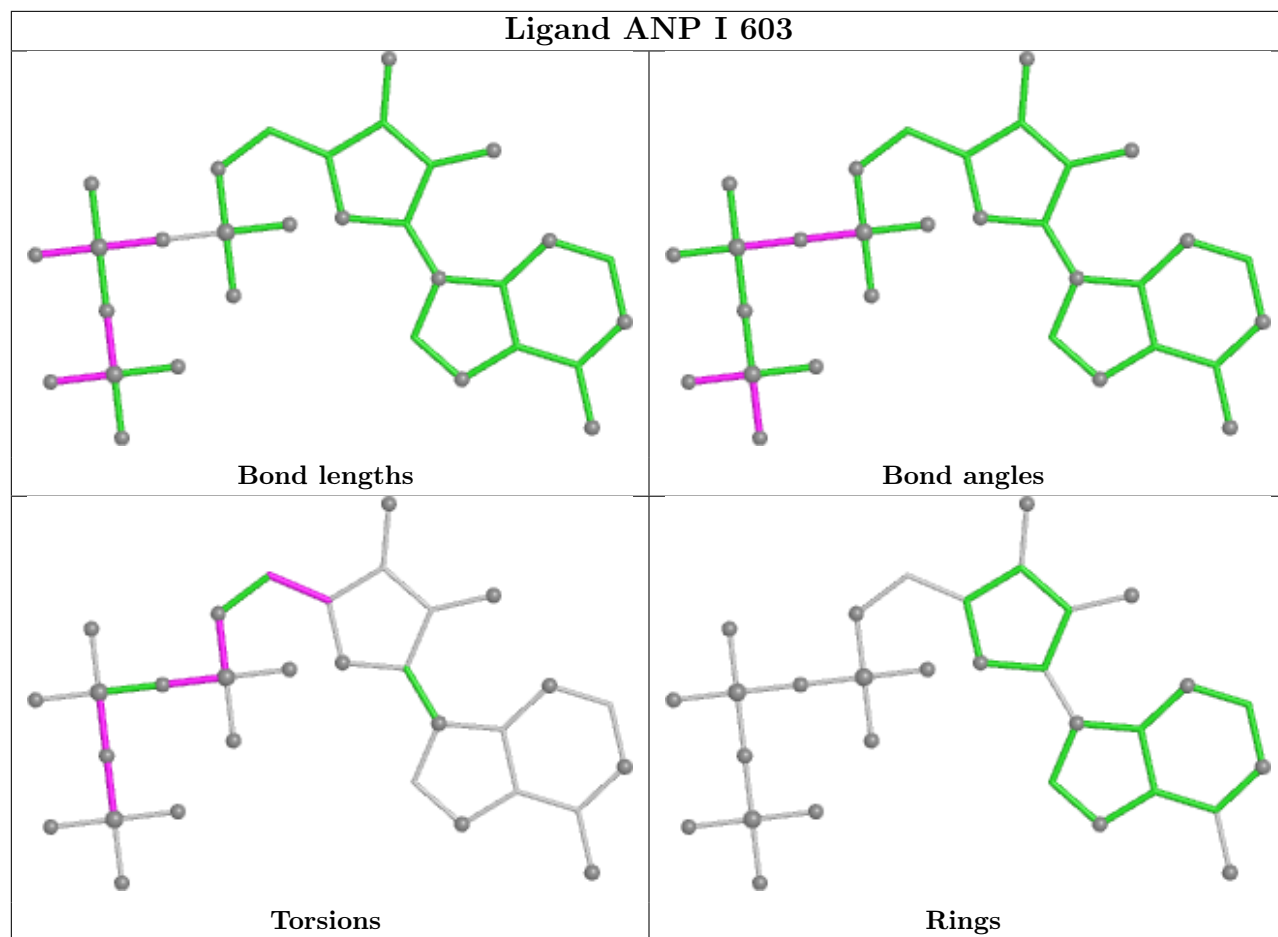
Ligand ANP V 602

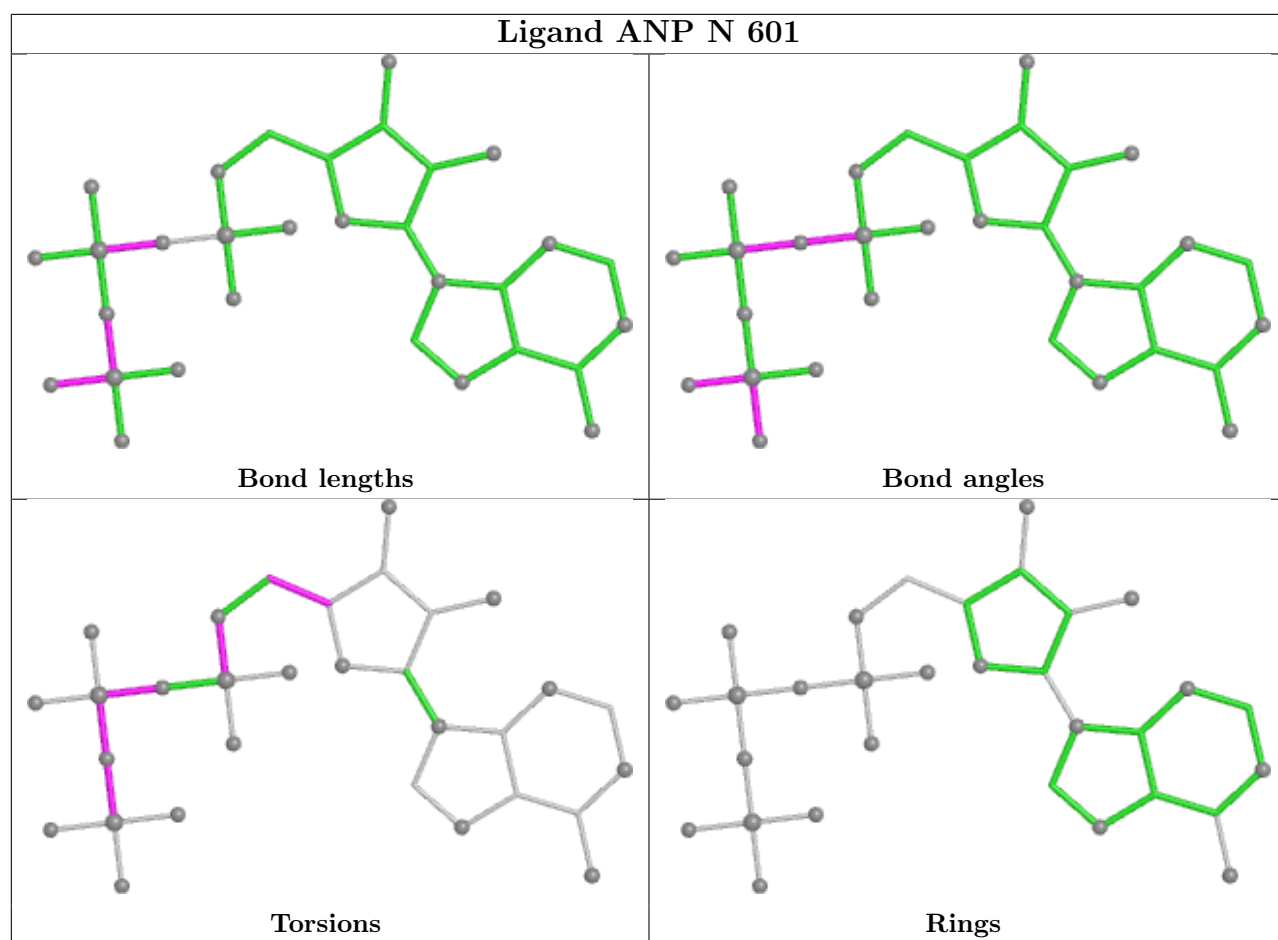
The figure displays four panels of structural analysis for Ligand ANP V 602. Each panel shows a 3D ball-and-stick model of the ligand, which consists of a central metal complex (two metal atoms, likely copper, coordinated by two nitrogen atoms and two oxygen atoms) and a large organic ligand system (a fused ring system, likely a porphyrin derivative). The panels are labeled as follows:

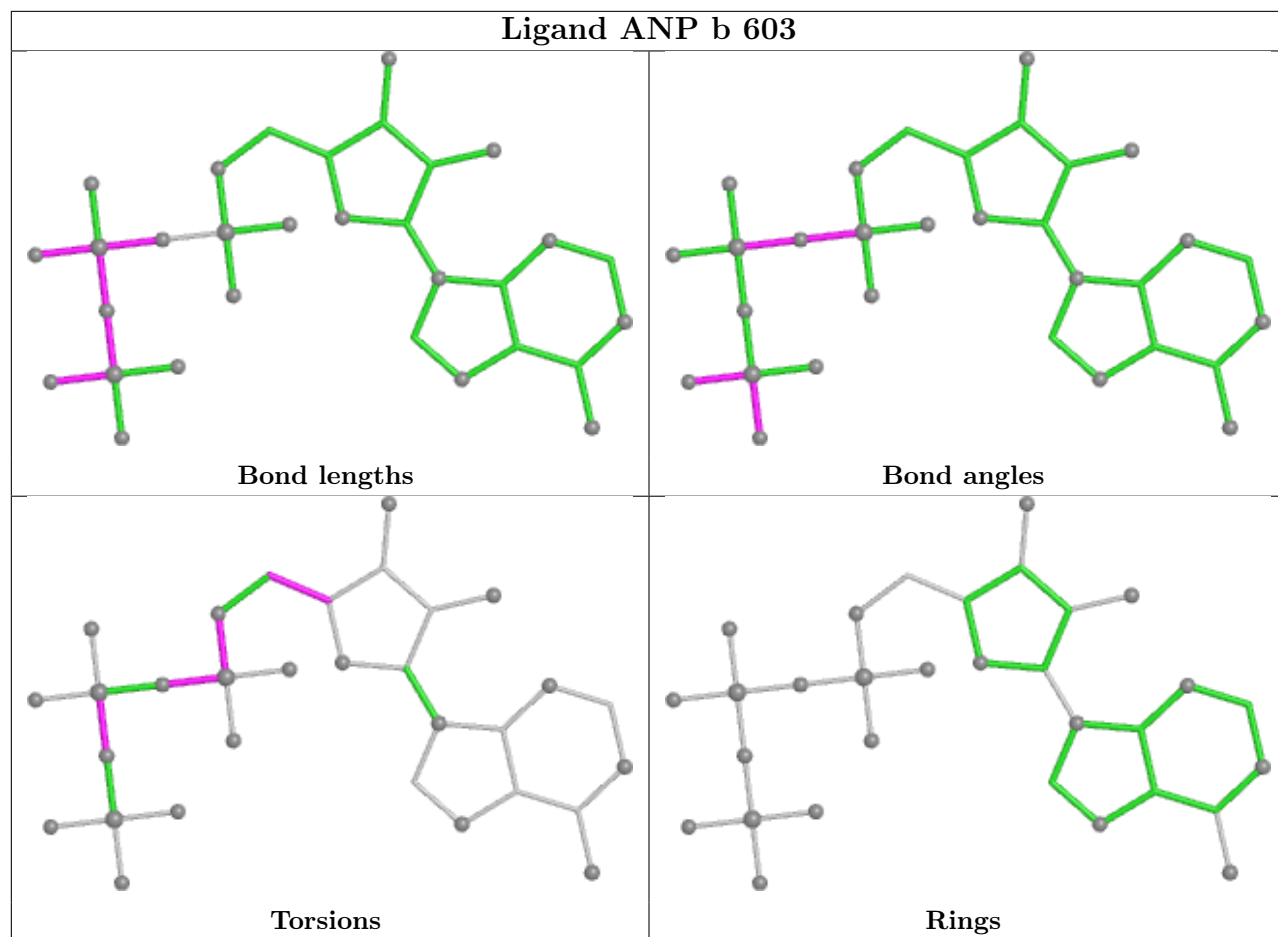
- Bond lengths:** Shows the bond lengths for the ligand. The central metal complex is highlighted in magenta, and the organic ligand is highlighted in green.
- Bond angles:** Shows the bond angles for the ligand. The central metal complex is highlighted in magenta, and the organic ligand is highlighted in green.
- Torsions:** Shows the torsion angles for the ligand. The central metal complex is highlighted in magenta, and the organic ligand is highlighted in green.
- Rings:** Shows the rings for the ligand. The central metal complex is highlighted in magenta, and the organic ligand is highlighted in green.

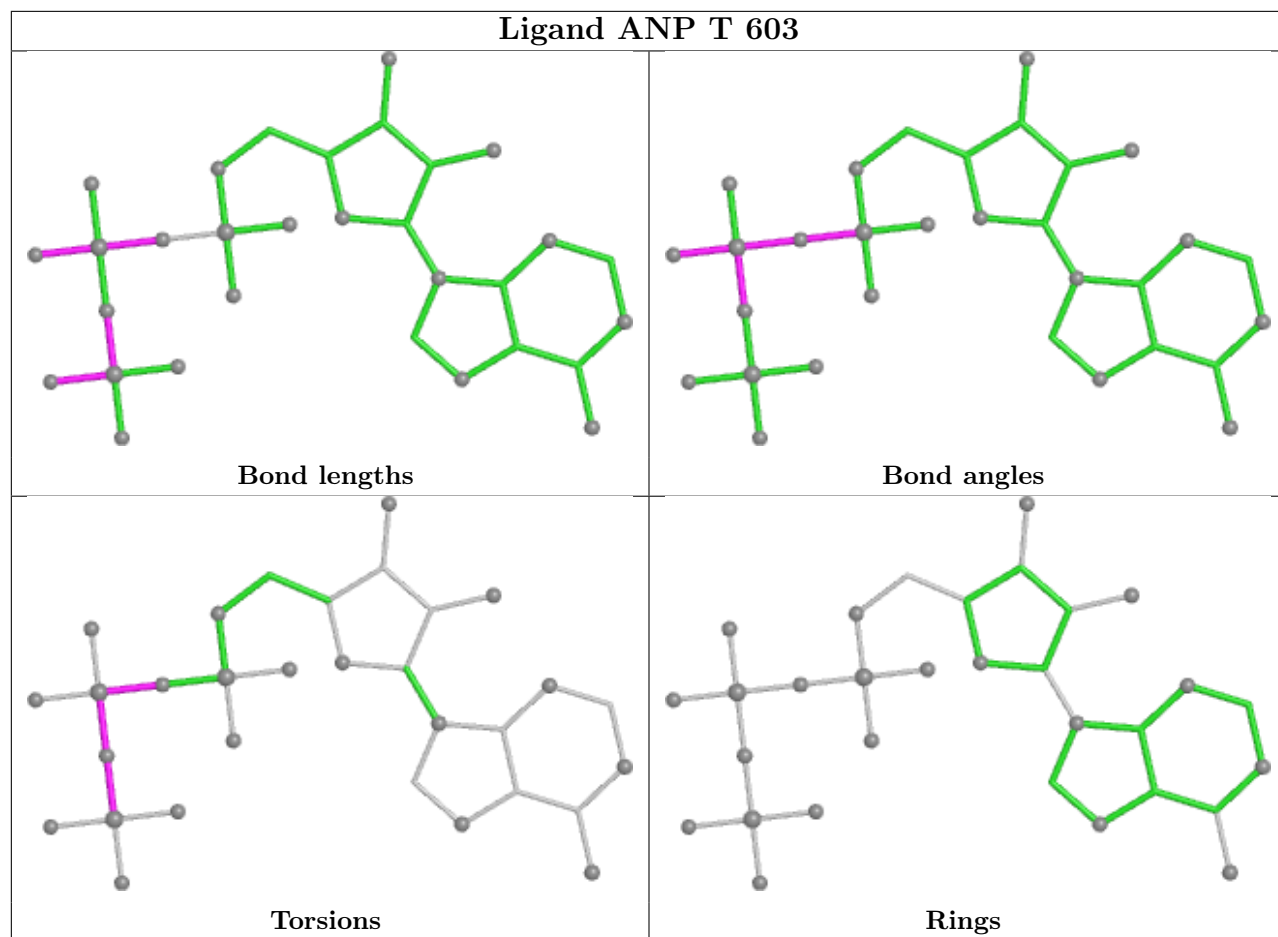


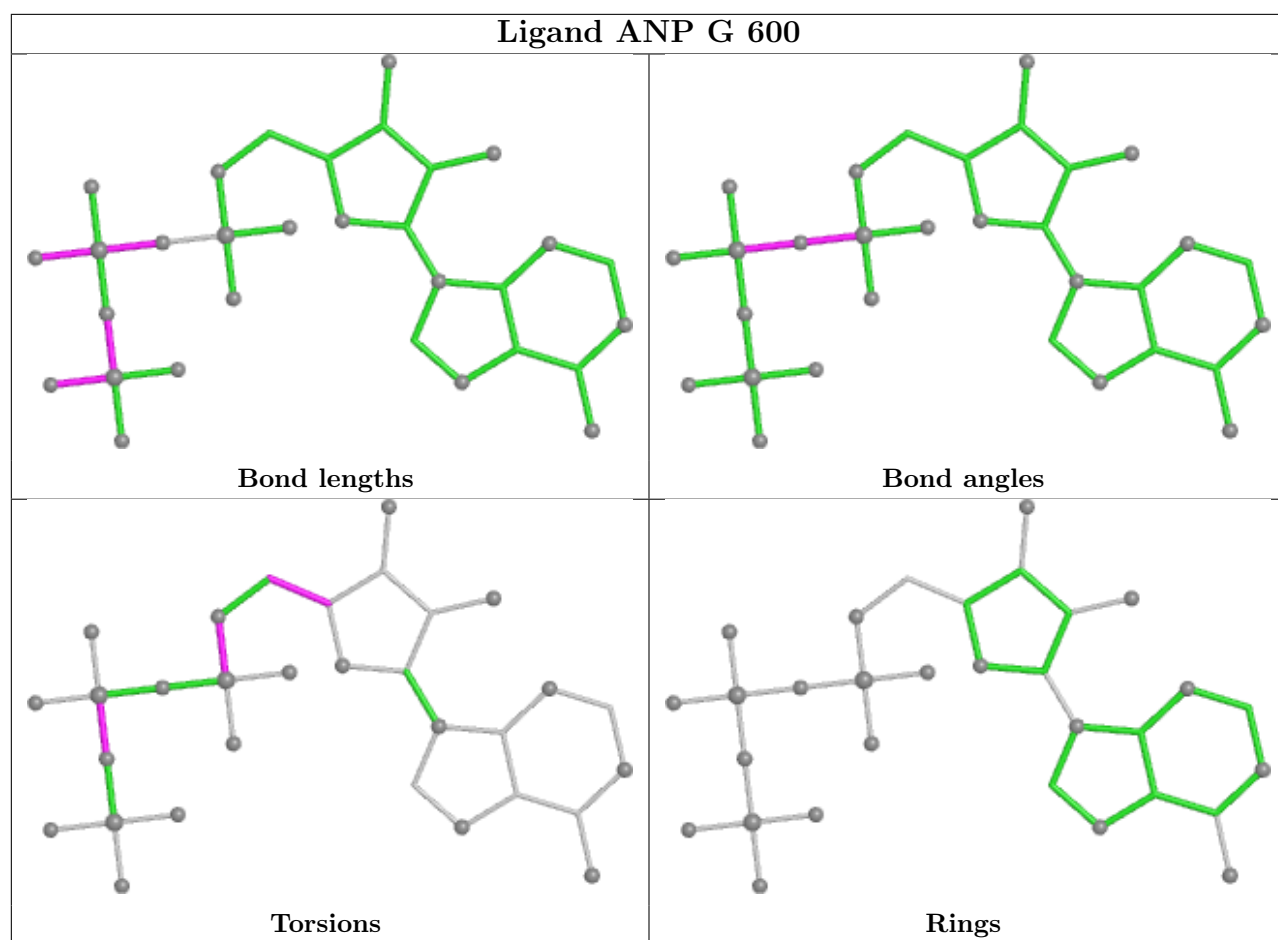
Ligand ANP I 603

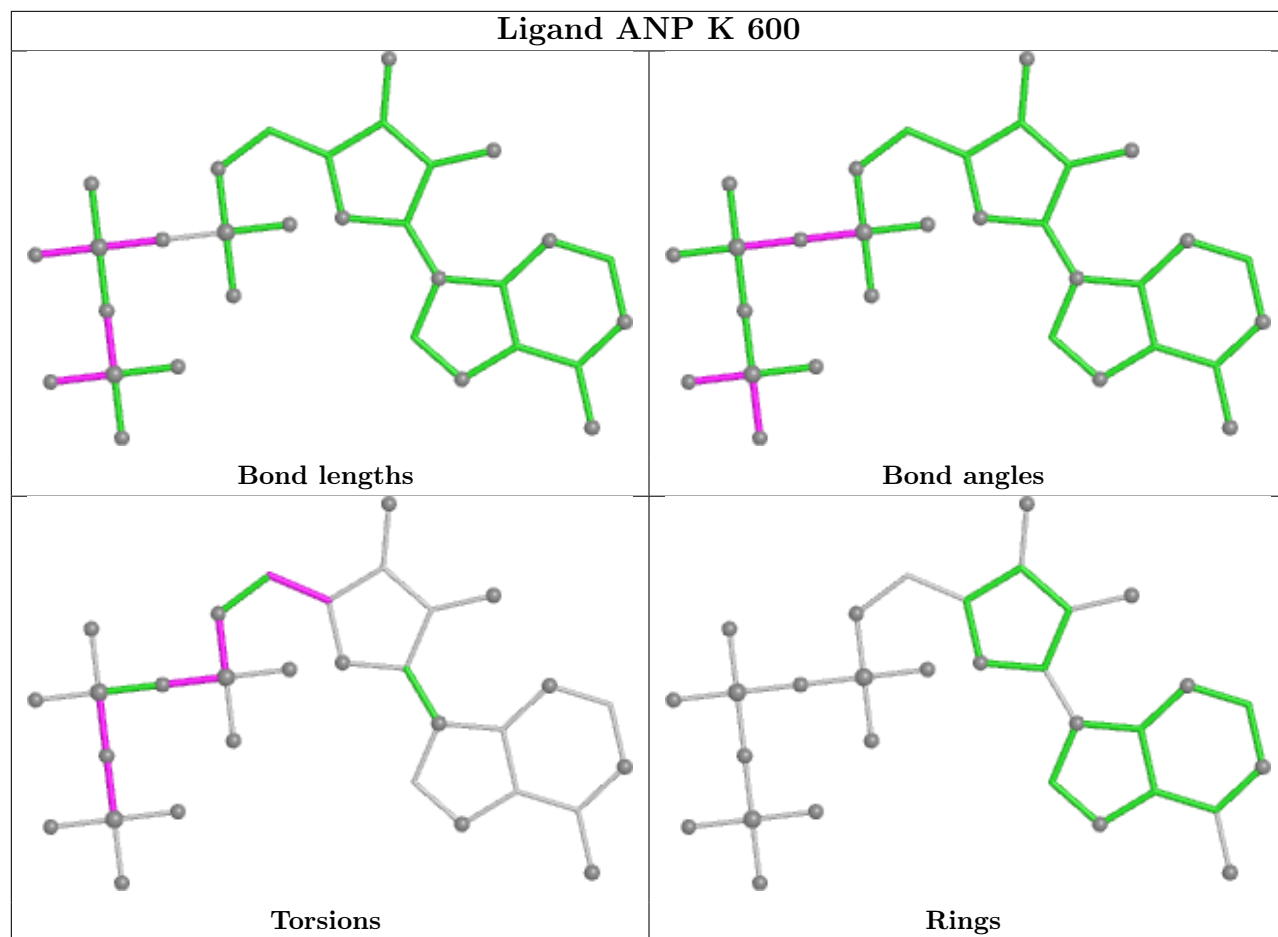












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

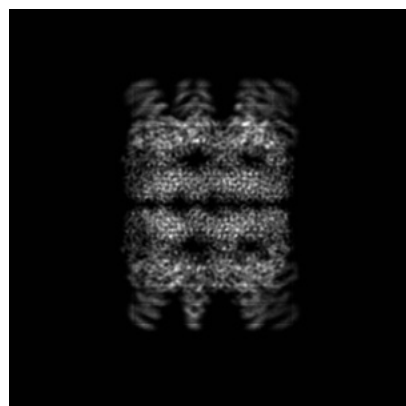
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65877. These allow visual inspection of the internal detail of the map and identification of artifacts.

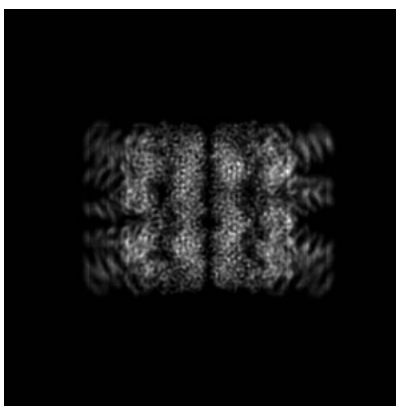
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

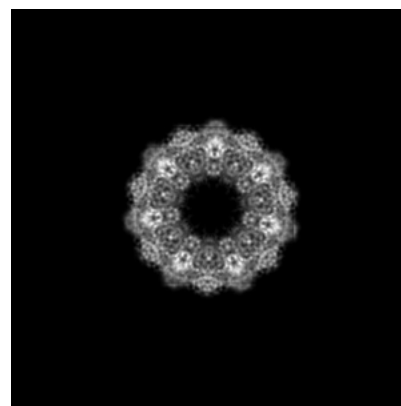
6.1.1 Primary map



X

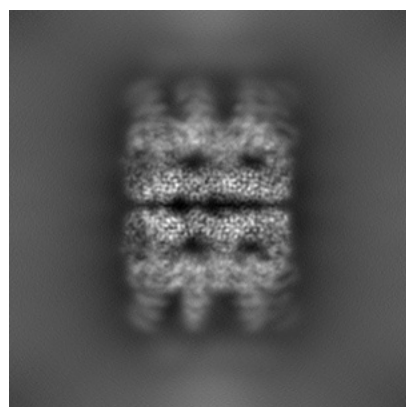


Y

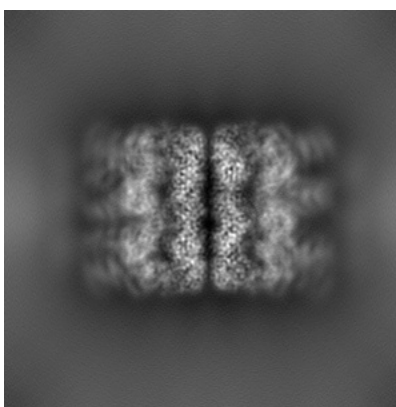


Z

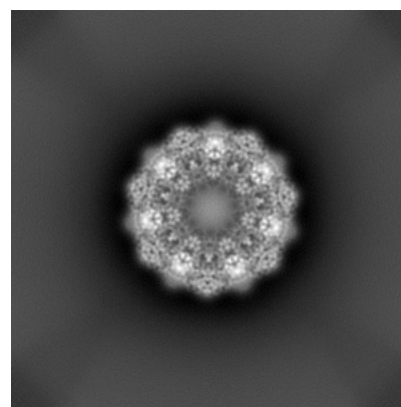
6.1.2 Raw map



X



Y

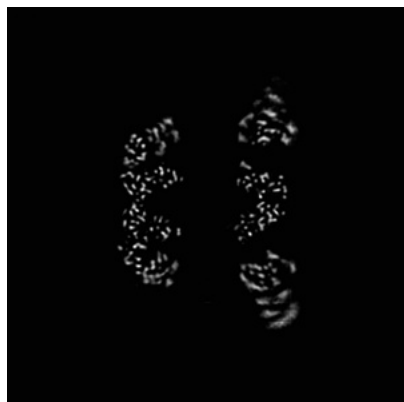


Z

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

6.2 Central slices [i](#)

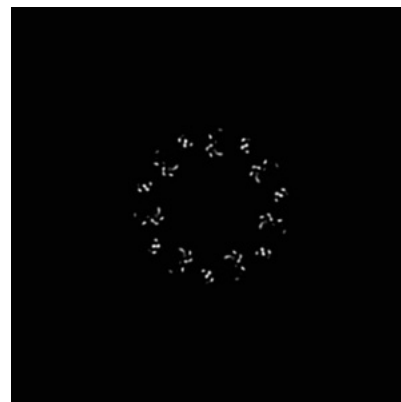
6.2.1 Primary map



X Index: 150

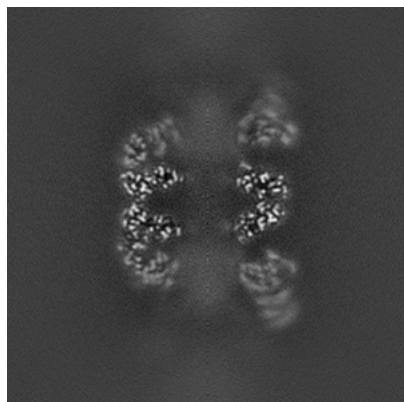


Y Index: 150

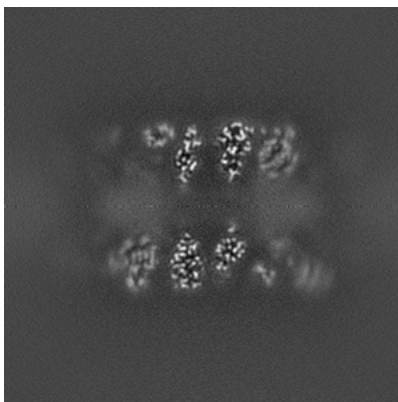


Z Index: 150

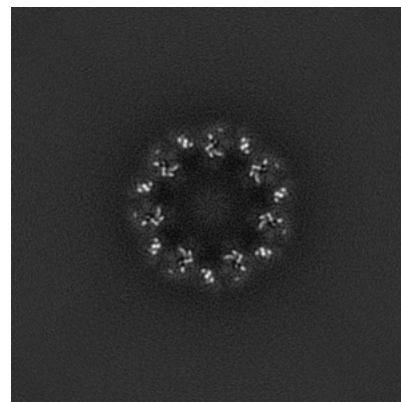
6.2.2 Raw map



X Index: 150



Y Index: 150

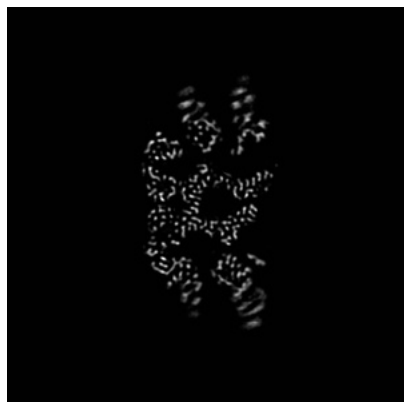


Z Index: 150

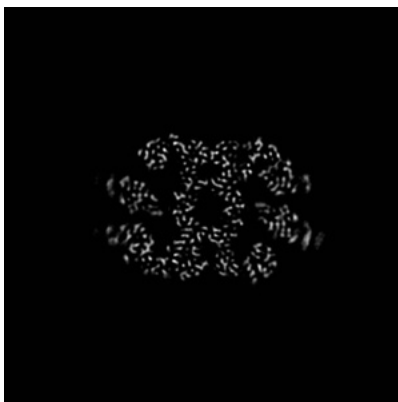
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 190

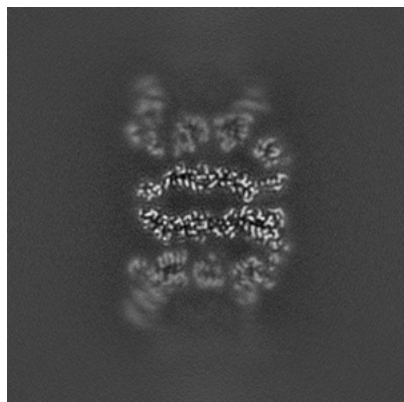


Y Index: 115

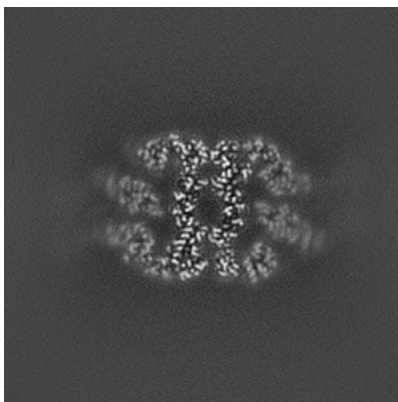


Z Index: 200

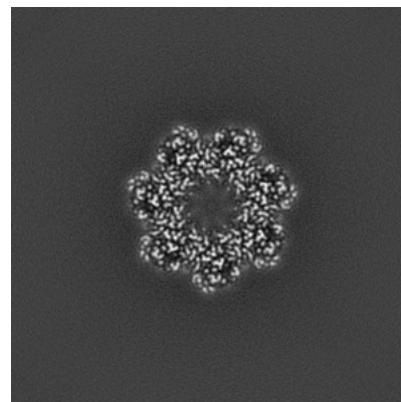
6.3.2 Raw map



X Index: 122



Y Index: 115

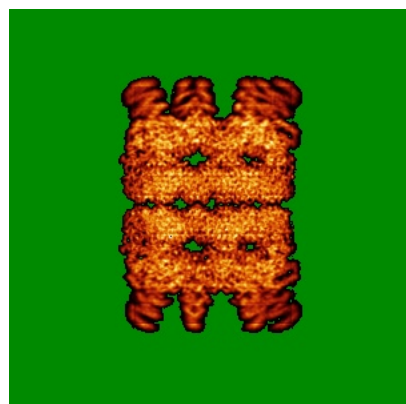


Z Index: 138

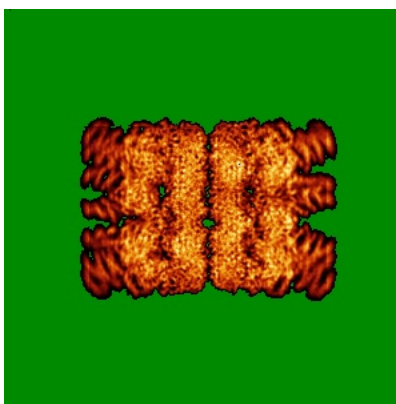
The images above show the largest variance slices of the map in three orthogonal directions.

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

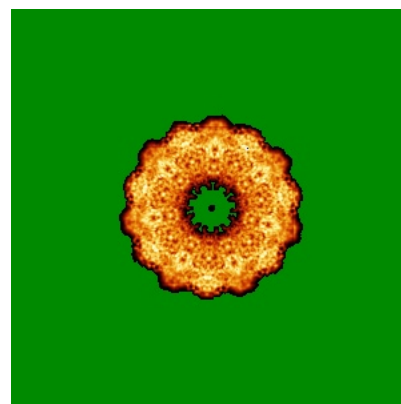
6.4.1 Primary map



X

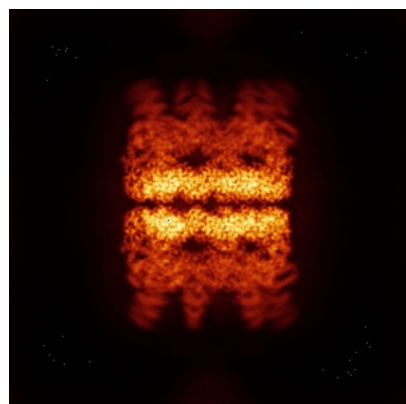


Y

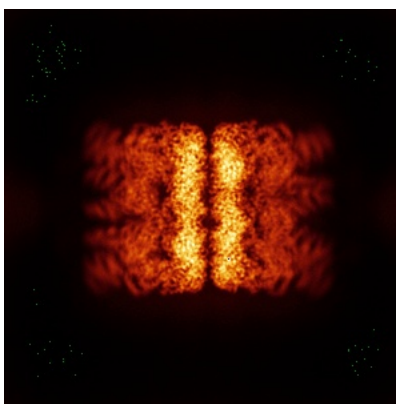


Z

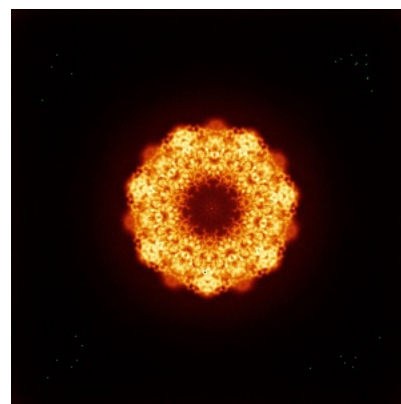
6.4.2 Raw map



X



Y

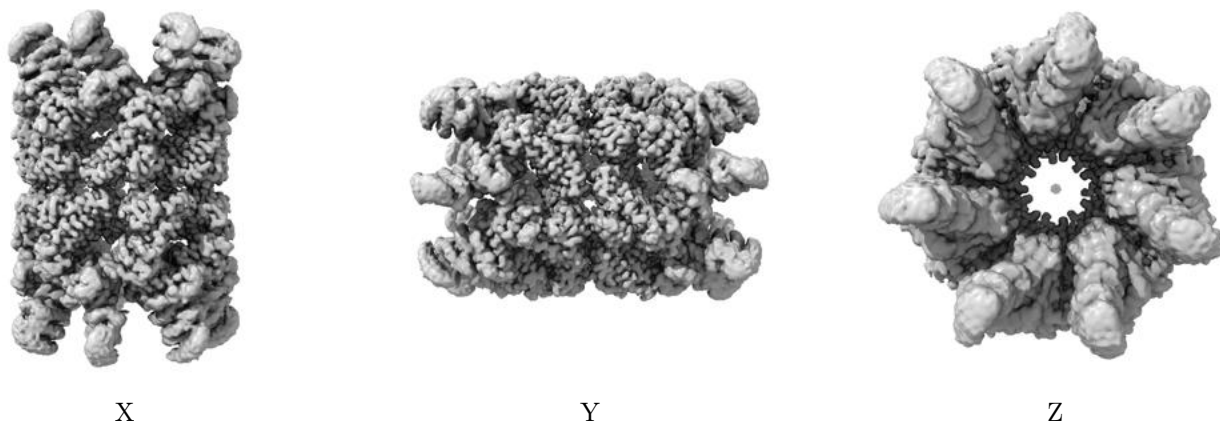


Z

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

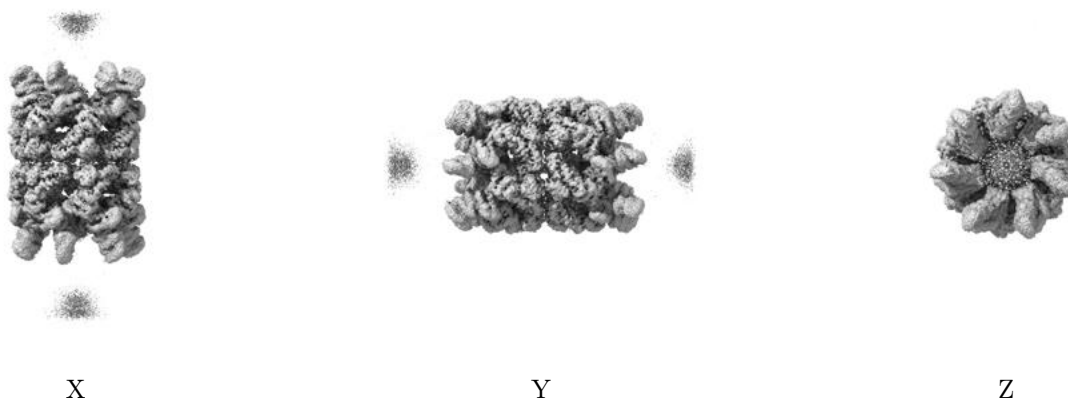
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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.

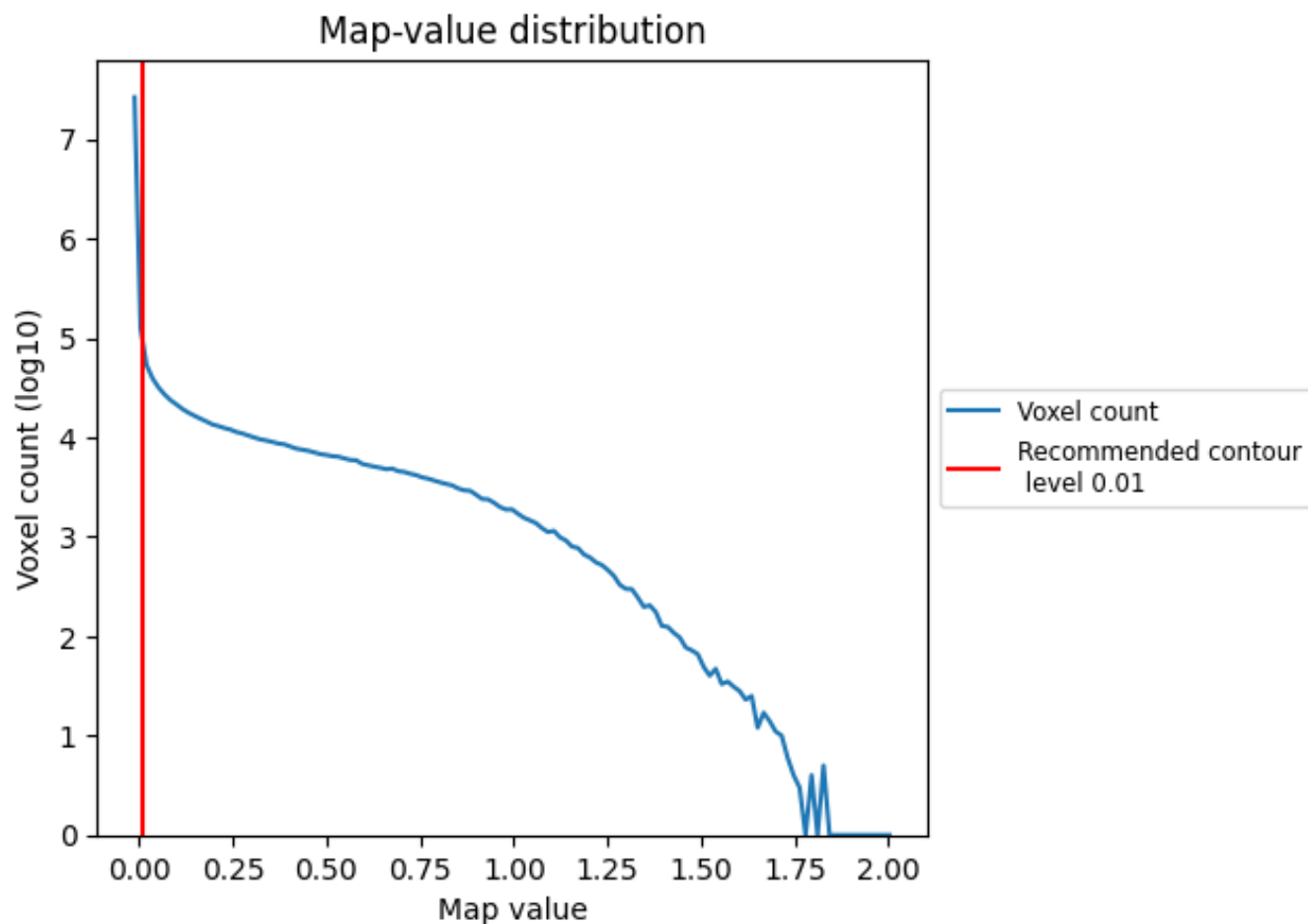
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

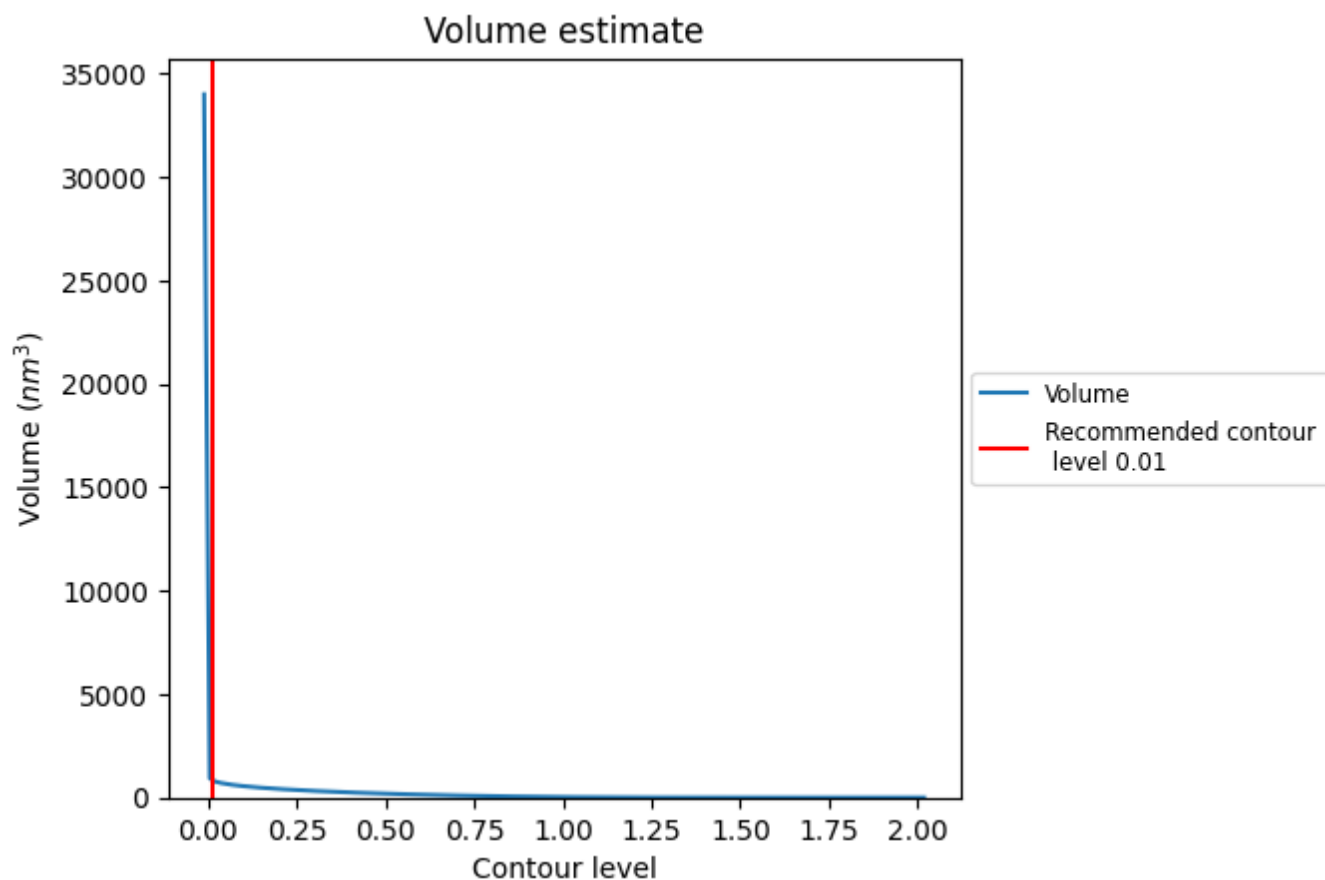
This section contains the results of statistical analysis of the map.

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.

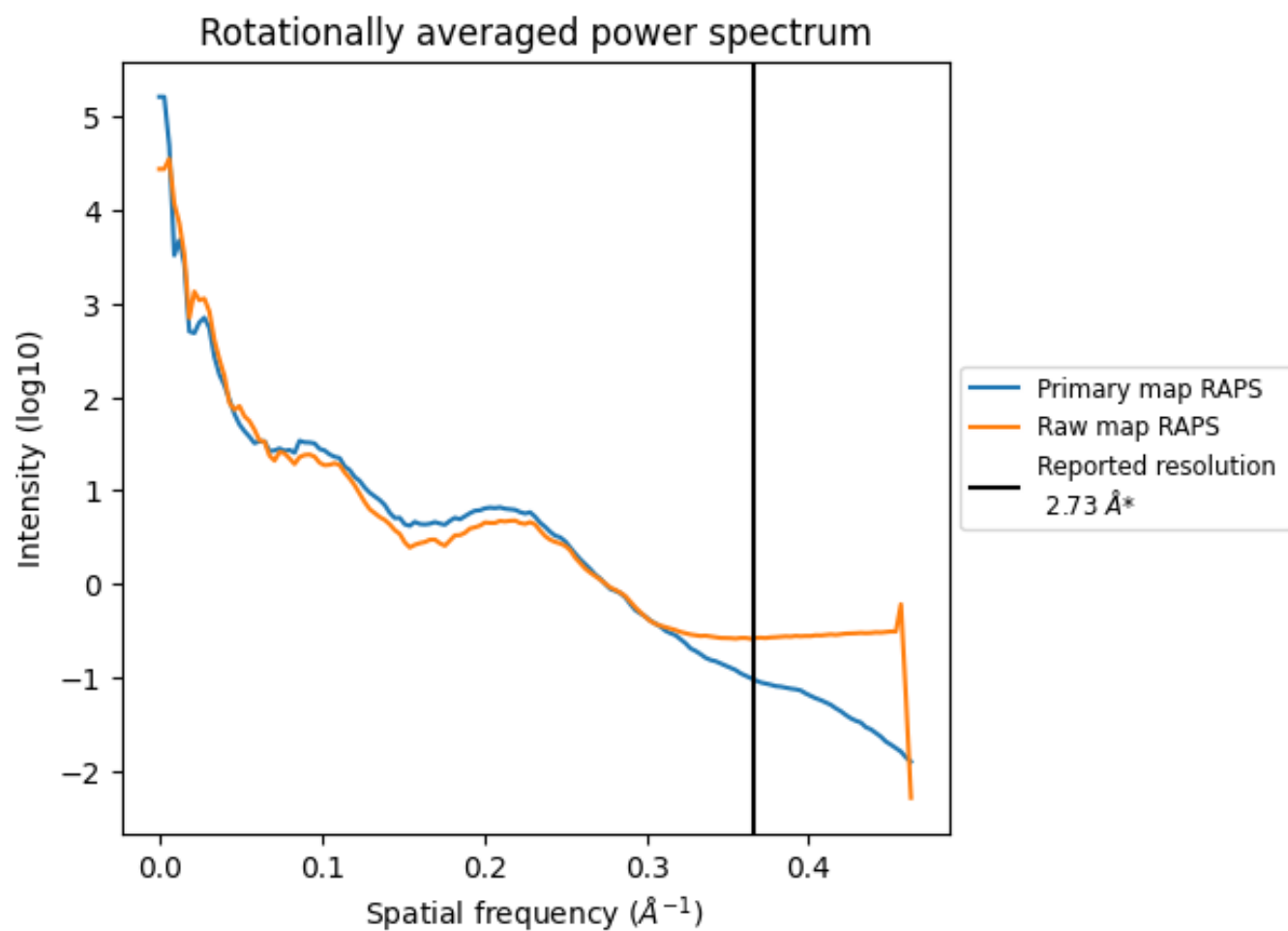
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 870 nm^3 ; this corresponds to an approximate mass of 786 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 ⓘ

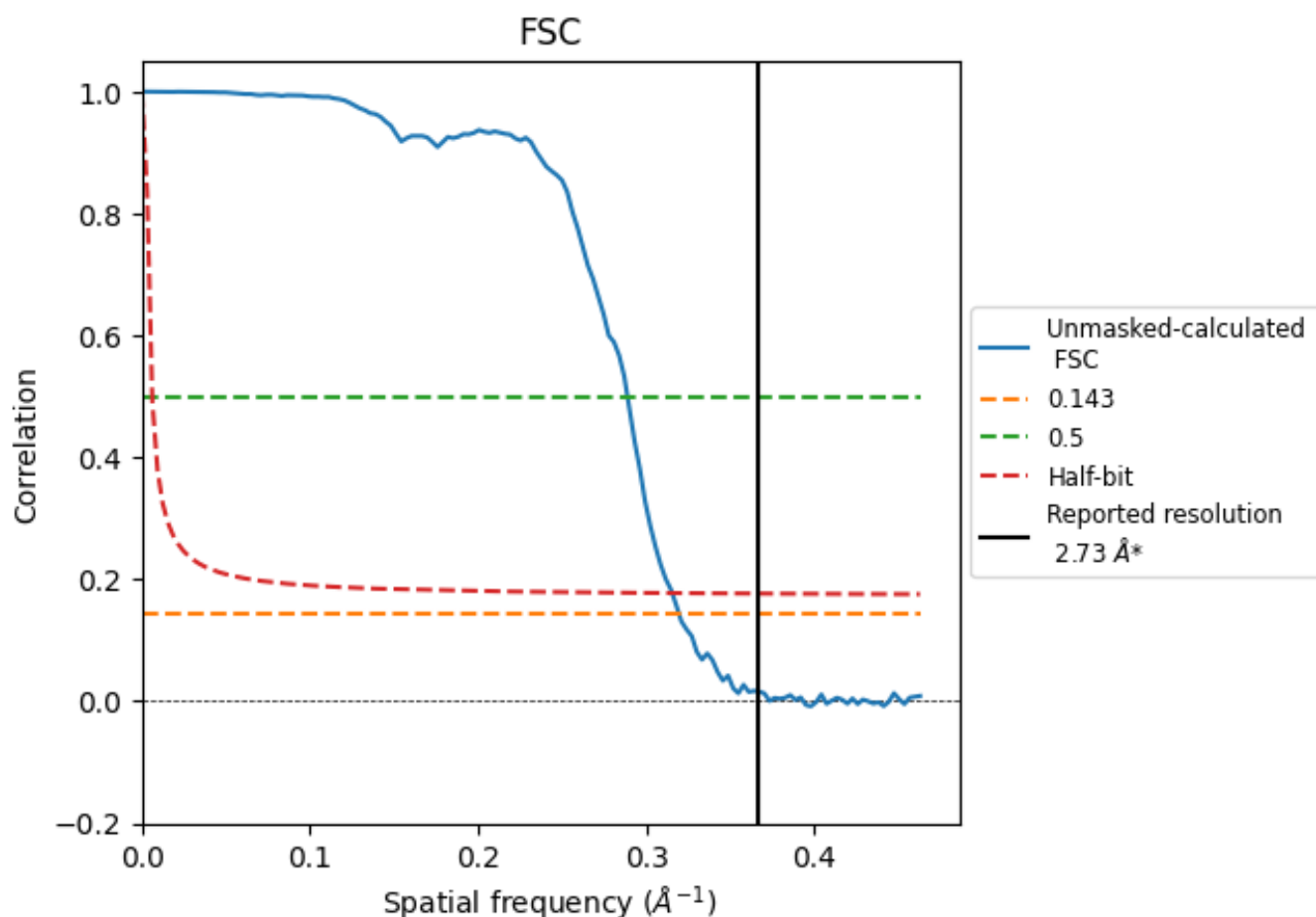


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 0.366 Å⁻¹

8.2 Resolution estimates [i](#)

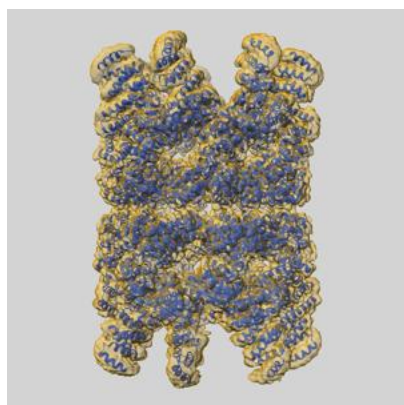
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	3.46	3.17

*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 3.13 differs from the reported value 2.73 by more than 10 %

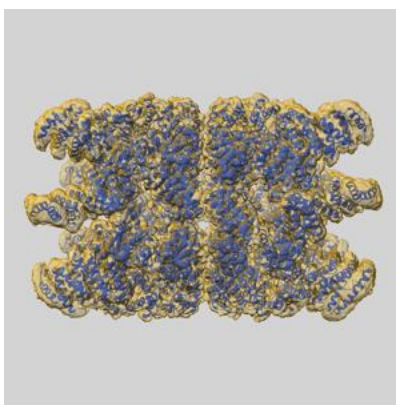
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65877 and PDB model 9WCW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

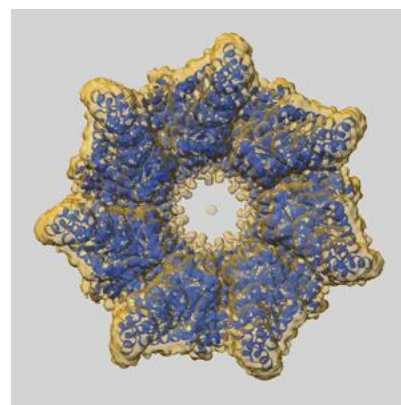
9.1 Map-model overlay [i](#)



X



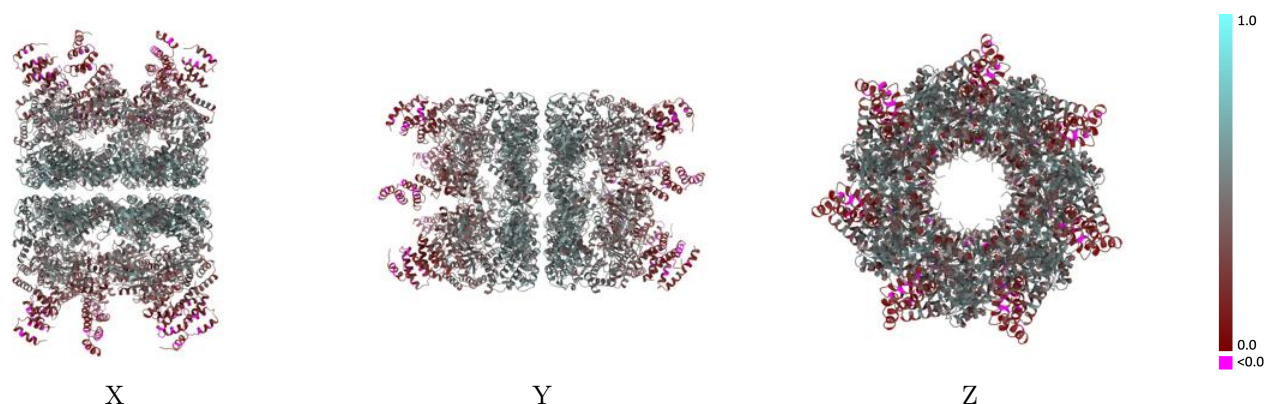
Y



Z

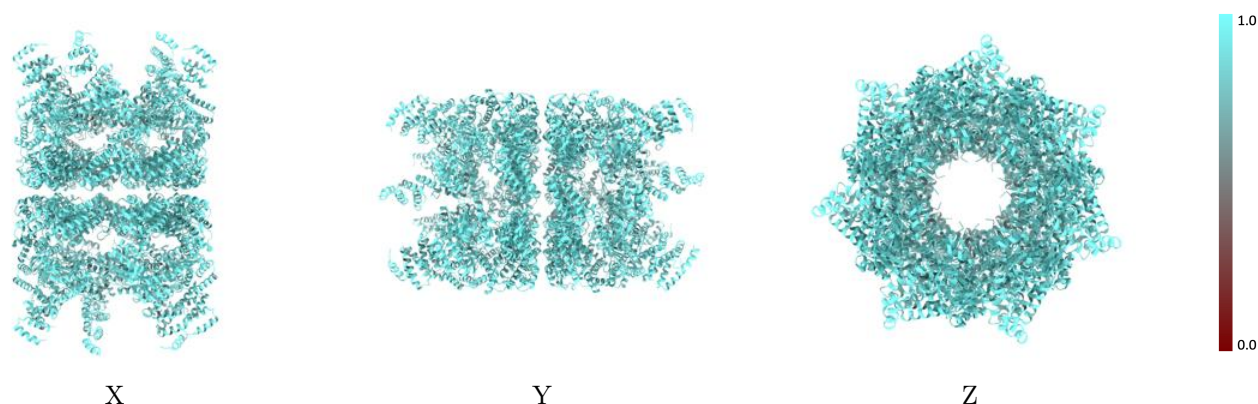
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



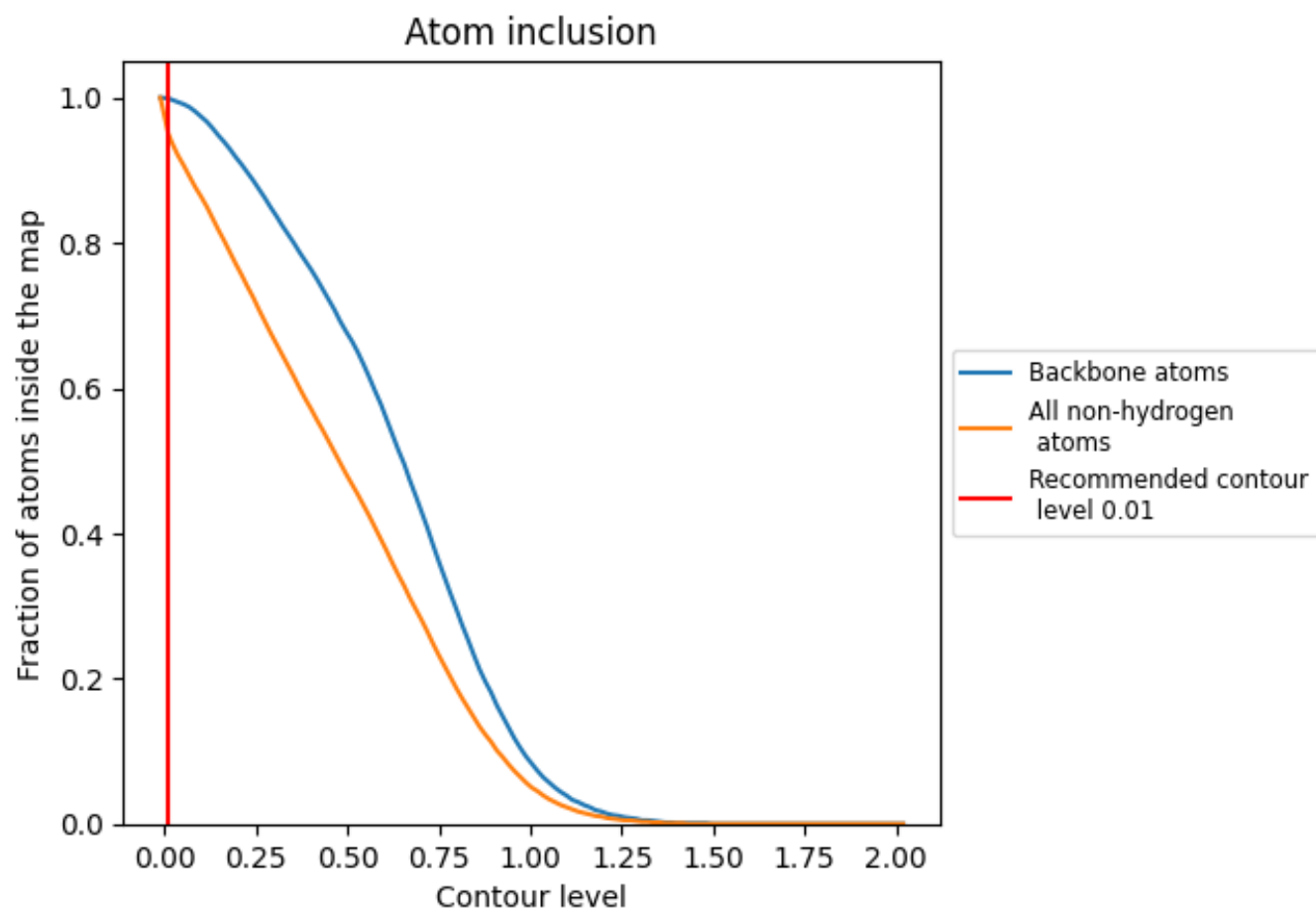
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.4050
A	 0.9100	 0.1720
B	 0.9080	 0.1730
C	 0.9130	 0.1710
D	 0.9040	 0.1680
E	 0.9110	 0.1700
F	 0.9170	 0.1680
G	 0.9570	 0.4480
I	 0.9570	 0.4440
J	 0.9560	 0.4440
K	 0.9550	 0.4440
L	 0.9560	 0.4450
M	 0.9140	 0.1710
N	 0.9570	 0.4480
O	 0.9290	 0.1790
P	 0.9560	 0.4480
Q	 0.9320	 0.1810
R	 0.9530	 0.4470
S	 0.9250	 0.1790
T	 0.9550	 0.4470
U	 0.9260	 0.1730
V	 0.9560	 0.4470
W	 0.9140	 0.1700
X	 0.9550	 0.4440
Y	 0.9230	 0.1750
Z	 0.9590	 0.4470
a	 0.9170	 0.1730
b	 0.9570	 0.4410
c	 0.9580	 0.4470

