



wwPDB EM Validation Summary Report ⓘ

Apr 9, 2026 – 09:42 PM UTC

PDB ID : 9RWG / pdb_00009rwg
EMDB ID : EMD-54328
Title : Pentameric AAV2 Rep40 in complex with AAV8
Authors : Rouse, S.L.; Bubeck, D.; Barritt, J.D.; Xu, V.; Wake, M.
Deposited on : 2025-07-09
Resolution : 2.19 Å(reported)
Based on initial model : 6v12

This is a wwPDB EM Validation Summary 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

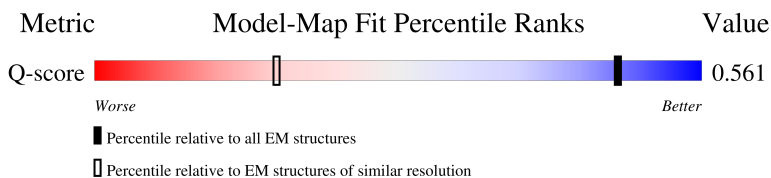
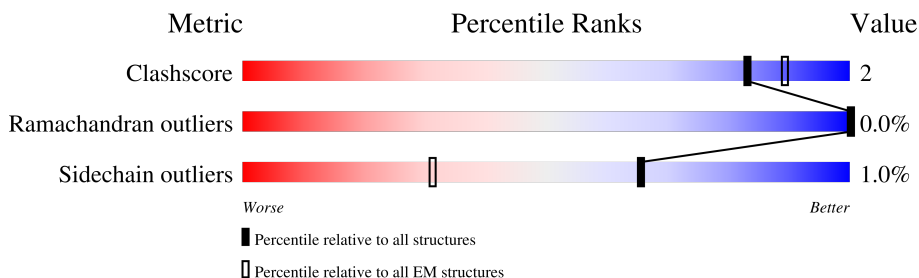
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.19 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.



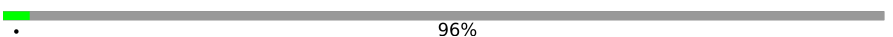
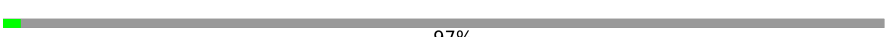
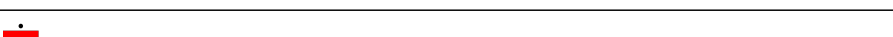
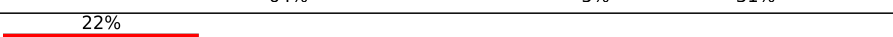
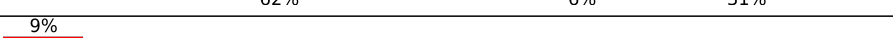
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2745 (1.70 - 2.69)

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	738	
1	B	738	
1	E	738	
1	F	738	

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Mol	Chain	Length	Quality of chain
1	G	738	
1	H	738	
1	I	738	
1	Q	738	
1	R	738	
1	S	738	
1	U	738	
1	V	738	
1	W	738	
1	X	738	
1	Y	738	
2	a	397	
2	b	397	
2	c	397	
2	d	397	
2	e	397	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 36961 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	202	Total	C	N	O	S	0	0
			1625	1007	293	320	5		
1	B	15	Total	C	N	O		0	0
			112	62	24	26			
1	E	39	Total	C	N	O		0	0
			287	171	59	57			
1	F	438	Total	C	N	O	S	0	0
			3515	2226	604	674	11		
1	G	434	Total	C	N	O	S	0	0
			3486	2210	598	668	10		
1	H	184	Total	C	N	O	S	0	0
			1477	912	267	293	5		
1	I	27	Total	C	N	O		0	0
			199	118	40	41			
1	Q	195	Total	C	N	O	S	0	0
			1571	973	283	309	6		
1	R	435	Total	C	N	O	S	0	0
			3490	2212	599	669	10		
1	S	20	Total	C	N	O		0	0
			144	83	29	32			
1	U	180	Total	C	N	O	S	0	0
			1445	891	261	288	5		
1	V	427	Total	C	N	O	S	0	0
			3436	2179	588	659	10		
1	W	426	Total	C	N	O	S	0	0
			3429	2174	587	658	10		
1	X	180	Total	C	N	O	S	0	0
			1446	891	262	288	5		
1	Y	14	Total	C	N	O		0	0
			105	57	23	25			

- Molecule 2 is a protein called Protein Rep68.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	273	Total	C	N	O	S	0	0
			2172	1383	370	409	10		
2	b	273	Total	C	N	O	S	0	0
			2172	1383	370	409	10		
2	c	273	Total	C	N	O	S	0	0
			2172	1383	370	409	10		
2	d	273	Total	C	N	O	S	0	0
			2172	1383	370	409	10		
2	e	273	Total	C	N	O	S	0	0
			2172	1383	370	409	10		

There are 305 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	337	GLY	-	expression tag	UNP P03132
a	338	SER	-	expression tag	UNP P03132
a	339	LEU	-	expression tag	UNP P03132
a	340	VAL	-	expression tag	UNP P03132
a	341	PRO	-	expression tag	UNP P03132
a	342	ARG	-	expression tag	UNP P03132
a	343	GLY	-	expression tag	UNP P03132
a	344	SER	-	expression tag	UNP P03132
a	345	GLY	-	expression tag	UNP P03132
a	346	GLY	-	expression tag	UNP P03132
a	347	GLY	-	expression tag	UNP P03132
a	348	GLY	-	expression tag	UNP P03132
a	349	SER	-	expression tag	UNP P03132
a	350	GLY	-	expression tag	UNP P03132
a	351	GLY	-	expression tag	UNP P03132
a	352	GLY	-	expression tag	UNP P03132
a	353	GLY	-	expression tag	UNP P03132
a	354	SER	-	expression tag	UNP P03132
a	355	GLY	-	expression tag	UNP P03132
a	356	GLY	-	expression tag	UNP P03132
a	357	GLY	-	expression tag	UNP P03132
a	358	GLY	-	expression tag	UNP P03132
a	359	SER	-	expression tag	UNP P03132
a	360	MET	-	expression tag	UNP P03132
a	361	ASP	-	expression tag	UNP P03132
a	362	TYR	-	expression tag	UNP P03132
a	363	LYS	-	expression tag	UNP P03132
a	364	ASP	-	expression tag	UNP P03132
a	365	HIS	-	expression tag	UNP P03132
a	366	ASP	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
a	367	GLY	-	expression tag	UNP P03132
a	368	ASP	-	expression tag	UNP P03132
a	369	TYR	-	expression tag	UNP P03132
a	370	LYS	-	expression tag	UNP P03132
a	371	ASP	-	expression tag	UNP P03132
a	372	HIS	-	expression tag	UNP P03132
a	373	ASP	-	expression tag	UNP P03132
a	374	ILE	-	expression tag	UNP P03132
a	375	ASP	-	expression tag	UNP P03132
a	376	TYR	-	expression tag	UNP P03132
a	377	LYS	-	expression tag	UNP P03132
a	378	ASP	-	expression tag	UNP P03132
a	379	ASP	-	expression tag	UNP P03132
a	380	ASP	-	expression tag	UNP P03132
a	381	ASP	-	expression tag	UNP P03132
a	382	LYS	-	expression tag	UNP P03132
a	383	GLY	-	expression tag	UNP P03132
a	384	SER	-	expression tag	UNP P03132
a	385	GLU	-	expression tag	UNP P03132
a	386	ASN	-	expression tag	UNP P03132
a	387	LEU	-	expression tag	UNP P03132
a	388	TYR	-	expression tag	UNP P03132
a	389	PHE	-	expression tag	UNP P03132
a	390	GLN	-	expression tag	UNP P03132
a	391	SER	-	expression tag	UNP P03132
a	392	HIS	-	expression tag	UNP P03132
a	393	HIS	-	expression tag	UNP P03132
a	394	HIS	-	expression tag	UNP P03132
a	395	HIS	-	expression tag	UNP P03132
a	396	HIS	-	expression tag	UNP P03132
a	397	HIS	-	expression tag	UNP P03132
b	337	GLY	-	expression tag	UNP P03132
b	338	SER	-	expression tag	UNP P03132
b	339	LEU	-	expression tag	UNP P03132
b	340	VAL	-	expression tag	UNP P03132
b	341	PRO	-	expression tag	UNP P03132
b	342	ARG	-	expression tag	UNP P03132
b	343	GLY	-	expression tag	UNP P03132
b	344	SER	-	expression tag	UNP P03132
b	345	GLY	-	expression tag	UNP P03132
b	346	GLY	-	expression tag	UNP P03132
b	347	GLY	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
b	348	GLY	-	expression tag	UNP P03132
b	349	SER	-	expression tag	UNP P03132
b	350	GLY	-	expression tag	UNP P03132
b	351	GLY	-	expression tag	UNP P03132
b	352	GLY	-	expression tag	UNP P03132
b	353	GLY	-	expression tag	UNP P03132
b	354	SER	-	expression tag	UNP P03132
b	355	GLY	-	expression tag	UNP P03132
b	356	GLY	-	expression tag	UNP P03132
b	357	GLY	-	expression tag	UNP P03132
b	358	GLY	-	expression tag	UNP P03132
b	359	SER	-	expression tag	UNP P03132
b	360	MET	-	expression tag	UNP P03132
b	361	ASP	-	expression tag	UNP P03132
b	362	TYR	-	expression tag	UNP P03132
b	363	LYS	-	expression tag	UNP P03132
b	364	ASP	-	expression tag	UNP P03132
b	365	HIS	-	expression tag	UNP P03132
b	366	ASP	-	expression tag	UNP P03132
b	367	GLY	-	expression tag	UNP P03132
b	368	ASP	-	expression tag	UNP P03132
b	369	TYR	-	expression tag	UNP P03132
b	370	LYS	-	expression tag	UNP P03132
b	371	ASP	-	expression tag	UNP P03132
b	372	HIS	-	expression tag	UNP P03132
b	373	ASP	-	expression tag	UNP P03132
b	374	ILE	-	expression tag	UNP P03132
b	375	ASP	-	expression tag	UNP P03132
b	376	TYR	-	expression tag	UNP P03132
b	377	LYS	-	expression tag	UNP P03132
b	378	ASP	-	expression tag	UNP P03132
b	379	ASP	-	expression tag	UNP P03132
b	380	ASP	-	expression tag	UNP P03132
b	381	ASP	-	expression tag	UNP P03132
b	382	LYS	-	expression tag	UNP P03132
b	383	GLY	-	expression tag	UNP P03132
b	384	SER	-	expression tag	UNP P03132
b	385	GLU	-	expression tag	UNP P03132
b	386	ASN	-	expression tag	UNP P03132
b	387	LEU	-	expression tag	UNP P03132
b	388	TYR	-	expression tag	UNP P03132
b	389	PHE	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
b	390	GLN	-	expression tag	UNP P03132
b	391	SER	-	expression tag	UNP P03132
b	392	HIS	-	expression tag	UNP P03132
b	393	HIS	-	expression tag	UNP P03132
b	394	HIS	-	expression tag	UNP P03132
b	395	HIS	-	expression tag	UNP P03132
b	396	HIS	-	expression tag	UNP P03132
b	397	HIS	-	expression tag	UNP P03132
c	337	GLY	-	expression tag	UNP P03132
c	338	SER	-	expression tag	UNP P03132
c	339	LEU	-	expression tag	UNP P03132
c	340	VAL	-	expression tag	UNP P03132
c	341	PRO	-	expression tag	UNP P03132
c	342	ARG	-	expression tag	UNP P03132
c	343	GLY	-	expression tag	UNP P03132
c	344	SER	-	expression tag	UNP P03132
c	345	GLY	-	expression tag	UNP P03132
c	346	GLY	-	expression tag	UNP P03132
c	347	GLY	-	expression tag	UNP P03132
c	348	GLY	-	expression tag	UNP P03132
c	349	SER	-	expression tag	UNP P03132
c	350	GLY	-	expression tag	UNP P03132
c	351	GLY	-	expression tag	UNP P03132
c	352	GLY	-	expression tag	UNP P03132
c	353	GLY	-	expression tag	UNP P03132
c	354	SER	-	expression tag	UNP P03132
c	355	GLY	-	expression tag	UNP P03132
c	356	GLY	-	expression tag	UNP P03132
c	357	GLY	-	expression tag	UNP P03132
c	358	GLY	-	expression tag	UNP P03132
c	359	SER	-	expression tag	UNP P03132
c	360	MET	-	expression tag	UNP P03132
c	361	ASP	-	expression tag	UNP P03132
c	362	TYR	-	expression tag	UNP P03132
c	363	LYS	-	expression tag	UNP P03132
c	364	ASP	-	expression tag	UNP P03132
c	365	HIS	-	expression tag	UNP P03132
c	366	ASP	-	expression tag	UNP P03132
c	367	GLY	-	expression tag	UNP P03132
c	368	ASP	-	expression tag	UNP P03132
c	369	TYR	-	expression tag	UNP P03132
c	370	LYS	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
c	371	ASP	-	expression tag	UNP P03132
c	372	HIS	-	expression tag	UNP P03132
c	373	ASP	-	expression tag	UNP P03132
c	374	ILE	-	expression tag	UNP P03132
c	375	ASP	-	expression tag	UNP P03132
c	376	TYR	-	expression tag	UNP P03132
c	377	LYS	-	expression tag	UNP P03132
c	378	ASP	-	expression tag	UNP P03132
c	379	ASP	-	expression tag	UNP P03132
c	380	ASP	-	expression tag	UNP P03132
c	381	ASP	-	expression tag	UNP P03132
c	382	LYS	-	expression tag	UNP P03132
c	383	GLY	-	expression tag	UNP P03132
c	384	SER	-	expression tag	UNP P03132
c	385	GLU	-	expression tag	UNP P03132
c	386	ASN	-	expression tag	UNP P03132
c	387	LEU	-	expression tag	UNP P03132
c	388	TYR	-	expression tag	UNP P03132
c	389	PHE	-	expression tag	UNP P03132
c	390	GLN	-	expression tag	UNP P03132
c	391	SER	-	expression tag	UNP P03132
c	392	HIS	-	expression tag	UNP P03132
c	393	HIS	-	expression tag	UNP P03132
c	394	HIS	-	expression tag	UNP P03132
c	395	HIS	-	expression tag	UNP P03132
c	396	HIS	-	expression tag	UNP P03132
c	397	HIS	-	expression tag	UNP P03132
d	337	GLY	-	expression tag	UNP P03132
d	338	SER	-	expression tag	UNP P03132
d	339	LEU	-	expression tag	UNP P03132
d	340	VAL	-	expression tag	UNP P03132
d	341	PRO	-	expression tag	UNP P03132
d	342	ARG	-	expression tag	UNP P03132
d	343	GLY	-	expression tag	UNP P03132
d	344	SER	-	expression tag	UNP P03132
d	345	GLY	-	expression tag	UNP P03132
d	346	GLY	-	expression tag	UNP P03132
d	347	GLY	-	expression tag	UNP P03132
d	348	GLY	-	expression tag	UNP P03132
d	349	SER	-	expression tag	UNP P03132
d	350	GLY	-	expression tag	UNP P03132
d	351	GLY	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
d	352	GLY	-	expression tag	UNP P03132
d	353	GLY	-	expression tag	UNP P03132
d	354	SER	-	expression tag	UNP P03132
d	355	GLY	-	expression tag	UNP P03132
d	356	GLY	-	expression tag	UNP P03132
d	357	GLY	-	expression tag	UNP P03132
d	358	GLY	-	expression tag	UNP P03132
d	359	SER	-	expression tag	UNP P03132
d	360	MET	-	expression tag	UNP P03132
d	361	ASP	-	expression tag	UNP P03132
d	362	TYR	-	expression tag	UNP P03132
d	363	LYS	-	expression tag	UNP P03132
d	364	ASP	-	expression tag	UNP P03132
d	365	HIS	-	expression tag	UNP P03132
d	366	ASP	-	expression tag	UNP P03132
d	367	GLY	-	expression tag	UNP P03132
d	368	ASP	-	expression tag	UNP P03132
d	369	TYR	-	expression tag	UNP P03132
d	370	LYS	-	expression tag	UNP P03132
d	371	ASP	-	expression tag	UNP P03132
d	372	HIS	-	expression tag	UNP P03132
d	373	ASP	-	expression tag	UNP P03132
d	374	ILE	-	expression tag	UNP P03132
d	375	ASP	-	expression tag	UNP P03132
d	376	TYR	-	expression tag	UNP P03132
d	377	LYS	-	expression tag	UNP P03132
d	378	ASP	-	expression tag	UNP P03132
d	379	ASP	-	expression tag	UNP P03132
d	380	ASP	-	expression tag	UNP P03132
d	381	ASP	-	expression tag	UNP P03132
d	382	LYS	-	expression tag	UNP P03132
d	383	GLY	-	expression tag	UNP P03132
d	384	SER	-	expression tag	UNP P03132
d	385	GLU	-	expression tag	UNP P03132
d	386	ASN	-	expression tag	UNP P03132
d	387	LEU	-	expression tag	UNP P03132
d	388	TYR	-	expression tag	UNP P03132
d	389	PHE	-	expression tag	UNP P03132
d	390	GLN	-	expression tag	UNP P03132
d	391	SER	-	expression tag	UNP P03132
d	392	HIS	-	expression tag	UNP P03132
d	393	HIS	-	expression tag	UNP P03132

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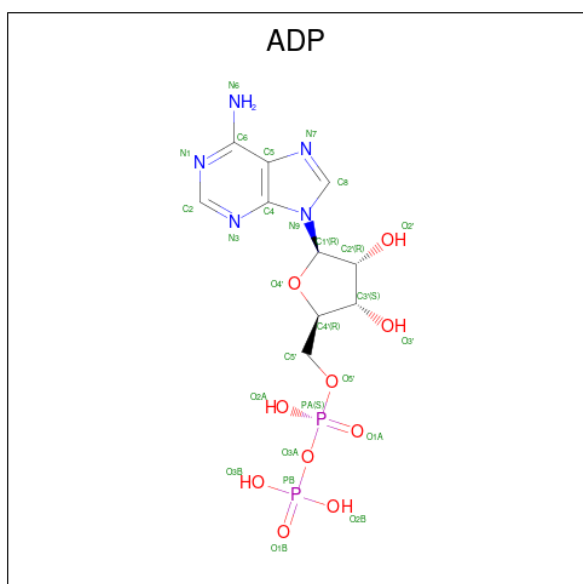
Chain	Residue	Modelled	Actual	Comment	Reference
d	394	HIS	-	expression tag	UNP P03132
d	395	HIS	-	expression tag	UNP P03132
d	396	HIS	-	expression tag	UNP P03132
d	397	HIS	-	expression tag	UNP P03132
e	337	GLY	-	expression tag	UNP P03132
e	338	SER	-	expression tag	UNP P03132
e	339	LEU	-	expression tag	UNP P03132
e	340	VAL	-	expression tag	UNP P03132
e	341	PRO	-	expression tag	UNP P03132
e	342	ARG	-	expression tag	UNP P03132
e	343	GLY	-	expression tag	UNP P03132
e	344	SER	-	expression tag	UNP P03132
e	345	GLY	-	expression tag	UNP P03132
e	346	GLY	-	expression tag	UNP P03132
e	347	GLY	-	expression tag	UNP P03132
e	348	GLY	-	expression tag	UNP P03132
e	349	SER	-	expression tag	UNP P03132
e	350	GLY	-	expression tag	UNP P03132
e	351	GLY	-	expression tag	UNP P03132
e	352	GLY	-	expression tag	UNP P03132
e	353	GLY	-	expression tag	UNP P03132
e	354	SER	-	expression tag	UNP P03132
e	355	GLY	-	expression tag	UNP P03132
e	356	GLY	-	expression tag	UNP P03132
e	357	GLY	-	expression tag	UNP P03132
e	358	GLY	-	expression tag	UNP P03132
e	359	SER	-	expression tag	UNP P03132
e	360	MET	-	expression tag	UNP P03132
e	361	ASP	-	expression tag	UNP P03132
e	362	TYR	-	expression tag	UNP P03132
e	363	LYS	-	expression tag	UNP P03132
e	364	ASP	-	expression tag	UNP P03132
e	365	HIS	-	expression tag	UNP P03132
e	366	ASP	-	expression tag	UNP P03132
e	367	GLY	-	expression tag	UNP P03132
e	368	ASP	-	expression tag	UNP P03132
e	369	TYR	-	expression tag	UNP P03132
e	370	LYS	-	expression tag	UNP P03132
e	371	ASP	-	expression tag	UNP P03132
e	372	HIS	-	expression tag	UNP P03132
e	373	ASP	-	expression tag	UNP P03132
e	374	ILE	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
e	375	ASP	-	expression tag	UNP P03132
e	376	TYR	-	expression tag	UNP P03132
e	377	LYS	-	expression tag	UNP P03132
e	378	ASP	-	expression tag	UNP P03132
e	379	ASP	-	expression tag	UNP P03132
e	380	ASP	-	expression tag	UNP P03132
e	381	ASP	-	expression tag	UNP P03132
e	382	LYS	-	expression tag	UNP P03132
e	383	GLY	-	expression tag	UNP P03132
e	384	SER	-	expression tag	UNP P03132
e	385	GLU	-	expression tag	UNP P03132
e	386	ASN	-	expression tag	UNP P03132
e	387	LEU	-	expression tag	UNP P03132
e	388	TYR	-	expression tag	UNP P03132
e	389	PHE	-	expression tag	UNP P03132
e	390	GLN	-	expression tag	UNP P03132
e	391	SER	-	expression tag	UNP P03132
e	392	HIS	-	expression tag	UNP P03132
e	393	HIS	-	expression tag	UNP P03132
e	394	HIS	-	expression tag	UNP P03132
e	395	HIS	-	expression tag	UNP P03132
e	396	HIS	-	expression tag	UNP P03132
e	397	HIS	-	expression tag	UNP P03132

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	
4	H	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	
4	R	1	Total	Mg	0
			1	1	
4	U	1	Total	Mg	0
			1	1	

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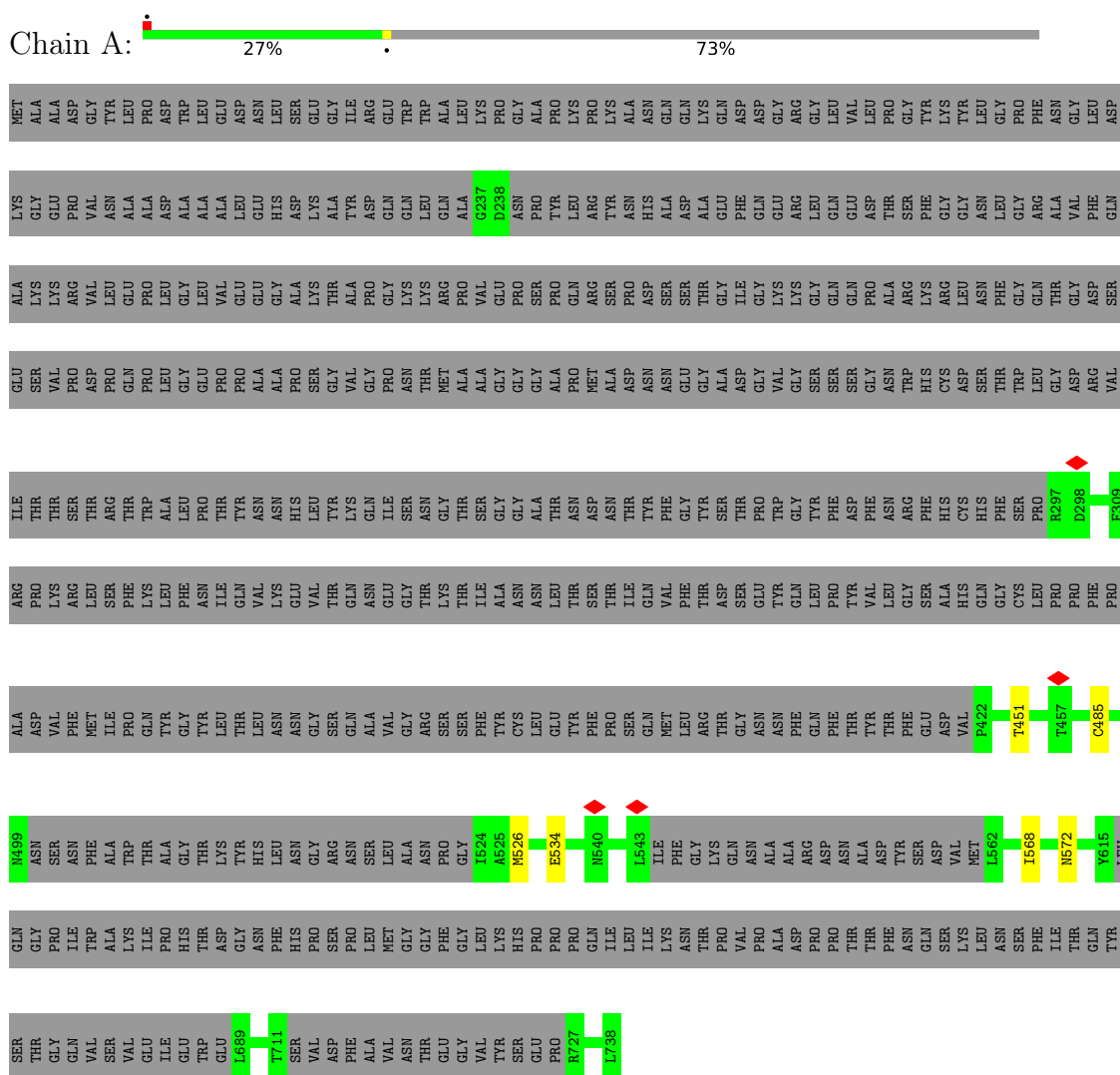
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Mol	Chain	Residues	Atoms		AltConf
4	V	1	Total 1	Mg 1	0
4	W	1	Total 1	Mg 1	0
4	X	1	Total 1	Mg 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

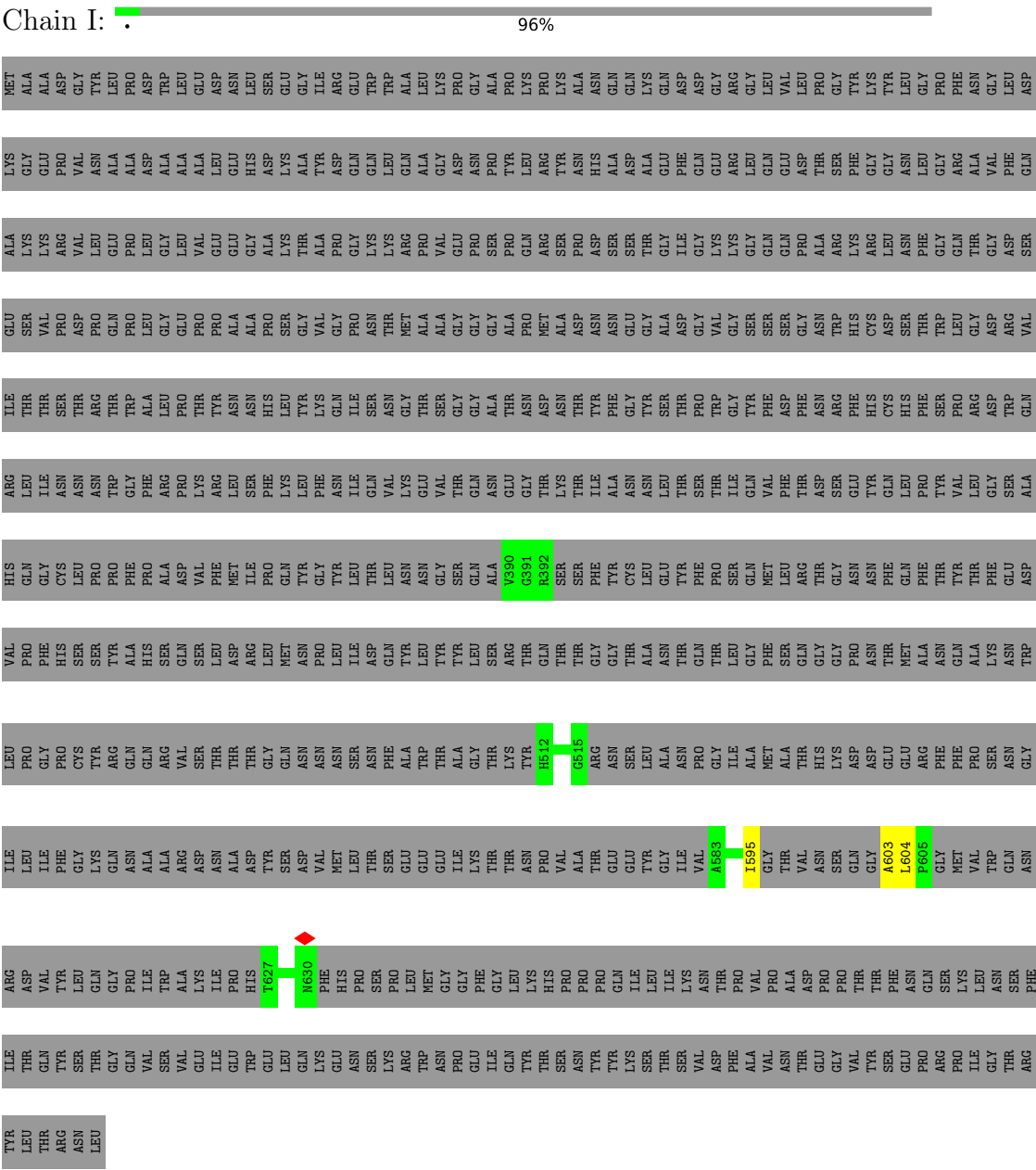
- Molecule 1: Capsid protein



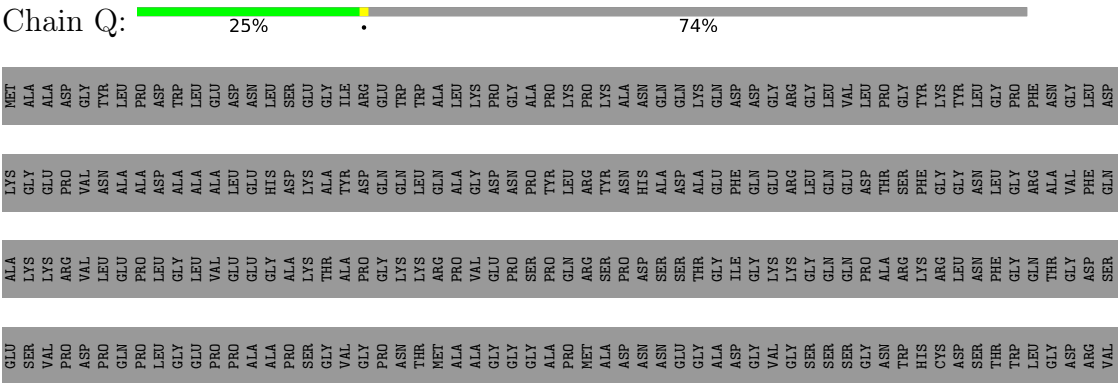
- Molecule 1: Capsid protein





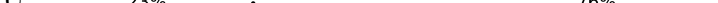


● Molecule 1: Capsid protein





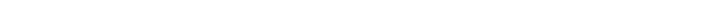
- Molecule 1: Capsid protein

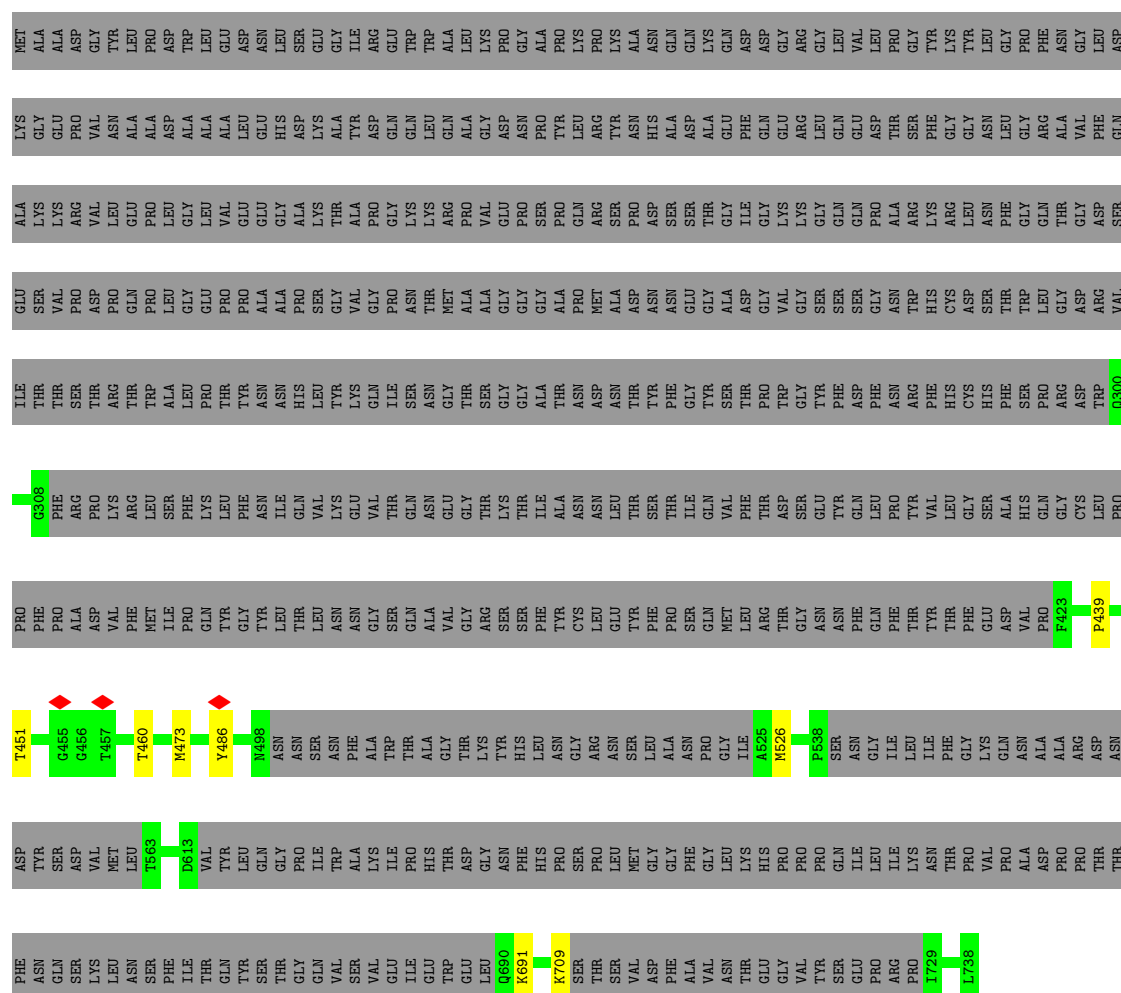
Chain U:  23% . 76%

G308	PHE	THR	THR	ILE	GLU	ALA	LYS	LYS	MET
	ARG	SER	THR	THR	VAL	LYS	ARG	GLY	ALA
	PRO	THR	THR	THR	ASP	VAL	VAL	PRO	ASP
	LYS	ARG	THR	ARG	PRO	LEU	LEU	ASN	TYR
	ARG	THR	THR	THR	GLN	GLU	ALA	ALA	LEU
	LEU	THR	THR	THR	PRO	PRO	ALA	ASP	PRO
	PHE	LEU	ALA	LEU	GLY	GLY	ALA	ASP	TRP
	LYS	PRO	THR	THR	GLU	LEU	VAL	ALA	LEU
	LEU	THR	THR	THR	PRO	VAL	VAL	ALA	GLU
	PHE	TYR	TYR	TYR	PRO	GLU	GLU	LEU	ASP
ASN	ASN	ASN	ASN	ALA	GLY	GLY	HIS	ASN	
ILE	ASN	ASN	ASN	ALA	GLY	GLY	ASP	SER	
GLN	HIS	THR	THR	PRO	ALA	ALA	ASP	GLY	
VAL	LEU	SER	GLY	SER	LYS	THR	LYS	GLU	
LYS	TYR	LYS	LYS	TYR	GLY	THR	ALA	GLY	
GLU	LYS	VAL	VAL	VAL	VAL	ALA	ASP	TYR	
GLU	VAL	GLN	ILE	ILE	PRO	PRO	GLY	GLN	
GLY	ASN	ASN	ASN	THR	LYS	LYS	LEU	TRP	
GLY	GLU	GLY	GLY	GLY	MET	ARG	GLN	ALA	
THR	THR	SER	THR	THR	ALA	VAL	PRO	LEU	
LYS	LYS	GLY	GLY	GLY	GLY	GLU	ASP	LYS	
ILE	ILE	ALA	ALA	ALA	GLY	PRO	ASN	ALA	
ALA	THR	THR	THR	THR	GLY	SER	HIS	ASN	
ASN	ASN	ASN	ASN	ASN	ALA	PRO	ALA	GLN	
ASN	ASN	THR	THR	THR	ASN	ASP	ASP	ASN	
THR	THR	PHE	PHE	PHE	ASN	SER	ALA	GLN	
ILE	GLY	GLY	GLY	GLY	GLU	SER	ASP	GLN	
GLN	VAL	THR	THR	THR	GLY	THR	ALA	LYS	
PHE	THR	THR	THR	THR	ASP	ILE	PHE	ASP	
THR	THR	THR	THR	THR	GLY	GLY	GLN	GLY	
ASP	THR	THR	THR	THR	VAL	LYS	GLU	GLY	
SER	SER	GLY	GLY	GLY	GLY	LYS	ARG	ARG	
GLU	GLU	TYR	TYR	TYR	GLY	LYS	LEU	LEU	
TYR	GLN	GLN	ASP	ASP	SER	GLN	GLN	VAL	
LEU	LEU	PHE	PHE	PHE	GLY	PRO	ASP	LEU	
PRO	PRO	ASN	ASN	ASN	ASN	ALA	THR	PRO	
TYR	TYR	ARG	ARG	ARG	TRP	ARG	SER	GLY	
VAL	PHE	PHE	HIS	HIS	HIS	LYS	PHE	TYR	
LEU	LEU	HIS	CYS	CYS	ASP	ARG	GLY	LYS	
GLY	GLY	CYS	THR	THR	SER	LEU	GLY	TYR	
ALA	ALA	PHE	HIS	PHE	SER	PHE	ASN	LEU	
HIS	HIS	SER	SER	THR	THR	GLY	LEU	GLY	
GLN	GLN	PRO	PRO	PRO	LEU	GLN	ARG	PRO	
GLY	GLY	ARG	ARG	ARG	GLY	THR	ALA	ASN	
CYS	CYS	ASP	ASP	ASP	ASP	GLY	VAL	GLY	
LEU	LEU	TRP	TRP	TRP	ARG	ASP	CHN	LEU	
LEU	LEU	VAL	VAL	VAL	VAL	SER	PHE	ASN	



- Molecule 1: Capsid protein

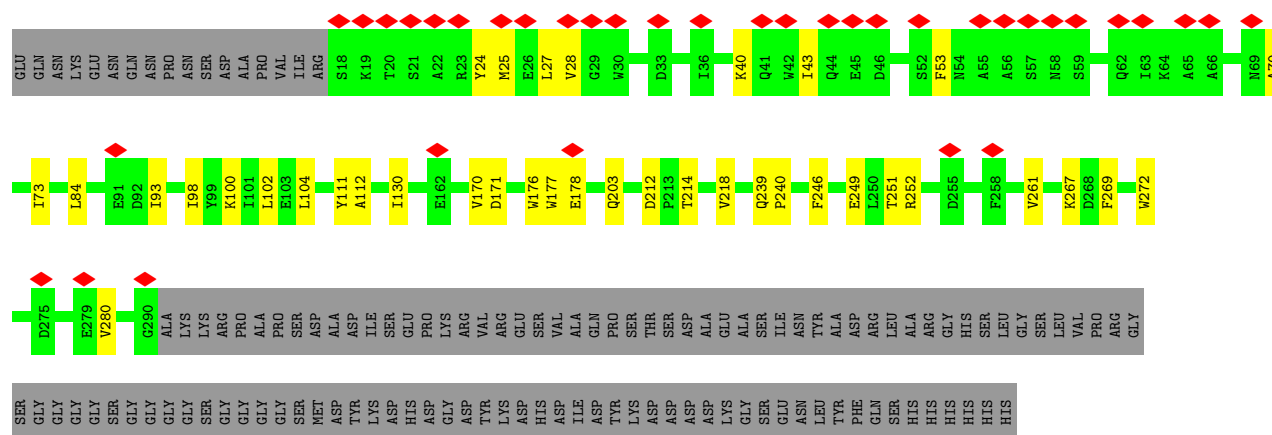
Chain X:  23% . 76%



- Molecule 1: Capsid protein

Chain Y: 98%

- Molecule 2: Protein Rep68



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	191887	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.360	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0397	Depositor
Map size (Å)	502.74, 502.74, 502.74	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.931, 0.931, 0.931	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/1658	0.39	0/2245
1	B	0.37	0/108	0.67	0/139
1	E	0.13	0/286	0.37	0/380
1	F	0.17	0/3622	0.36	0/4935
1	G	0.16	0/3593	0.37	1/4897 (0.0%)
1	H	0.15	0/1505	0.40	0/2038
1	I	0.13	0/197	0.39	0/262
1	Q	0.15	0/1604	0.38	0/2173
1	R	0.17	0/3597	0.36	0/4902
1	S	0.13	0/141	0.40	0/186
1	U	0.18	0/1473	0.43	0/1995
1	V	0.25	0/3542	0.44	0/4827
1	W	0.16	0/3534	0.34	0/4816
1	X	0.15	0/1474	0.37	0/1995
1	Y	0.14	0/101	0.46	0/129
2	a	0.12	0/2223	0.36	0/3008
2	b	0.13	0/2223	0.37	0/3008
2	c	0.14	0/2223	0.37	0/3008
2	d	0.37	0/2223	0.69	1/3008 (0.0%)
2	e	0.26	0/2223	0.54	0/3008
All	All	0.19	0/37550	0.41	2/50959 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	327	THR	OG1-CB-CG2	5.61	120.53	109.30
2	d	280	VAL	N-CA-C	5.44	120.65	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1625	0	1535	4	0
1	B	112	0	95	1	0
1	E	287	0	265	0	0
1	F	3515	0	3288	10	0
1	G	3486	0	3262	11	0
1	H	1477	0	1398	4	0
1	I	199	0	184	1	0
1	Q	1571	0	1481	5	0
1	R	3490	0	3265	13	0
1	S	144	0	130	1	0
1	U	1445	0	1359	7	0
1	V	3436	0	3206	14	0
1	W	3429	0	3198	11	0
1	X	1446	0	1361	7	0
1	Y	105	0	86	2	0
2	a	2172	0	2135	18	0
2	b	2172	0	2135	26	0
2	c	2172	0	2135	14	0
2	d	2172	0	2135	15	0
2	e	2172	0	2135	26	0
3	A	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
3	Q	27	0	12	0	0
3	R	27	0	12	0	0
3	U	27	0	12	0	0
3	V	27	0	12	0	0
3	W	27	0	12	0	0
3	X	27	0	12	0	0
3	c	27	0	12	0	0
3	e	27	0	12	0	0
4	A	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0
All	All	36961	0	34932	175	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 2.

The worst 5 of 175 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)
1:R:548:GLN:O	1:R:549:ASN:ND2	2.01	0.92
2:d:113:ALA:HB1	2:d:273:ALA:HB2	1.57	0.84
2:b:138:THR:HG22	2:b:253:ARG:NH2	1.93	0.83
1:F:372:VAL:HG11	1:G:657:PRO:HG3	1.65	0.79
1:F:657:PRO:HG3	1:R:372:VAL:HG11	1.67	0.75

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	188/738 (26%)	185 (98%)	3 (2%)	0	100	100
1	B	7/738 (1%)	7 (100%)	0	0	100	100
1	E	27/738 (4%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	428/738 (58%)	424 (99%)	4 (1%)	0	100	100
1	G	424/738 (58%)	415 (98%)	9 (2%)	0	100	100
1	H	172/738 (23%)	170 (99%)	2 (1%)	0	100	100
1	I	17/738 (2%)	17 (100%)	0	0	100	100
1	Q	183/738 (25%)	181 (99%)	2 (1%)	0	100	100
1	R	425/738 (58%)	421 (99%)	4 (1%)	0	100	100
1	S	12/738 (2%)	12 (100%)	0	0	100	100
1	U	168/738 (23%)	164 (98%)	4 (2%)	0	100	100
1	V	417/738 (56%)	412 (99%)	5 (1%)	0	100	100
1	W	416/738 (56%)	411 (99%)	5 (1%)	0	100	100
1	X	168/738 (23%)	163 (97%)	5 (3%)	0	100	100
1	Y	6/738 (1%)	6 (100%)	0	0	100	100
2	a	271/397 (68%)	262 (97%)	9 (3%)	0	100	100
2	b	271/397 (68%)	263 (97%)	8 (3%)	0	100	100
2	c	271/397 (68%)	263 (97%)	7 (3%)	1 (0%)	30	34
2	d	271/397 (68%)	262 (97%)	8 (3%)	1 (0%)	30	34
2	e	271/397 (68%)	263 (97%)	8 (3%)	0	100	100
All	All	4413/13055 (34%)	4327 (98%)	84 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	d	280	VAL
2	c	90	VAL

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	177/618 (29%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	12/618 (2%)	12 (100%)	0	100	100
1	E	30/618 (5%)	29 (97%)	1 (3%)	33	45
1	F	386/618 (62%)	386 (100%)	0	100	100
1	G	383/618 (62%)	379 (99%)	4 (1%)	68	81
1	H	161/618 (26%)	160 (99%)	1 (1%)	78	89
1	I	21/618 (3%)	20 (95%)	1 (5%)	23	30
1	Q	171/618 (28%)	167 (98%)	4 (2%)	44	59
1	R	383/618 (62%)	378 (99%)	5 (1%)	61	76
1	S	15/618 (2%)	14 (93%)	1 (7%)	15	17
1	U	157/618 (25%)	155 (99%)	2 (1%)	61	76
1	V	377/618 (61%)	375 (100%)	2 (0%)	81	90
1	W	376/618 (61%)	371 (99%)	5 (1%)	61	76
1	X	157/618 (25%)	156 (99%)	1 (1%)	78	89
1	Y	11/618 (2%)	11 (100%)	0	100	100
2	a	235/333 (71%)	232 (99%)	3 (1%)	61	76
2	b	235/333 (71%)	234 (100%)	1 (0%)	84	92
2	c	235/333 (71%)	233 (99%)	2 (1%)	70	84
2	d	235/333 (71%)	230 (98%)	5 (2%)	47	63
2	e	235/333 (71%)	235 (100%)	0	100	100
All	All	3992/10935 (36%)	3954 (99%)	38 (1%)	65	81

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	284	PHE
2	d	161	ASN
2	a	285	TYR
2	c	233	THR
2	d	280	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	237	HIS

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Mol	Chain	Res	Type
2	c	58	ASN
2	d	238	GLN
1	R	344	GLN
1	R	291	HIS

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 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	ADP	U	2000	4	28,29,29	1.36	4 (14%)	43,45,45	1.85	9 (20%)
3	ADP	c	1000	-	28,29,29	1.40	4 (14%)	43,45,45	1.90	11 (25%)
3	ADP	W	2000	4	28,29,29	1.37	4 (14%)	43,45,45	1.91	9 (20%)
3	ADP	A	2000	4	28,29,29	1.39	4 (14%)	43,45,45	1.88	11 (25%)
3	ADP	X	2000	4	28,29,29	1.37	4 (14%)	43,45,45	1.91	9 (20%)
3	ADP	F	2000	-	28,29,29	1.36	4 (14%)	43,45,45	1.88	10 (23%)
3	ADP	e	1000	-	28,29,29	1.01	1 (3%)	43,45,45	1.33	9 (20%)
3	ADP	H	2000	4	28,29,29	1.38	4 (14%)	43,45,45	1.88	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	R	2000	4	28,29,29	1.37	4 (14%)	43,45,45	1.88	8 (18%)
3	ADP	G	2000	4	28,29,29	1.36	4 (14%)	43,45,45	1.89	10 (23%)
3	ADP	V	2000	4	28,29,29	1.09	0	43,45,45	1.16	5 (11%)
3	ADP	Q	2000	4	28,29,29	1.36	4 (14%)	43,45,45	1.90	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	U	2000	4	-	5/16/32/32	0/3/3/3
3	ADP	c	1000	-	-	0/16/32/32	0/3/3/3
3	ADP	W	2000	4	-	2/16/32/32	0/3/3/3
3	ADP	A	2000	4	-	5/16/32/32	0/3/3/3
3	ADP	X	2000	4	-	3/16/32/32	0/3/3/3
3	ADP	F	2000	-	-	1/16/32/32	0/3/3/3
3	ADP	e	1000	-	-	2/16/32/32	0/3/3/3
3	ADP	H	2000	4	-	5/16/32/32	0/3/3/3
3	ADP	R	2000	4	-	0/16/32/32	0/3/3/3
3	ADP	G	2000	4	-	7/16/32/32	0/3/3/3
3	ADP	V	2000	4	-	0/16/32/32	0/3/3/3
3	ADP	Q	2000	4	-	2/16/32/32	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	1000	ADP	C5-C4	4.61	1.47	1.39
3	H	2000	ADP	C5-C4	4.50	1.47	1.39
3	W	2000	ADP	C5-C4	4.50	1.47	1.39
3	A	2000	ADP	C5-C4	4.50	1.47	1.39
3	X	2000	ADP	C5-C4	4.50	1.47	1.39

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	2000	ADP	C5-C4-N3	-6.05	118.38	126.72
3	W	2000	ADP	C5-C4-N3	-6.03	118.41	126.72
3	Q	2000	ADP	C5-C4-N3	-6.02	118.42	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2000	ADP	C5-C4-N3	-5.92	118.56	126.72
3	R	2000	ADP	C5-C4-N3	-5.92	118.56	126.72

There are no chirality outliers.

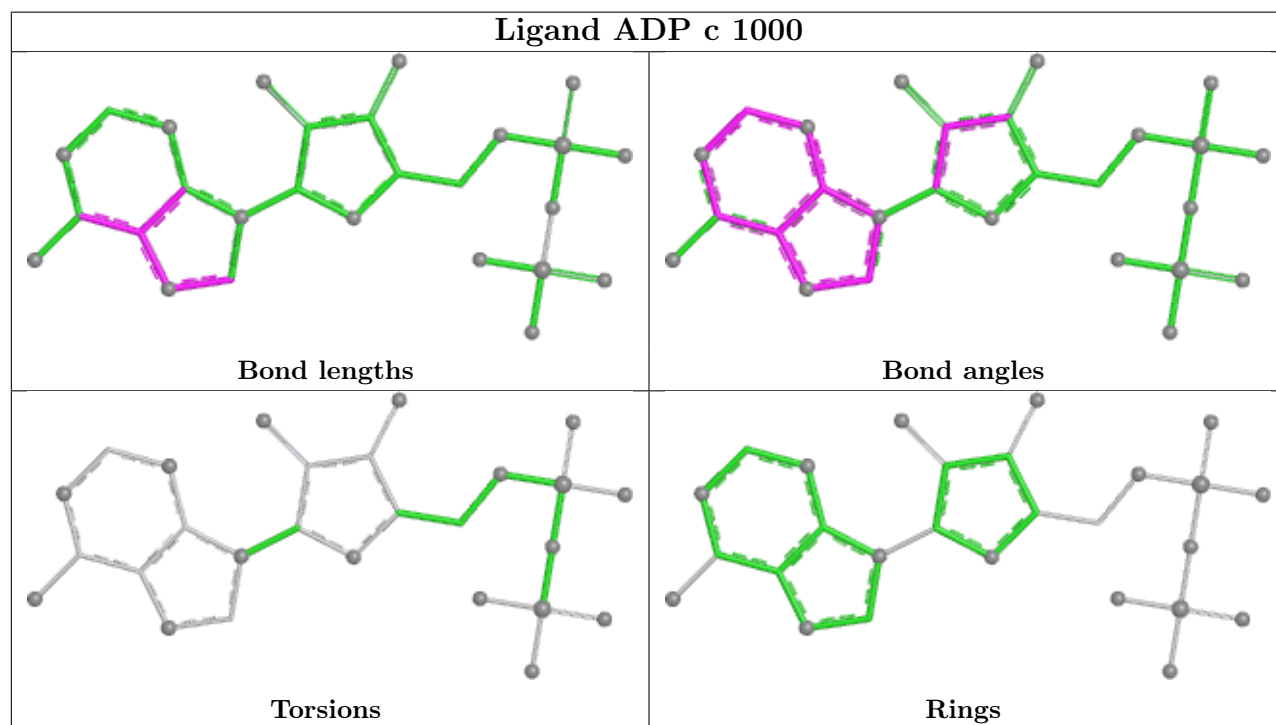
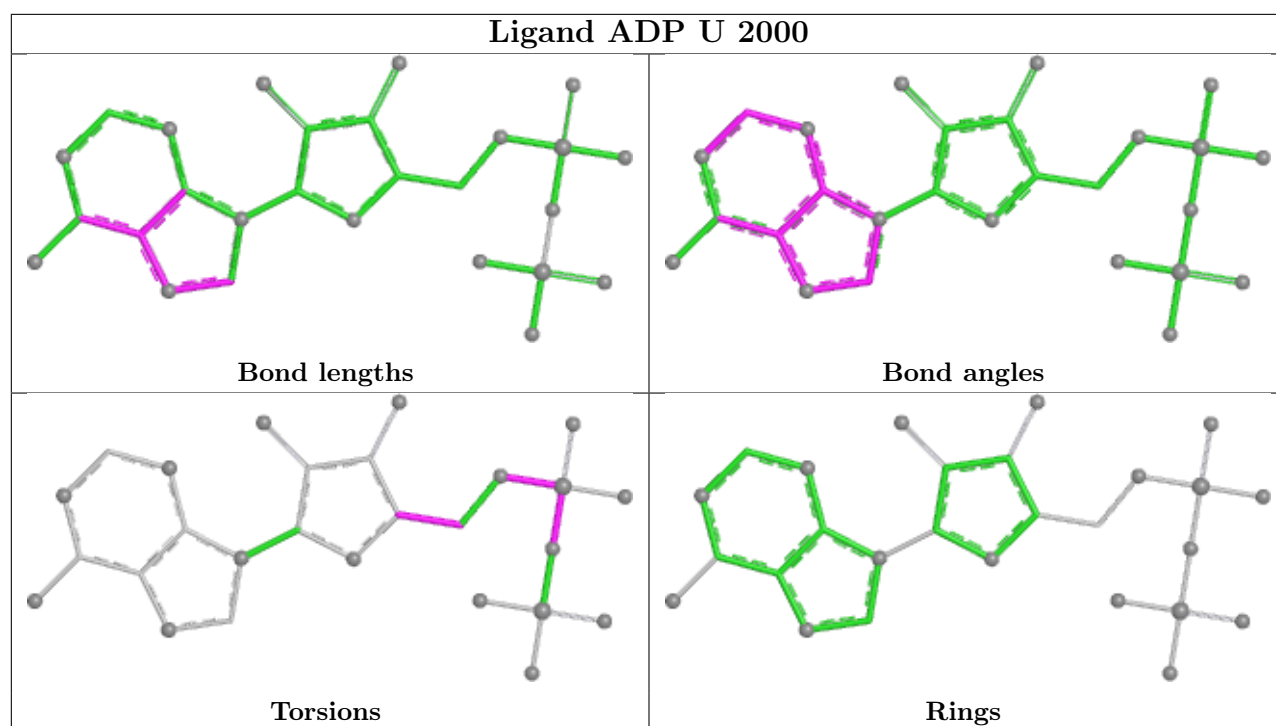
5 of 32 torsion outliers are listed below:

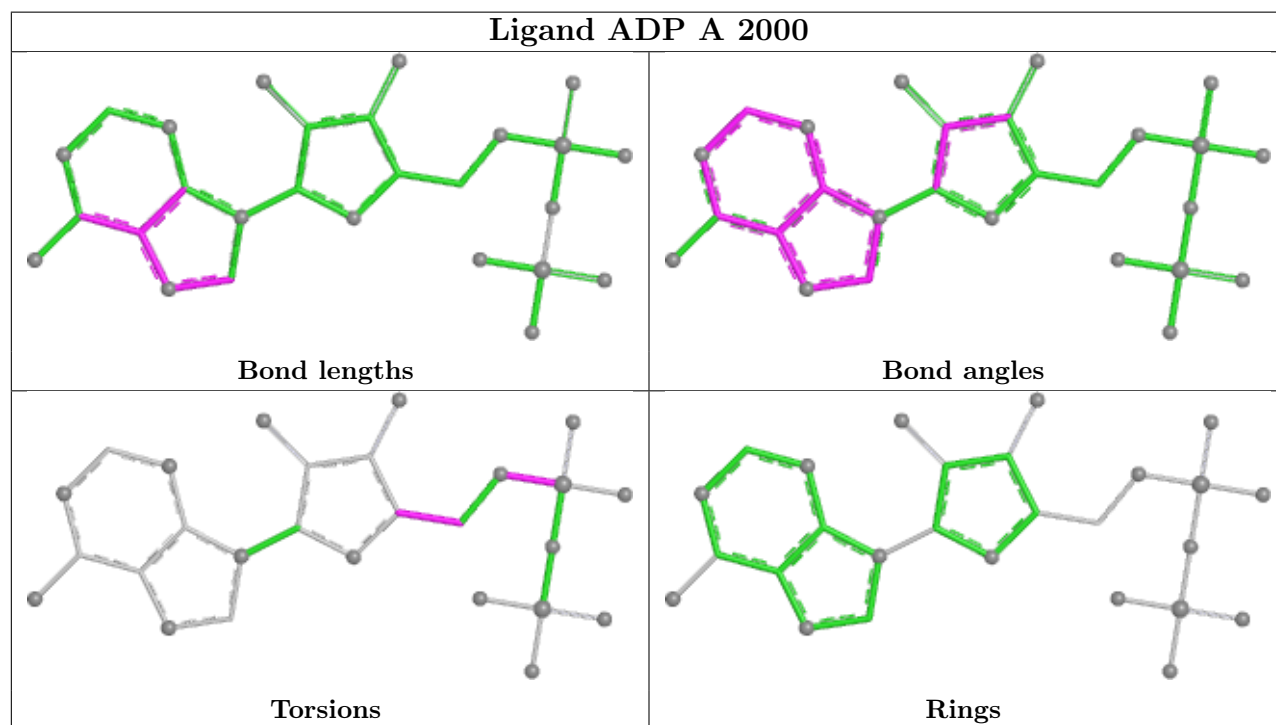
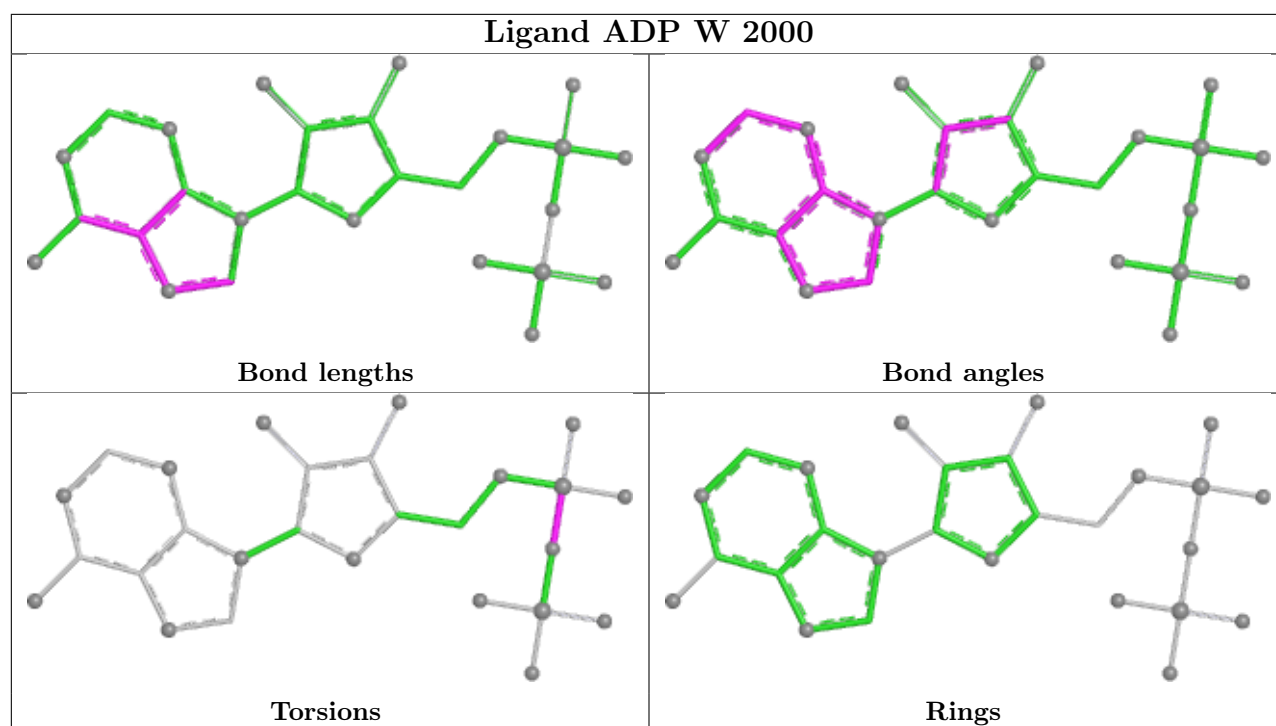
Mol	Chain	Res	Type	Atoms
3	A	2000	ADP	C5'-O5'-PA-O1A
3	A	2000	ADP	C5'-O5'-PA-O2A
3	A	2000	ADP	C5'-O5'-PA-O3A
3	G	2000	ADP	C5'-O5'-PA-O1A
3	G	2000	ADP	C5'-O5'-PA-O2A

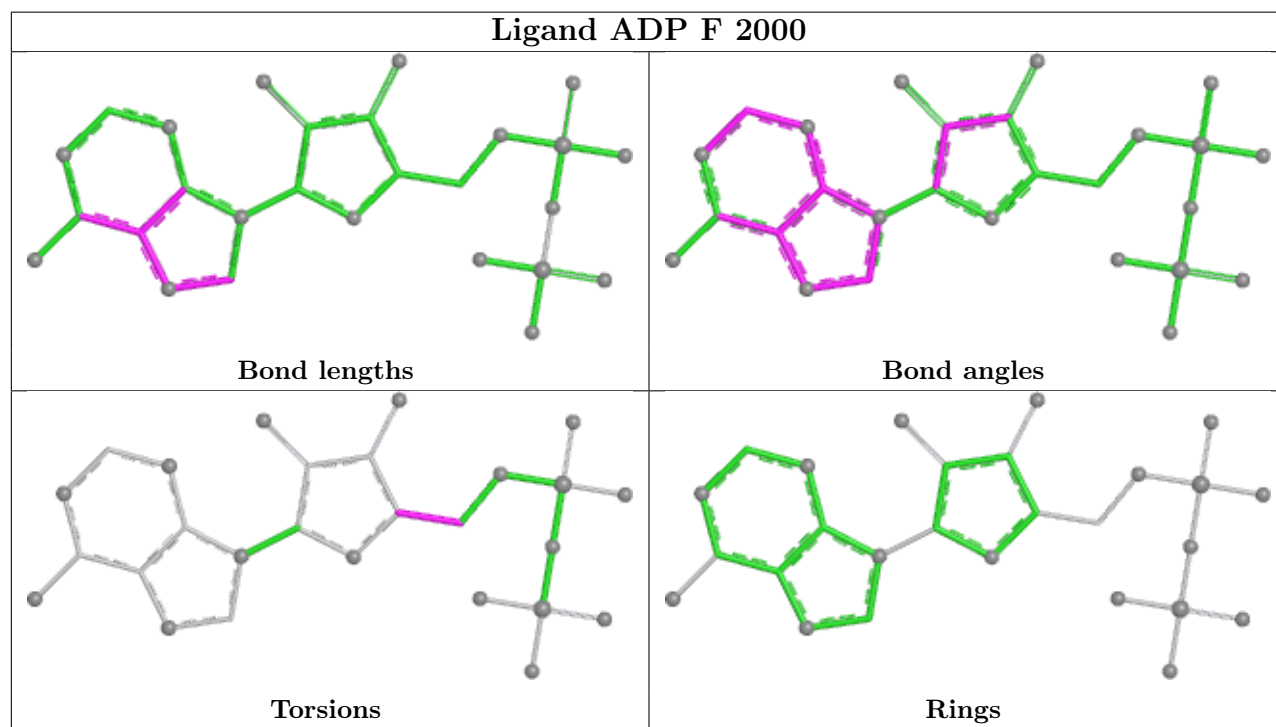
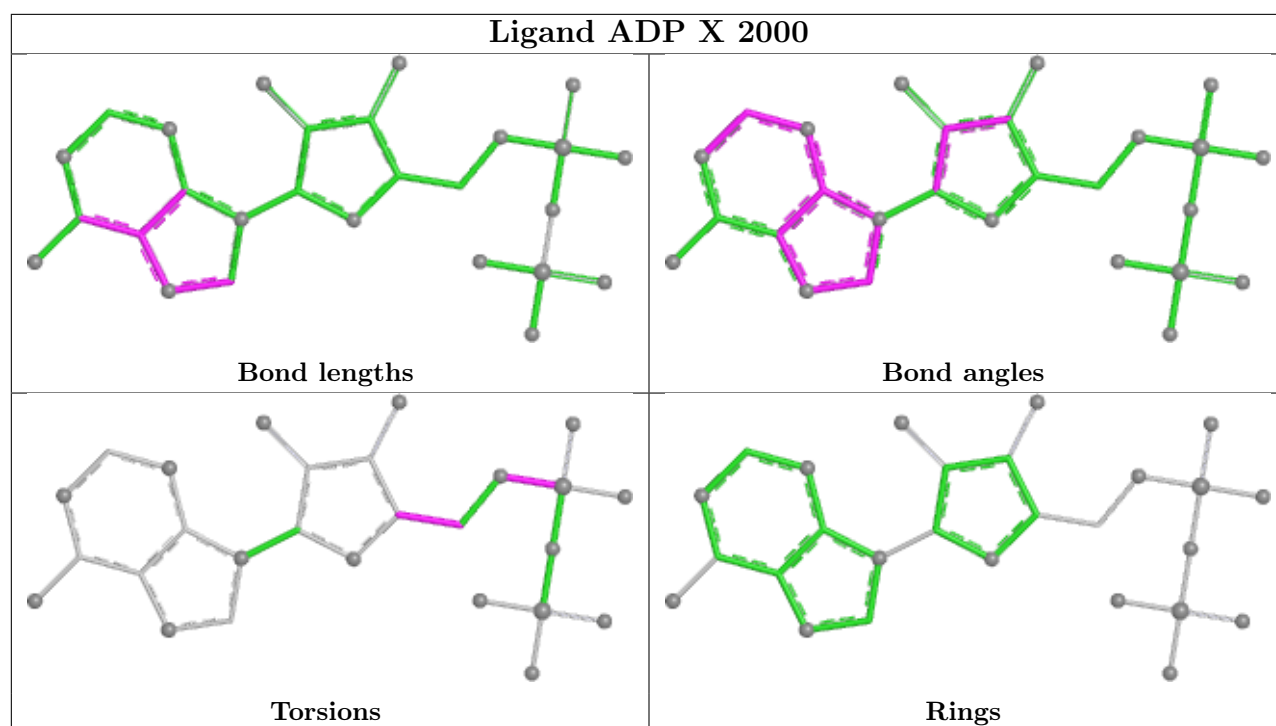
There are no ring outliers.

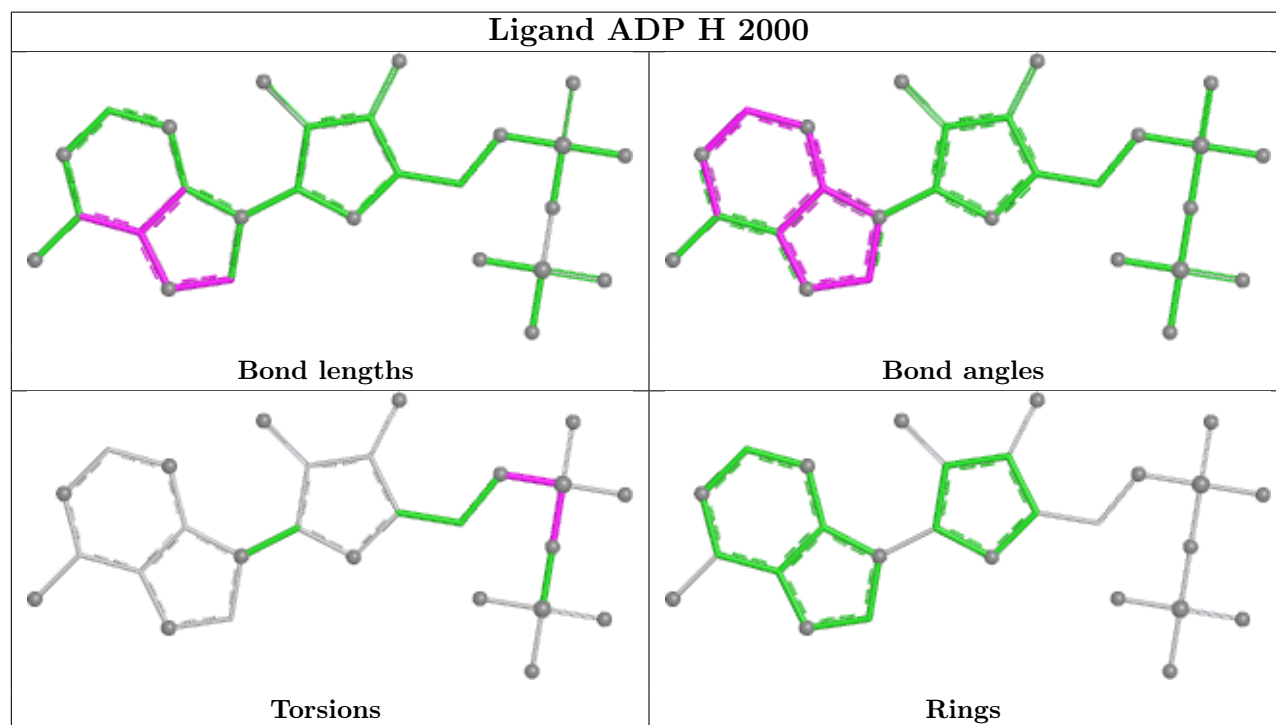
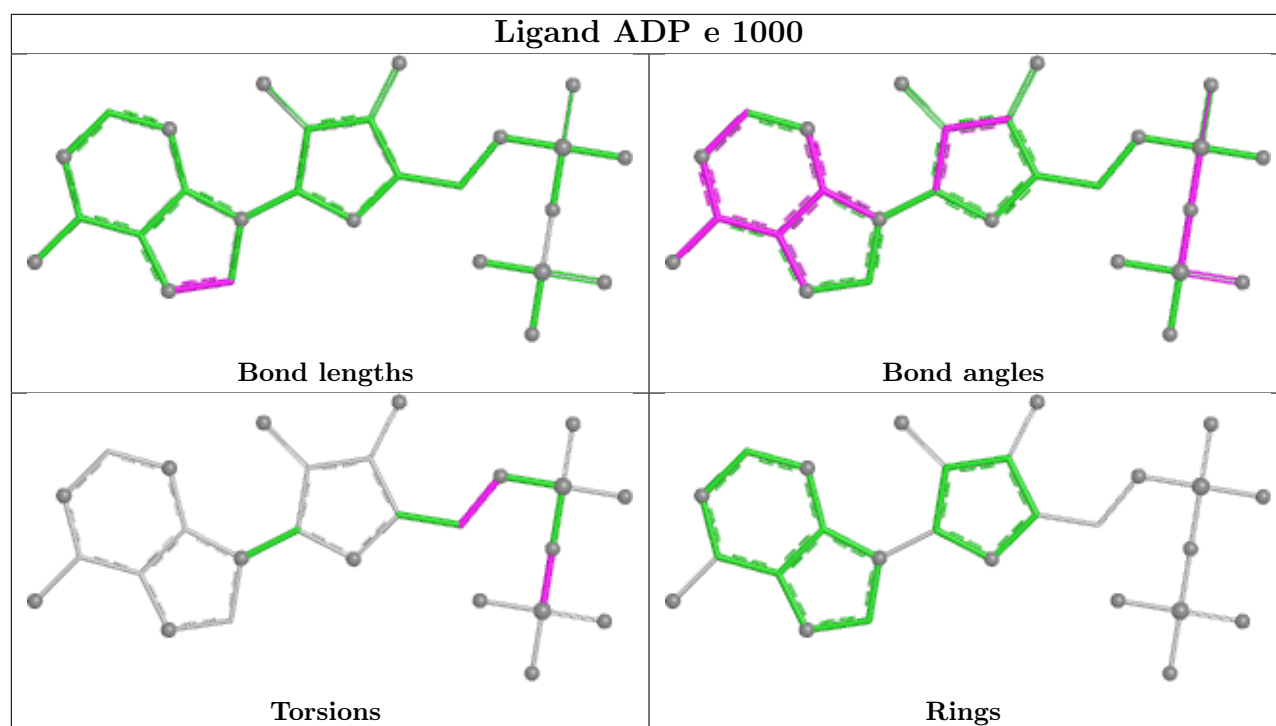
No monomer is involved in short contacts.

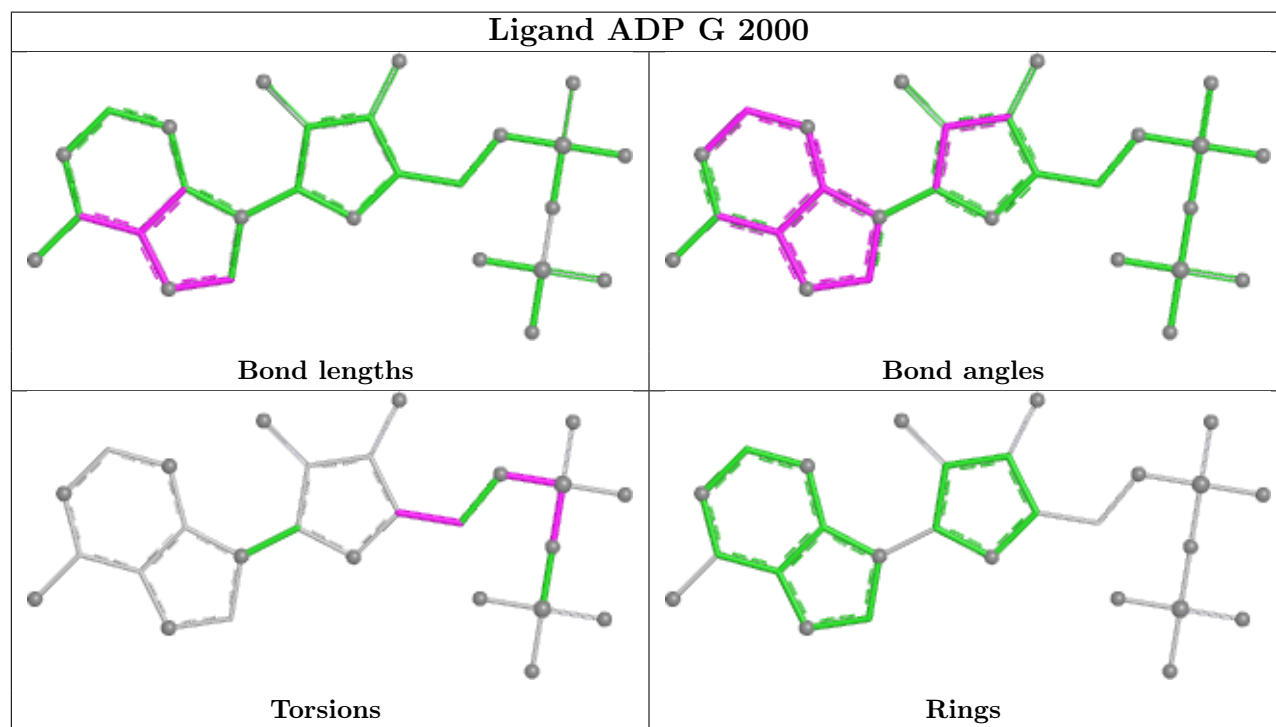
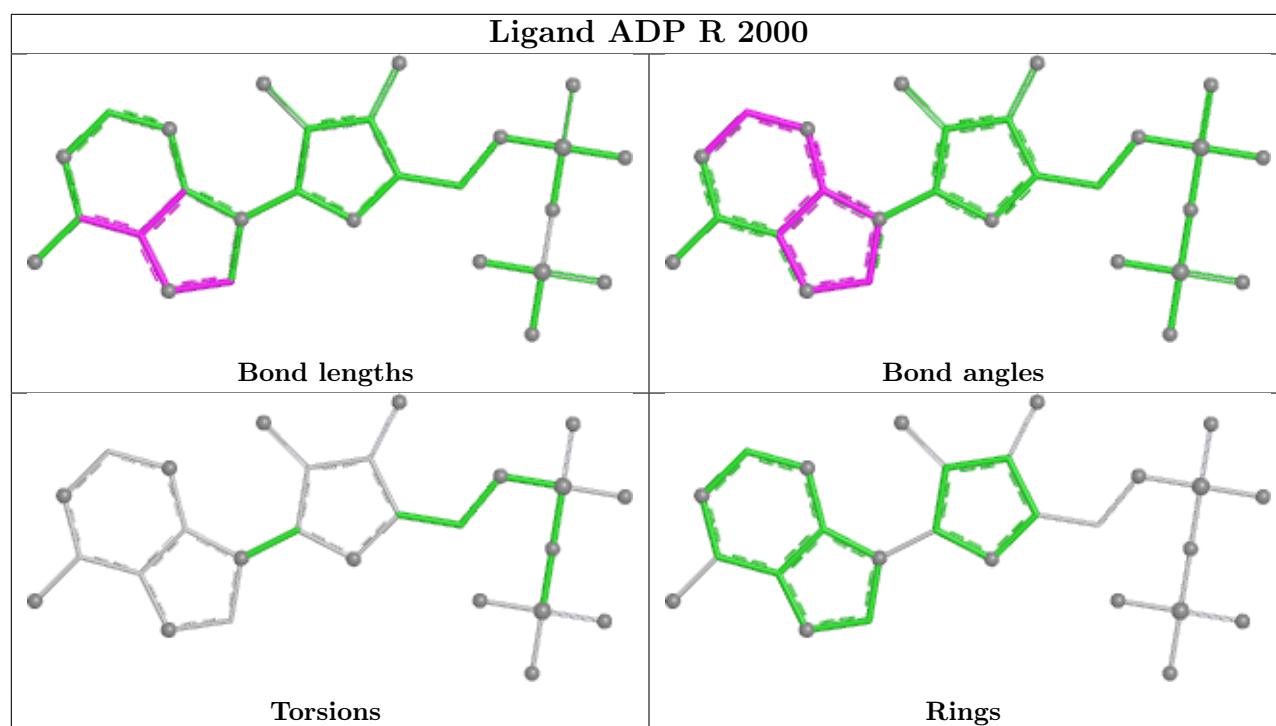
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

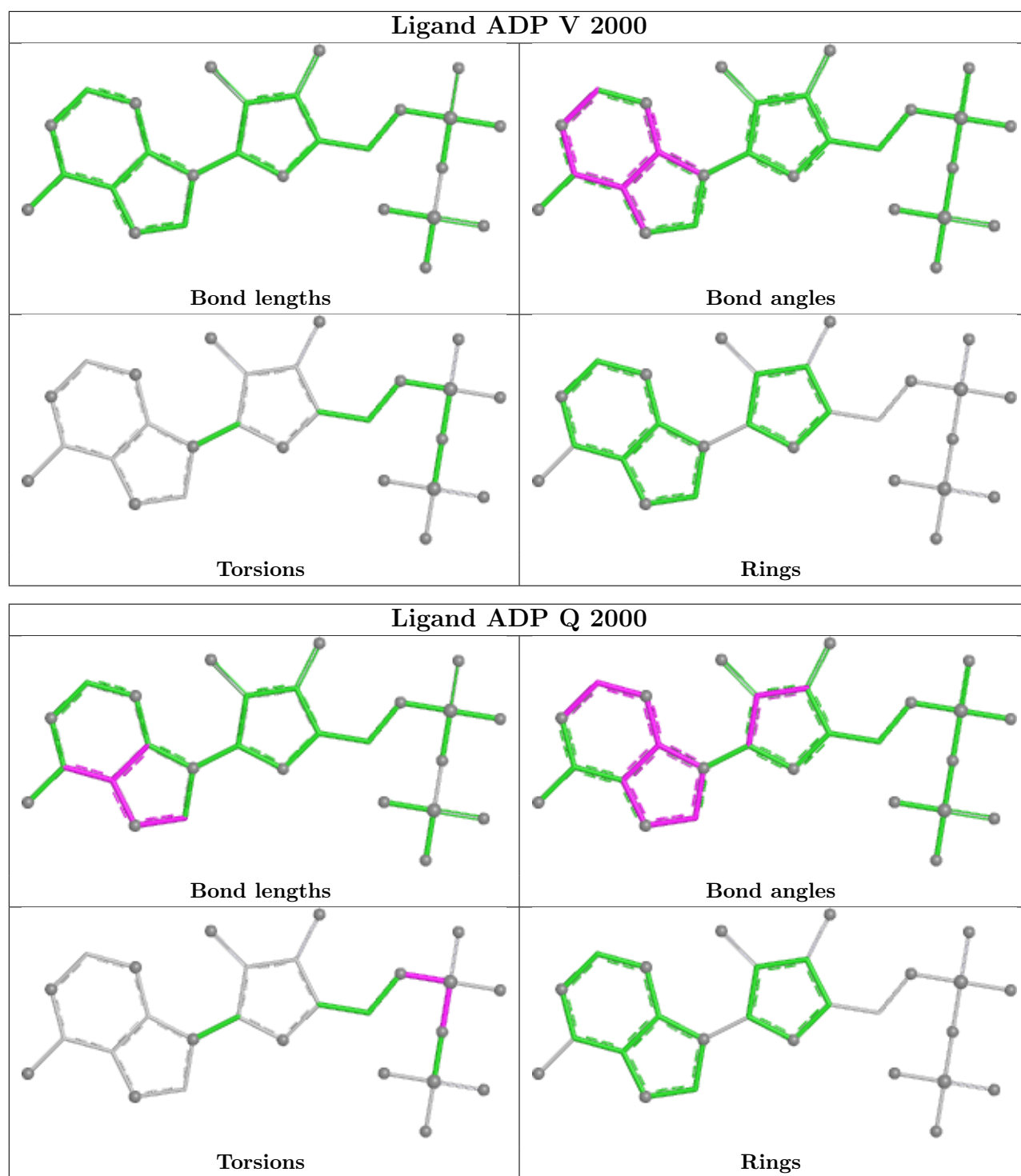












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

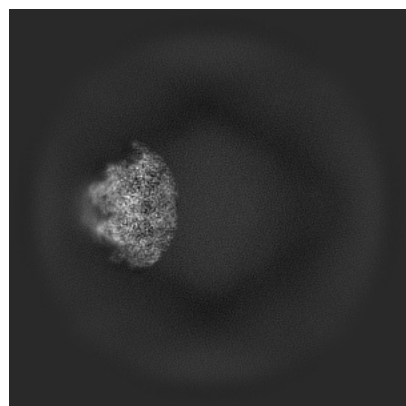
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54328. These allow visual inspection of the internal detail of the map and identification of artifacts.

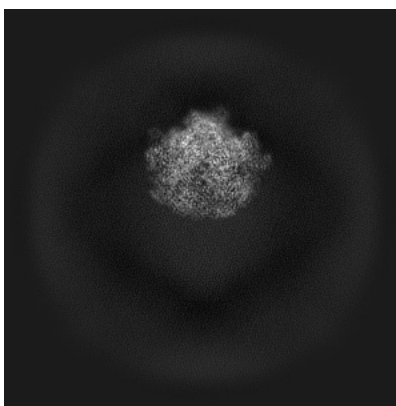
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

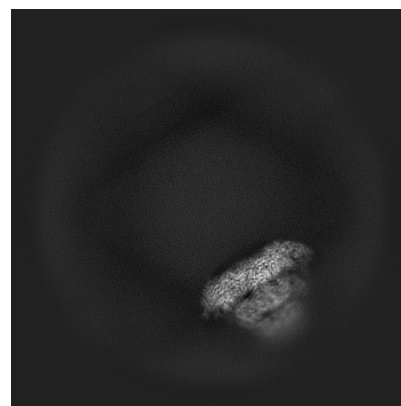
6.1.1 Primary map



X

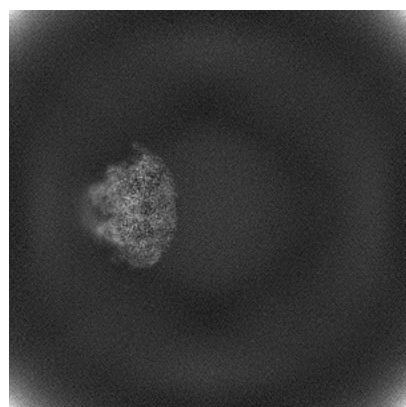


Y

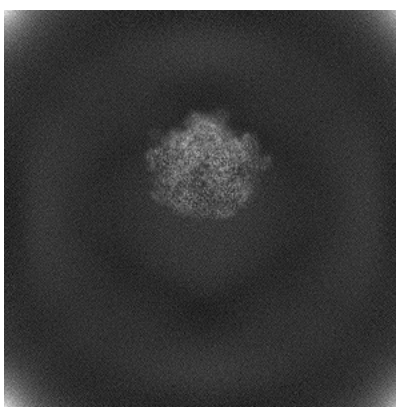


Z

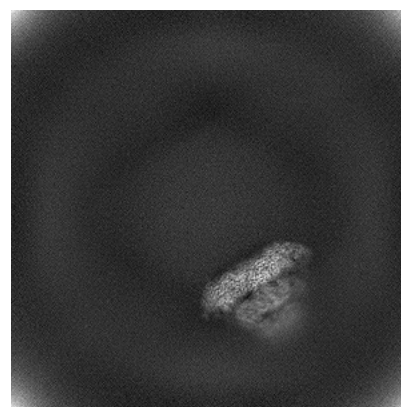
6.1.2 Raw map



X



Y

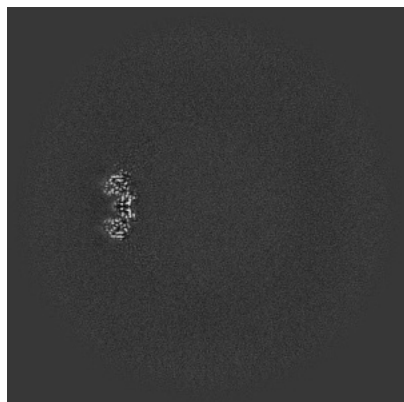


Z

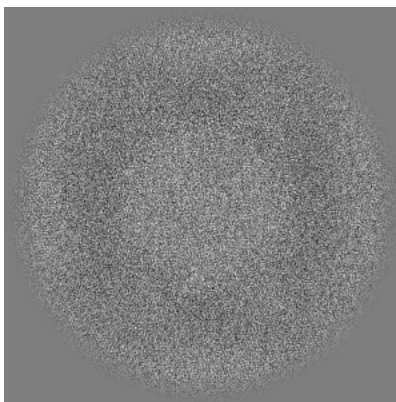
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 270

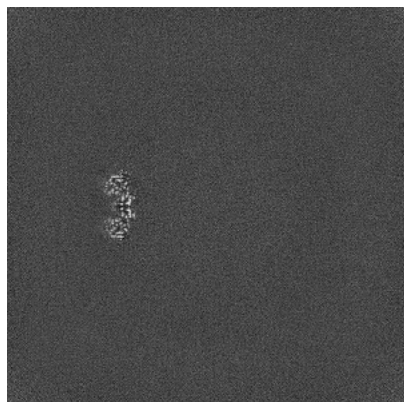


Y Index: 270

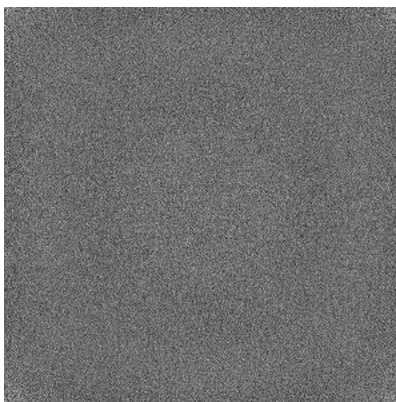


Z Index: 270

6.2.2 Raw map



X Index: 270



Y Index: 270

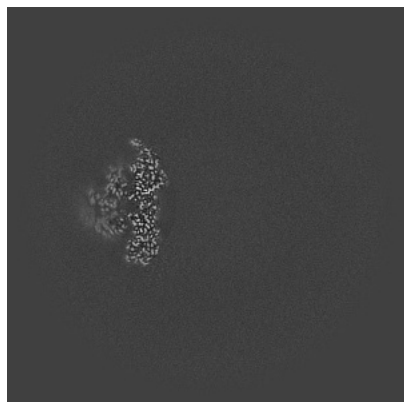


Z Index: 270

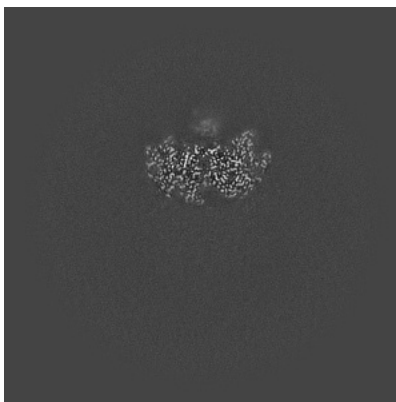
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

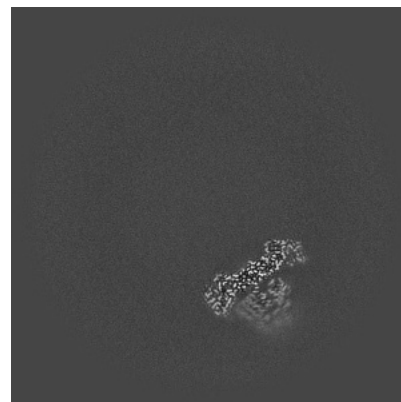
6.3.1 Primary map



X Index: 336

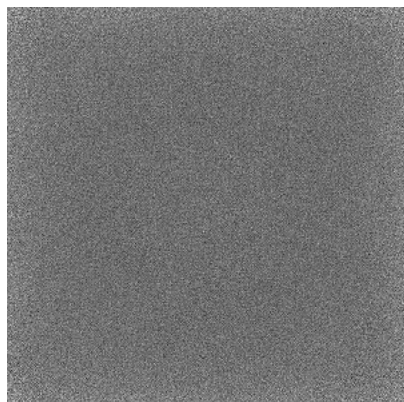


Y Index: 178

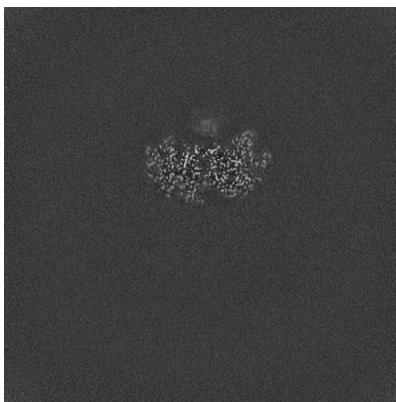


Z Index: 247

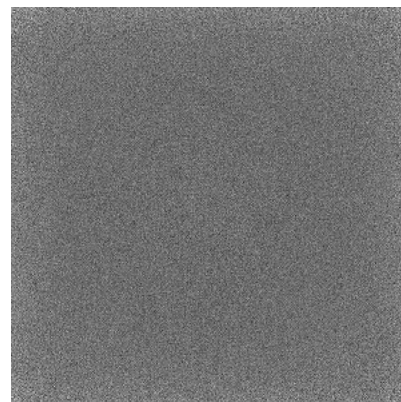
6.3.2 Raw map



X Index: 0



Y Index: 178

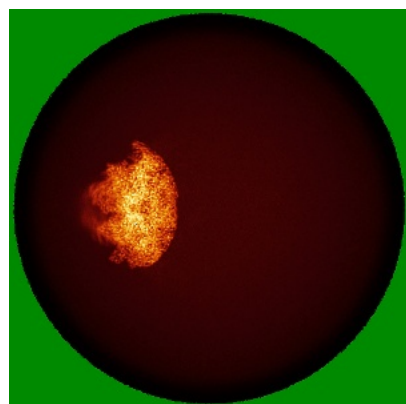


Z Index: 0

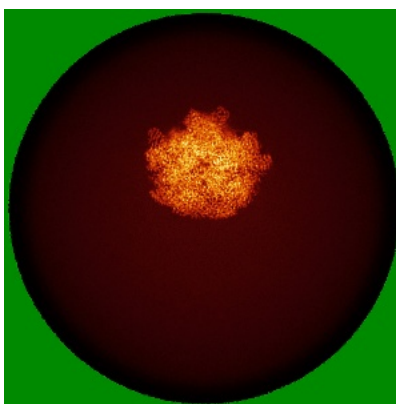
The images above show the largest variance slices of the map in three orthogonal directions.

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

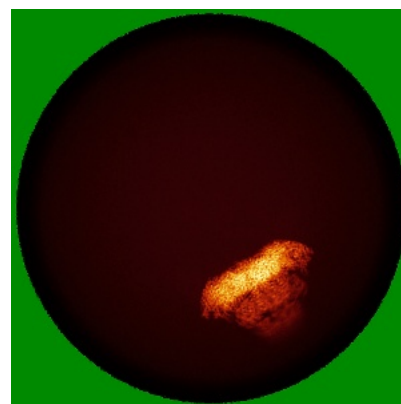
6.4.1 Primary map



X

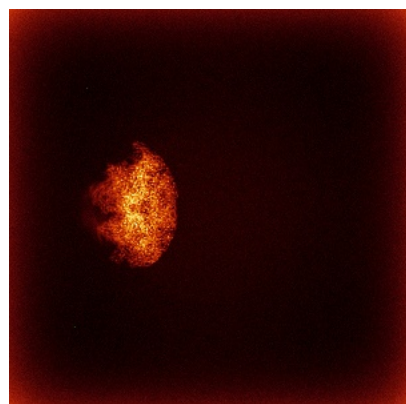


Y

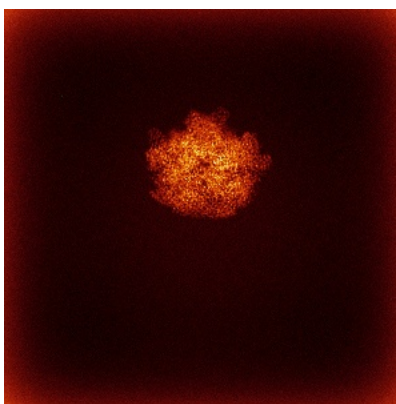


Z

6.4.2 Raw map



X



Y

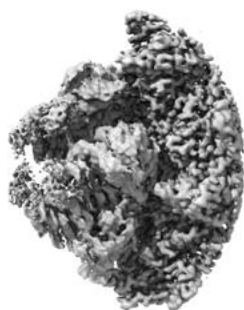


Z

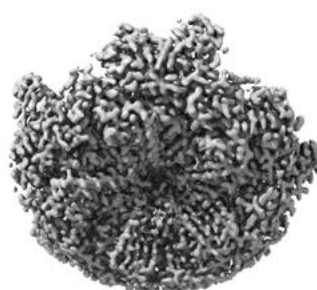
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

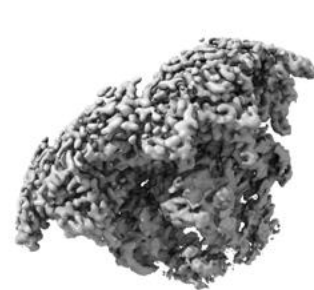
6.5.1 Primary map



X



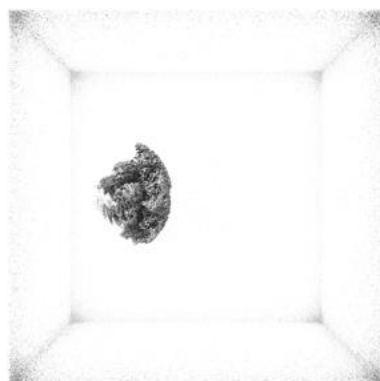
Y



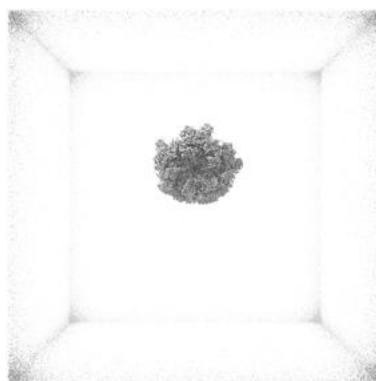
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0397. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

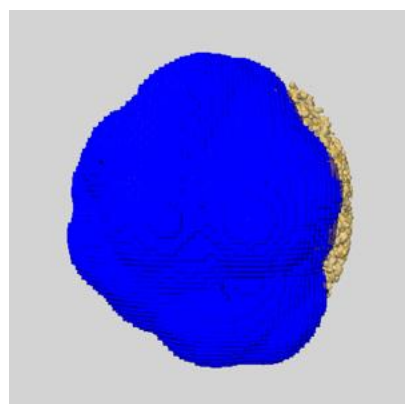
6.6 Mask visualisation [i](#)

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

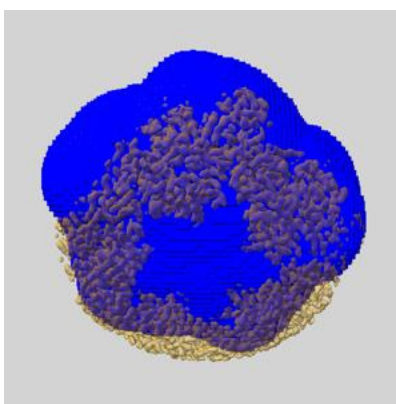
A mask typically either:

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

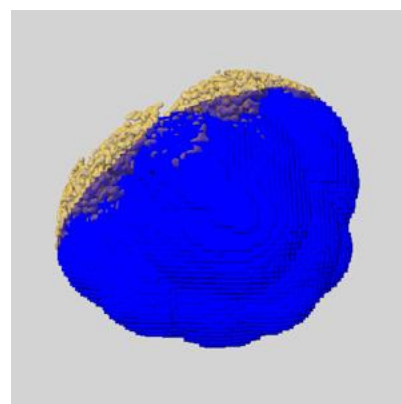
6.6.1 emd_54328_msk_1.map [i](#)



X



Y

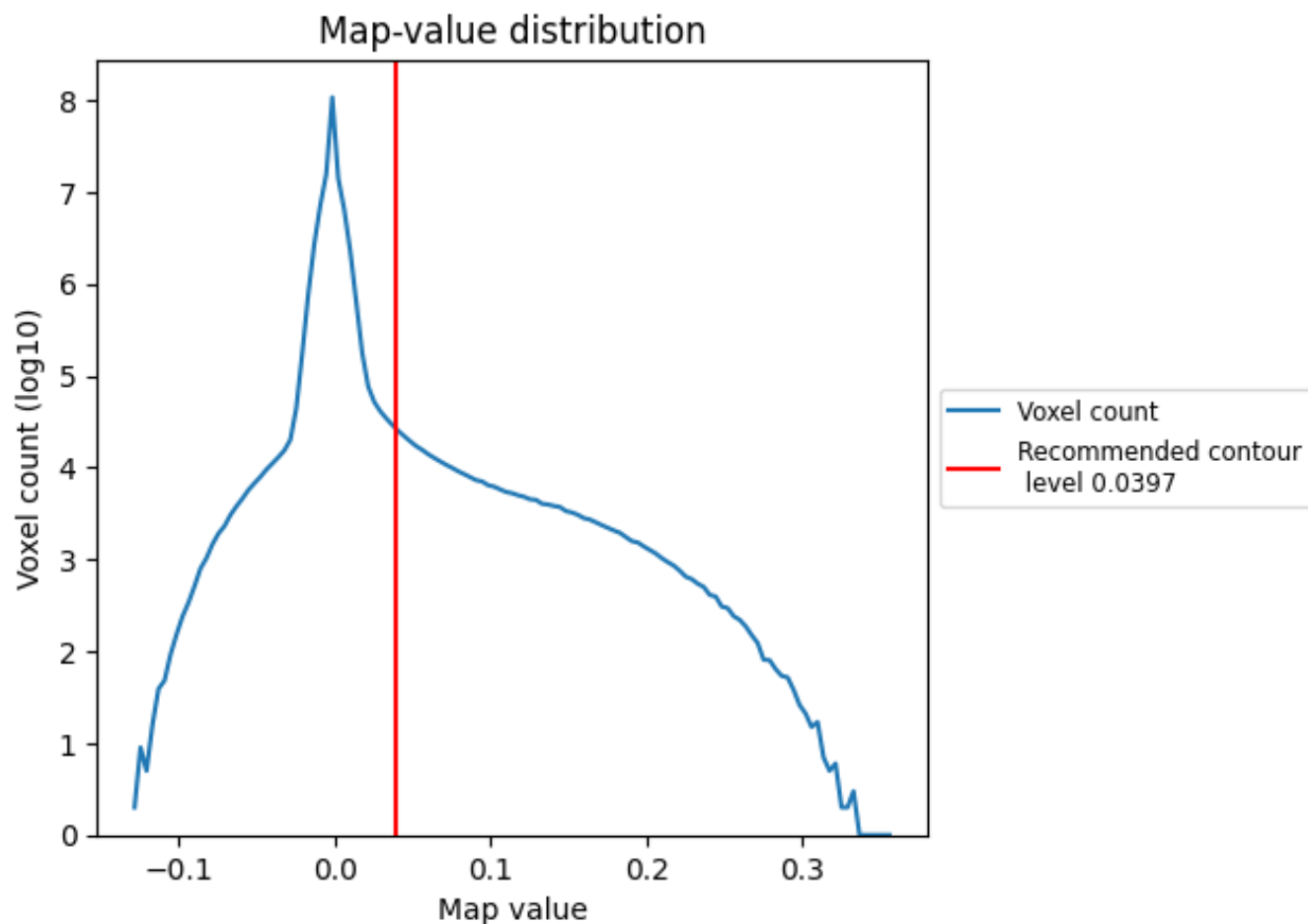


Z

7 Map analysis [i](#)

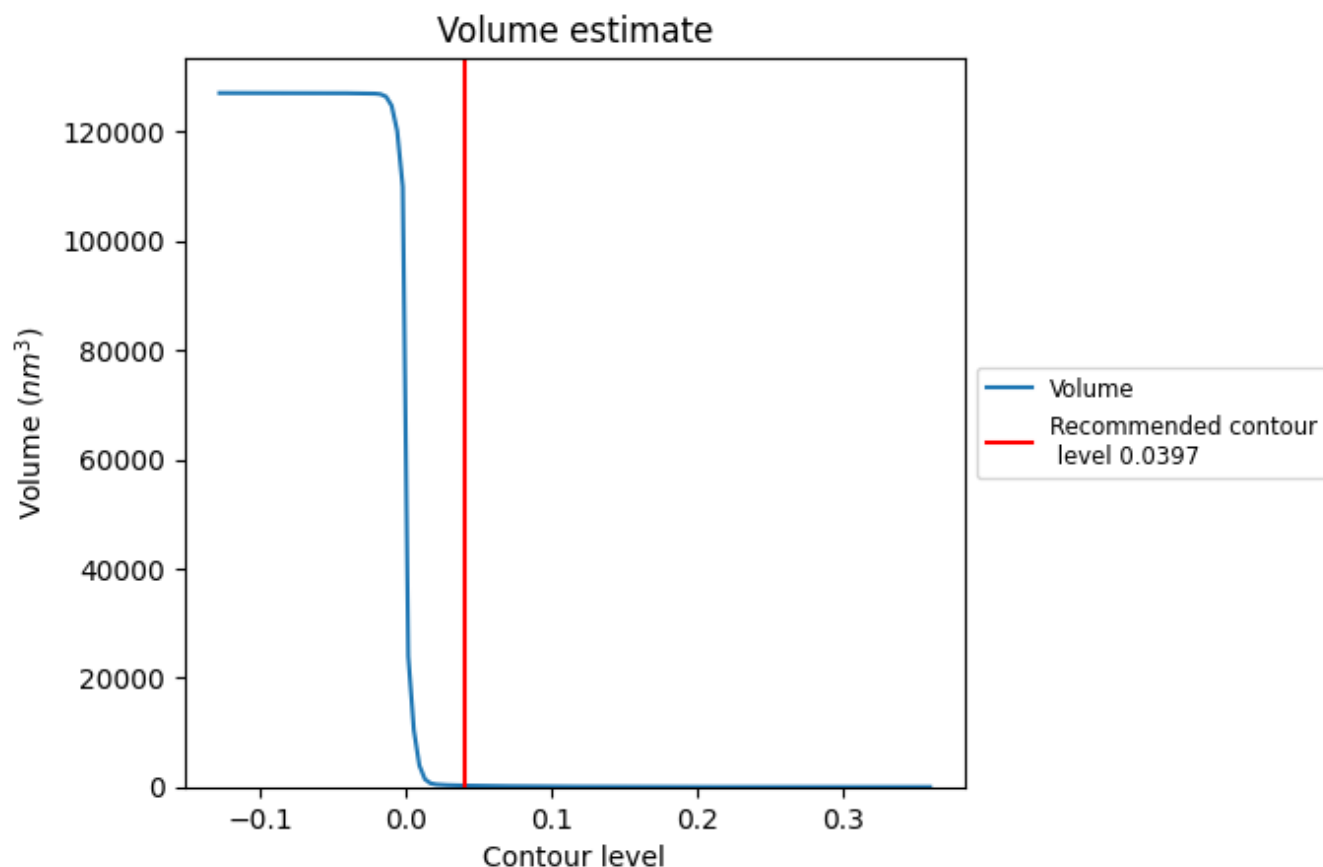
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

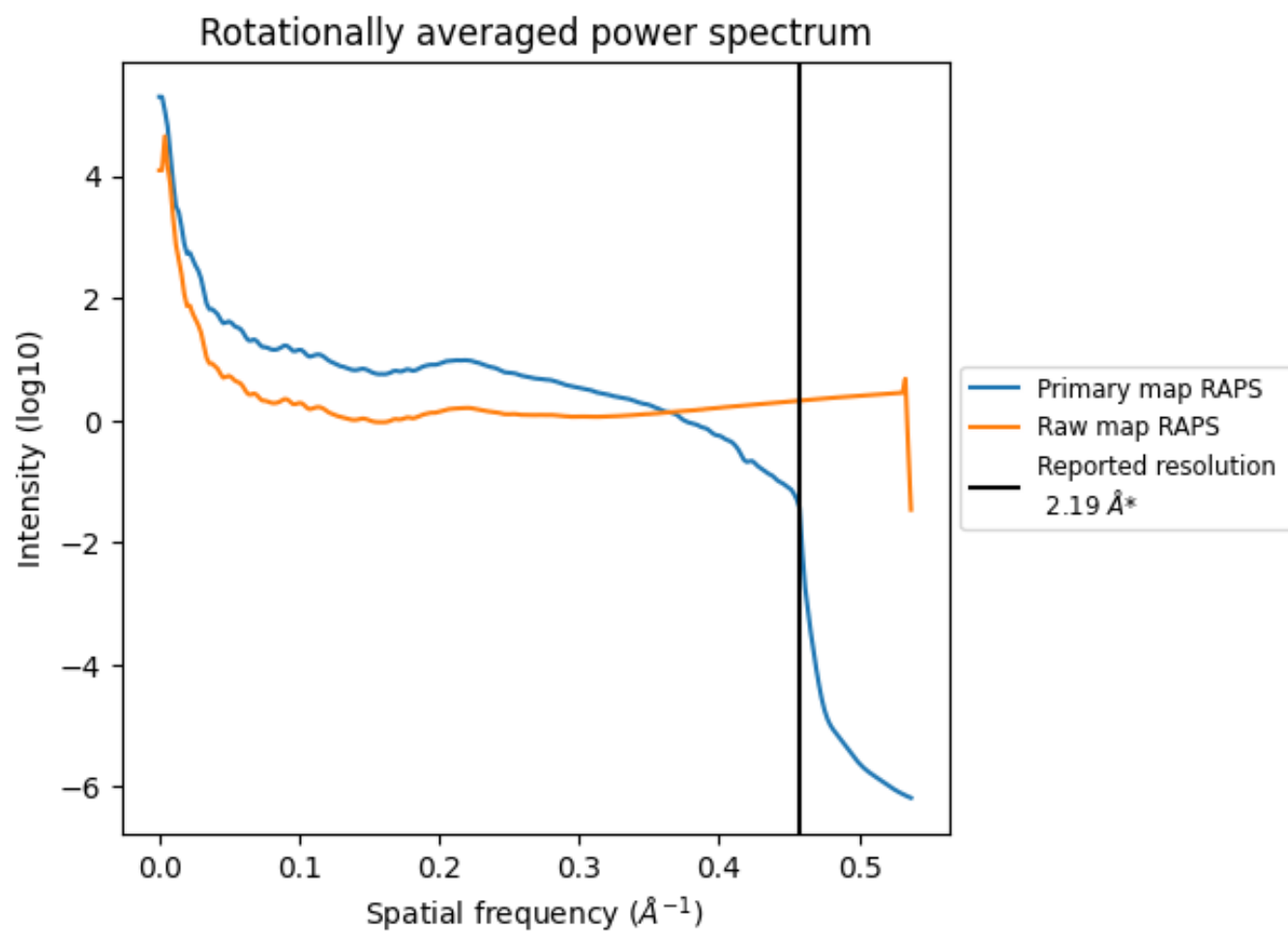
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm^3 ; this corresponds to an approximate mass of 229 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 ⓘ

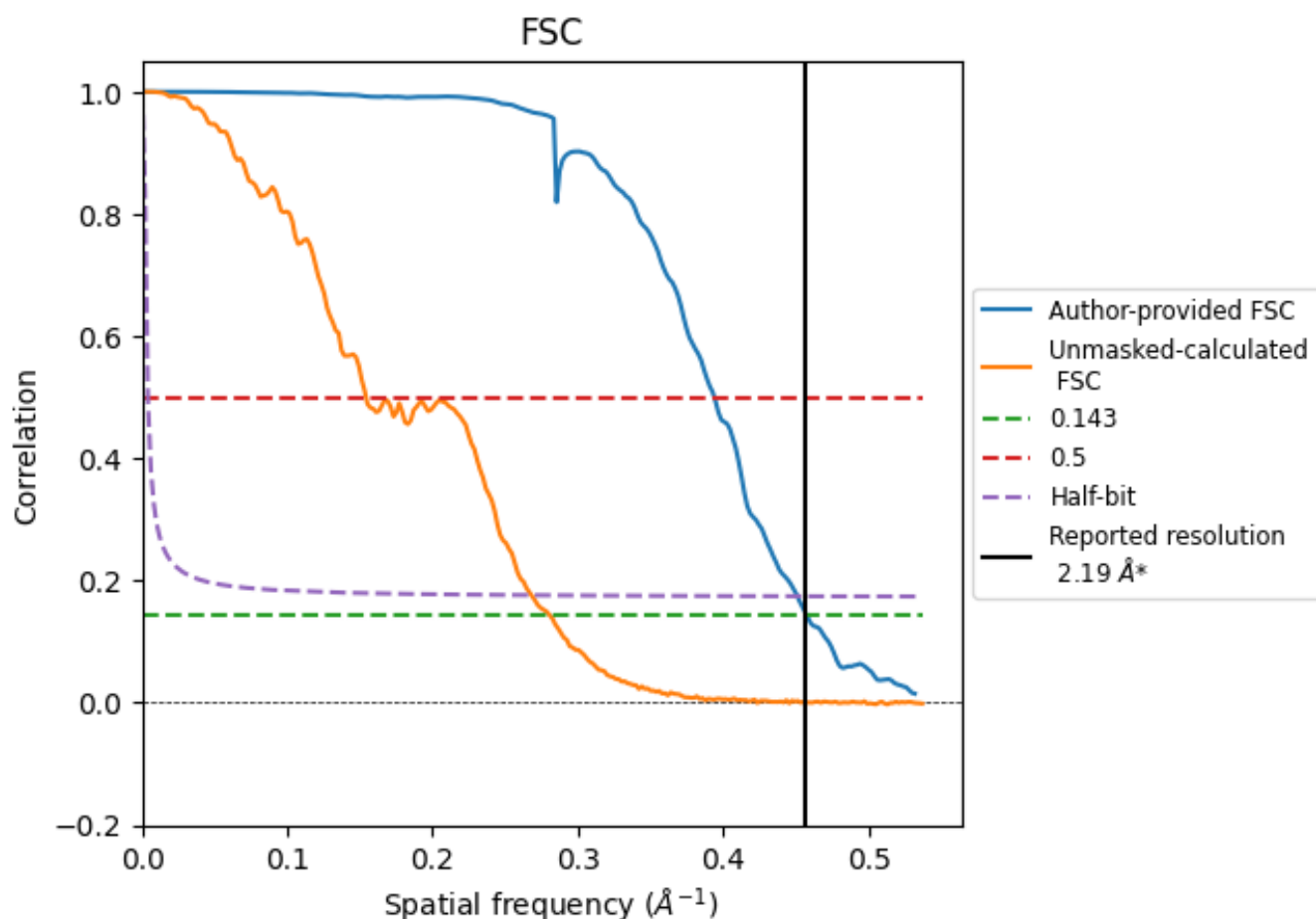


*Reported resolution corresponds to spatial frequency of 0.457 Å⁻¹

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 $0.457 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

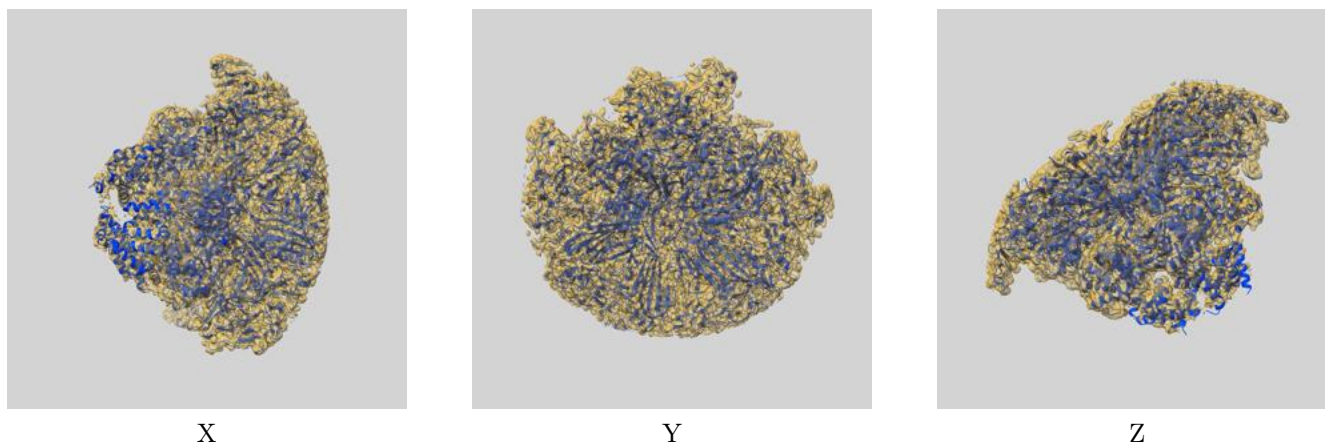
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.54	2.22
Unmasked-calculated*	3.56	6.49	3.73

*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 3.56 differs from the reported value 2.19 by more than 10 %

9 Map-model fit [i](#)

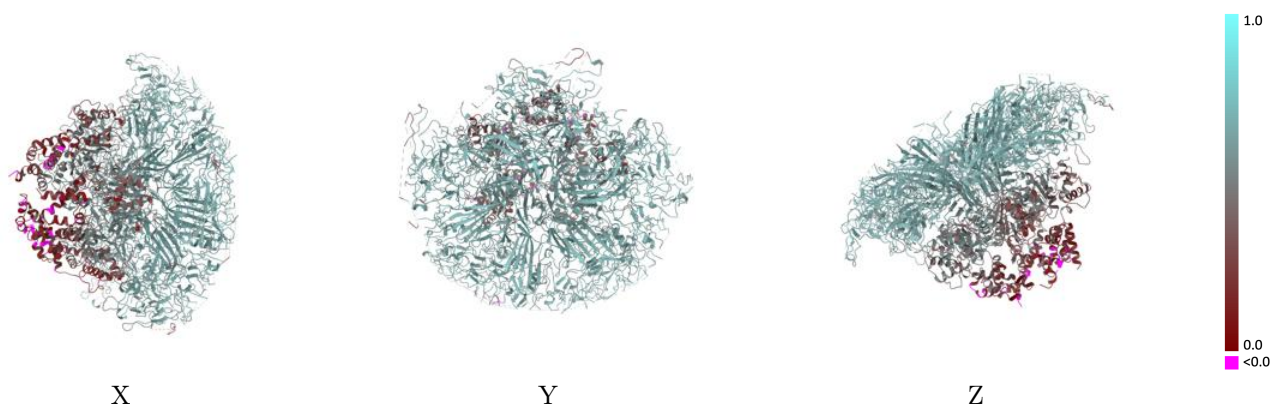
This section contains information regarding the fit between EMDB map EMD-54328 and PDB model 9RWG. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



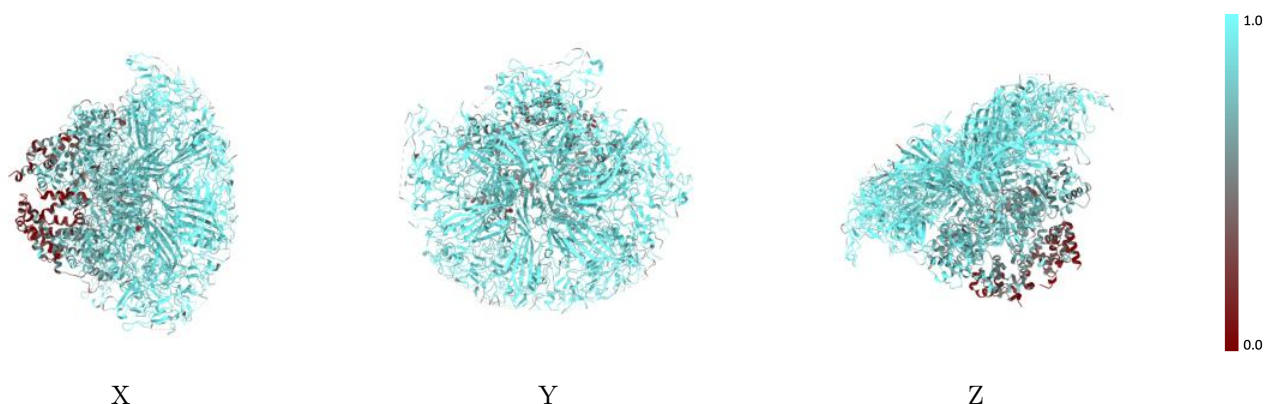
The images above show the 3D surface view of the map at the recommended contour level 0.0397 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



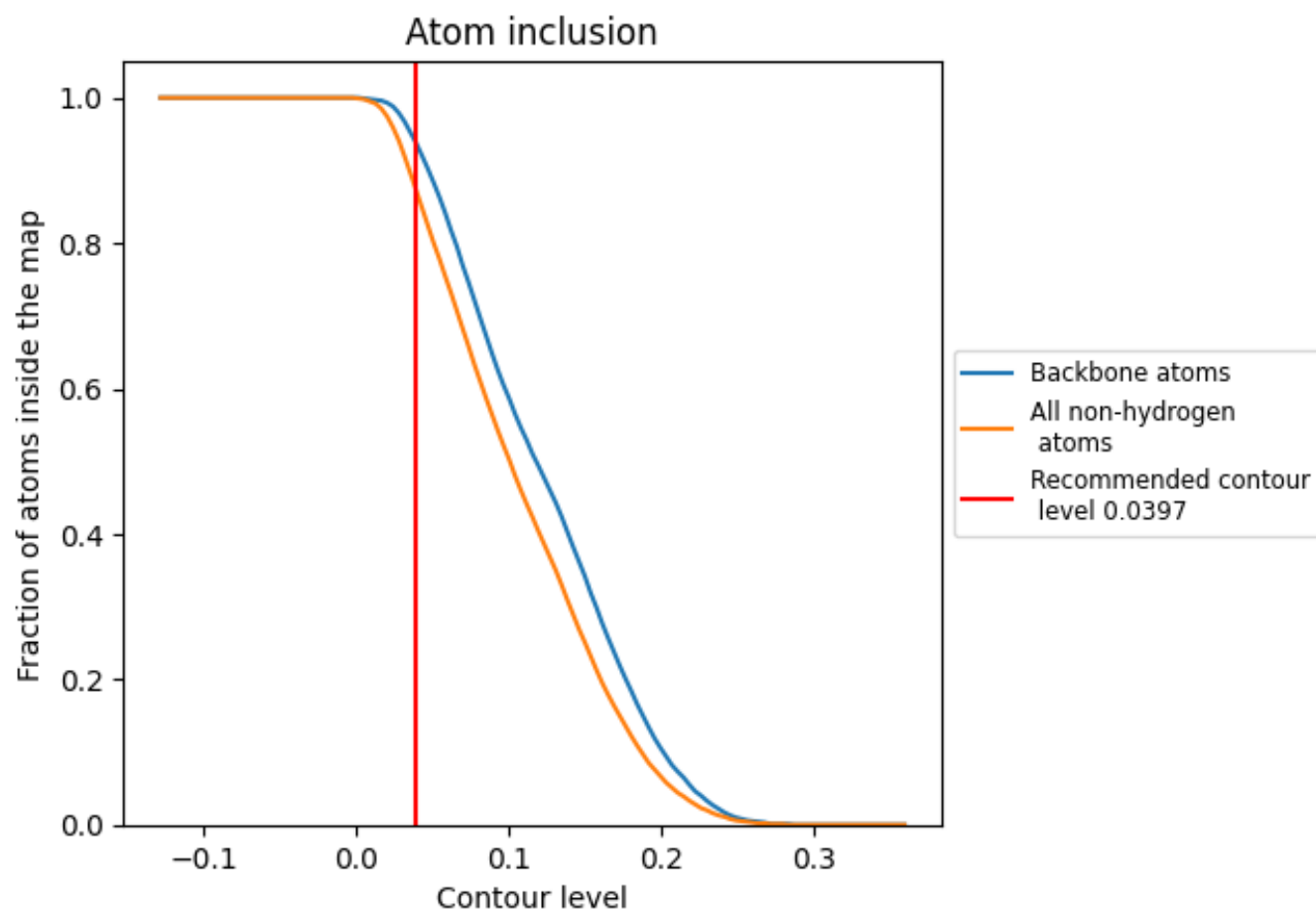
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0397).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.0397) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.5610
A	 0.9410	 0.6280
B	 0.7270	 0.3580
E	 0.8160	 0.5830
F	 0.9610	 0.6440
G	 0.9620	 0.6490
H	 0.9350	 0.6180
I	 0.8430	 0.5750
Q	 0.9520	 0.6290
R	 0.9650	 0.6450
S	 0.8240	 0.5030
U	 0.9420	 0.6210
V	 0.9600	 0.6450
W	 0.9590	 0.6450
X	 0.9210	 0.6190
Y	 0.6700	 0.3320
a	 0.6470	 0.3750
b	 0.7150	 0.3900
c	 0.8080	 0.4780
d	 0.5620	 0.3130
e	 0.7130	 0.3800

