Full wwPDB EM Validation Report

Oct 28, 2026 – 04:26 PM EDT

PDB ID	:	39QW / pdb_000039qw
EMDB ID	:	EMD-79708
Title	:	SaPIbov1 Rep:dsDNA component 1 frame 0
Authors	:	Shin, H.; Rice, P.A.
Deposited on	:	2026-10-22
Resolution	:	3.45 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:

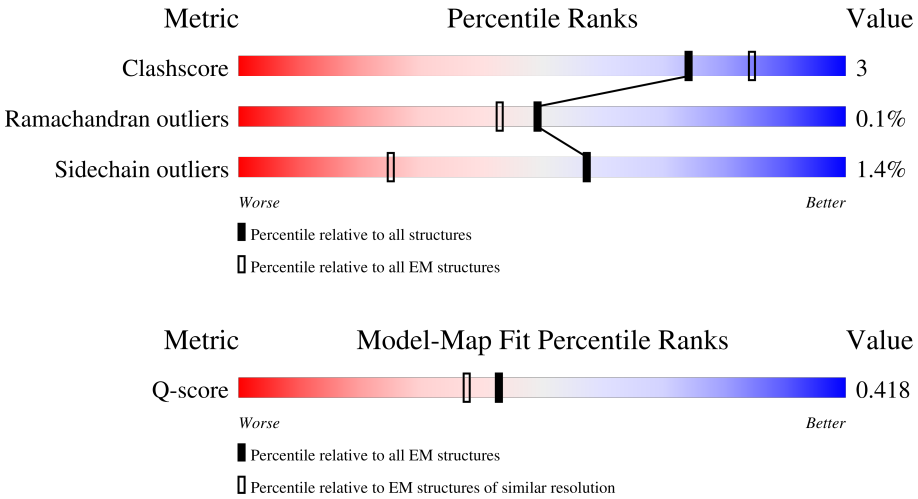
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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.



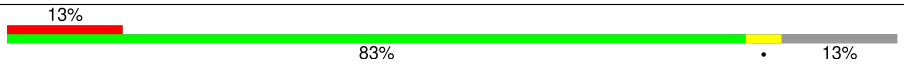
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 (2.95 - 3.95)

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 <=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	602	8% 53% 28% • 16%
1	B	602	• 75% 9% 15%
1	C	602	• 80% 7% 12%
1	D	602	• 77% 10% 13%

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Mol	Chain	Length	Quality of chain
1	E	602	
1	F	602	
2	G	25	
2	H	25	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 50788 atoms, of which 25295 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 Pathogenicity island protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F	524	Total	C	H	N	O	S	0	0
			8405	2674	4208	703	808	12		
1	B	509	Total	C	H	N	O	S	0	0
			8182	2607	4094	684	786	11		
1	D	524	Total	C	H	N	O	S	0	0
			8405	2674	4208	703	808	12		
1	A	504	Total	C	H	N	O	S	0	0
			8112	2588	4060	675	778	11		
1	E	524	Total	C	H	N	O	S	0	0
			8415	2677	4215	703	809	11		
1	C	527	Total	C	H	N	O	S	0	0
			8458	2691	4231	711	813	12		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	350	PRO	GLN	conflict	UNP A0A2X2JYA8
F	462	LEU	ILE	conflict	UNP A0A2X2JYA8
F	474	ALA	VAL	conflict	UNP A0A2X2JYA8
F	548	LYS	ARG	conflict	UNP A0A2X2JYA8
F	555	LEU	PHE	conflict	UNP A0A2X2JYA8
F	570	GLY	-	expression tag	UNP A0A2X2JYA8
F	571	SER	-	expression tag	UNP A0A2X2JYA8
F	572	GLY	-	expression tag	UNP A0A2X2JYA8
F	573	SER	-	expression tag	UNP A0A2X2JYA8
F	574	GLY	-	expression tag	UNP A0A2X2JYA8
F	575	TRP	-	expression tag	UNP A0A2X2JYA8
F	576	SER	-	expression tag	UNP A0A2X2JYA8
F	577	HIS	-	expression tag	UNP A0A2X2JYA8
F	578	PRO	-	expression tag	UNP A0A2X2JYA8
F	579	GLN	-	expression tag	UNP A0A2X2JYA8
F	580	PHE	-	expression tag	UNP A0A2X2JYA8
F	581	GLU	-	expression tag	UNP A0A2X2JYA8
F	582	LYS	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	583	GLY	-	expression tag	UNP A0A2X2JYA8
F	584	GLY	-	expression tag	UNP A0A2X2JYA8
F	585	GLY	-	expression tag	UNP A0A2X2JYA8
F	586	SER	-	expression tag	UNP A0A2X2JYA8
F	587	GLY	-	expression tag	UNP A0A2X2JYA8
F	588	GLY	-	expression tag	UNP A0A2X2JYA8
F	589	GLY	-	expression tag	UNP A0A2X2JYA8
F	590	SER	-	expression tag	UNP A0A2X2JYA8
F	591	GLY	-	expression tag	UNP A0A2X2JYA8
F	592	GLY	-	expression tag	UNP A0A2X2JYA8
F	593	SER	-	expression tag	UNP A0A2X2JYA8
F	594	ALA	-	expression tag	UNP A0A2X2JYA8
F	595	TRP	-	expression tag	UNP A0A2X2JYA8
F	596	SER	-	expression tag	UNP A0A2X2JYA8
F	597	HIS	-	expression tag	UNP A0A2X2JYA8
F	598	PRO	-	expression tag	UNP A0A2X2JYA8
F	599	GLN	-	expression tag	UNP A0A2X2JYA8
F	600	PHE	-	expression tag	UNP A0A2X2JYA8
F	601	GLU	-	expression tag	UNP A0A2X2JYA8
F	602	LYS	-	expression tag	UNP A0A2X2JYA8
B	350	PRO	GLN	conflict	UNP A0A2X2JYA8
B	462	LEU	ILE	conflict	UNP A0A2X2JYA8
B	474	ALA	VAL	conflict	UNP A0A2X2JYA8
B	548	LYS	ARG	conflict	UNP A0A2X2JYA8
B	555	LEU	PHE	conflict	UNP A0A2X2JYA8
B	570	GLY	-	expression tag	UNP A0A2X2JYA8
B	571	SER	-	expression tag	UNP A0A2X2JYA8
B	572	GLY	-	expression tag	UNP A0A2X2JYA8
B	573	SER	-	expression tag	UNP A0A2X2JYA8
B	574	GLY	-	expression tag	UNP A0A2X2JYA8
B	575	TRP	-	expression tag	UNP A0A2X2JYA8
B	576	SER	-	expression tag	UNP A0A2X2JYA8
B	577	HIS	-	expression tag	UNP A0A2X2JYA8
B	578	PRO	-	expression tag	UNP A0A2X2JYA8
B	579	GLN	-	expression tag	UNP A0A2X2JYA8
B	580	PHE	-	expression tag	UNP A0A2X2JYA8
B	581	GLU	-	expression tag	UNP A0A2X2JYA8
B	582	LYS	-	expression tag	UNP A0A2X2JYA8
B	583	GLY	-	expression tag	UNP A0A2X2JYA8
B	584	GLY	-	expression tag	UNP A0A2X2JYA8
B	585	GLY	-	expression tag	UNP A0A2X2JYA8
B	586	SER	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	587	GLY	-	expression tag	UNP A0A2X2JYA8
B	588	GLY	-	expression tag	UNP A0A2X2JYA8
B	589	GLY	-	expression tag	UNP A0A2X2JYA8
B	590	SER	-	expression tag	UNP A0A2X2JYA8
B	591	GLY	-	expression tag	UNP A0A2X2JYA8
B	592	GLY	-	expression tag	UNP A0A2X2JYA8
B	593	SER	-	expression tag	UNP A0A2X2JYA8
B	594	ALA	-	expression tag	UNP A0A2X2JYA8
B	595	TRP	-	expression tag	UNP A0A2X2JYA8
B	596	SER	-	expression tag	UNP A0A2X2JYA8
B	597	HIS	-	expression tag	UNP A0A2X2JYA8
B	598	PRO	-	expression tag	UNP A0A2X2JYA8
B	599	GLN	-	expression tag	UNP A0A2X2JYA8
B	600	PHE	-	expression tag	UNP A0A2X2JYA8
B	601	GLU	-	expression tag	UNP A0A2X2JYA8
B	602	LYS	-	expression tag	UNP A0A2X2JYA8
D	350	PRO	GLN	conflict	UNP A0A2X2JYA8
D	462	LEU	ILE	conflict	UNP A0A2X2JYA8
D	474	ALA	VAL	conflict	UNP A0A2X2JYA8
D	548	LYS	ARG	conflict	UNP A0A2X2JYA8
D	555	LEU	PHE	conflict	UNP A0A2X2JYA8
D	570	GLY	-	expression tag	UNP A0A2X2JYA8
D	571	SER	-	expression tag	UNP A0A2X2JYA8
D	572	GLY	-	expression tag	UNP A0A2X2JYA8
D	573	SER	-	expression tag	UNP A0A2X2JYA8
D	574	GLY	-	expression tag	UNP A0A2X2JYA8
D	575	TRP	-	expression tag	UNP A0A2X2JYA8
D	576	SER	-	expression tag	UNP A0A2X2JYA8
D	577	HIS	-	expression tag	UNP A0A2X2JYA8
D	578	PRO	-	expression tag	UNP A0A2X2JYA8
D	579	GLN	-	expression tag	UNP A0A2X2JYA8
D	580	PHE	-	expression tag	UNP A0A2X2JYA8
D	581	GLU	-	expression tag	UNP A0A2X2JYA8
D	582	LYS	-	expression tag	UNP A0A2X2JYA8
D	583	GLY	-	expression tag	UNP A0A2X2JYA8
D	584	GLY	-	expression tag	UNP A0A2X2JYA8
D	585	GLY	-	expression tag	UNP A0A2X2JYA8
D	586	SER	-	expression tag	UNP A0A2X2JYA8
D	587	GLY	-	expression tag	UNP A0A2X2JYA8
D	588	GLY	-	expression tag	UNP A0A2X2JYA8
D	589	GLY	-	expression tag	UNP A0A2X2JYA8
D	590	SER	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	591	GLY	-	expression tag	UNP A0A2X2JYA8
D	592	GLY	-	expression tag	UNP A0A2X2JYA8
D	593	SER	-	expression tag	UNP A0A2X2JYA8
D	594	ALA	-	expression tag	UNP A0A2X2JYA8
D	595	TRP	-	expression tag	UNP A0A2X2JYA8
D	596	SER	-	expression tag	UNP A0A2X2JYA8
D	597	HIS	-	expression tag	UNP A0A2X2JYA8
D	598	PRO	-	expression tag	UNP A0A2X2JYA8
D	599	GLN	-	expression tag	UNP A0A2X2JYA8
D	600	PHE	-	expression tag	UNP A0A2X2JYA8
D	601	GLU	-	expression tag	UNP A0A2X2JYA8
D	602	LYS	-	expression tag	UNP A0A2X2JYA8
A	350	PRO	GLN	conflict	UNP A0A2X2JYA8
A	462	LEU	ILE	conflict	UNP A0A2X2JYA8
A	474	ALA	VAL	conflict	UNP A0A2X2JYA8
A	548	LYS	ARG	conflict	UNP A0A2X2JYA8
A	555	LEU	PHE	conflict	UNP A0A2X2JYA8
A	570	GLY	-	expression tag	UNP A0A2X2JYA8
A	571	SER	-	expression tag	UNP A0A2X2JYA8
A	572	GLY	-	expression tag	UNP A0A2X2JYA8
A	573	SER	-	expression tag	UNP A0A2X2JYA8
A	574	GLY	-	expression tag	UNP A0A2X2JYA8
A	575	TRP	-	expression tag	UNP A0A2X2JYA8
A	576	SER	-	expression tag	UNP A0A2X2JYA8
A	577	HIS	-	expression tag	UNP A0A2X2JYA8
A	578	PRO	-	expression tag	UNP A0A2X2JYA8
A	579	GLN	-	expression tag	UNP A0A2X2JYA8
A	580	PHE	-	expression tag	UNP A0A2X2JYA8
A	581	GLU	-	expression tag	UNP A0A2X2JYA8
A	582	LYS	-	expression tag	UNP A0A2X2JYA8
A	583	GLY	-	expression tag	UNP A0A2X2JYA8
A	584	GLY	-	expression tag	UNP A0A2X2JYA8
A	585	GLY	-	expression tag	UNP A0A2X2JYA8
A	586	SER	-	expression tag	UNP A0A2X2JYA8
A	587	GLY	-	expression tag	UNP A0A2X2JYA8
A	588	GLY	-	expression tag	UNP A0A2X2JYA8
A	589	GLY	-	expression tag	UNP A0A2X2JYA8
A	590	SER	-	expression tag	UNP A0A2X2JYA8
A	591	GLY	-	expression tag	UNP A0A2X2JYA8
A	592	GLY	-	expression tag	UNP A0A2X2JYA8
A	593	SER	-	expression tag	UNP A0A2X2JYA8
A	594	ALA	-	expression tag	UNP A0A2X2JYA8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	595	TRP	-	expression tag	UNP A0A2X2JYA8
A	596	SER	-	expression tag	UNP A0A2X2JYA8
A	597	HIS	-	expression tag	UNP A0A2X2JYA8
A	598	PRO	-	expression tag	UNP A0A2X2JYA8
A	599	GLN	-	expression tag	UNP A0A2X2JYA8
A	600	PHE	-	expression tag	UNP A0A2X2JYA8
A	601	GLU	-	expression tag	UNP A0A2X2JYA8
A	602	LYS	-	expression tag	UNP A0A2X2JYA8
E	350	PRO	GLN	conflict	UNP A0A2X2JYA8
E	462	LEU	ILE	conflict	UNP A0A2X2JYA8
E	474	ALA	VAL	conflict	UNP A0A2X2JYA8
E	548	LYS	ARG	conflict	UNP A0A2X2JYA8
E	555	LEU	PHE	conflict	UNP A0A2X2JYA8
E	570	GLY	-	expression tag	UNP A0A2X2JYA8
E	571	SER	-	expression tag	UNP A0A2X2JYA8
E	572	GLY	-	expression tag	UNP A0A2X2JYA8
E	573	SER	-	expression tag	UNP A0A2X2JYA8
E	574	GLY	-	expression tag	UNP A0A2X2JYA8
E	575	TRP	-	expression tag	UNP A0A2X2JYA8
E	576	SER	-	expression tag	UNP A0A2X2JYA8
E	577	HIS	-	expression tag	UNP A0A2X2JYA8
E	578	PRO	-	expression tag	UNP A0A2X2JYA8
E	579	GLN	-	expression tag	UNP A0A2X2JYA8
E	580	PHE	-	expression tag	UNP A0A2X2JYA8
E	581	GLU	-	expression tag	UNP A0A2X2JYA8
E	582	LYS	-	expression tag	UNP A0A2X2JYA8
E	583	GLY	-	expression tag	UNP A0A2X2JYA8
E	584	GLY	-	expression tag	UNP A0A2X2JYA8
E	585	GLY	-	expression tag	UNP A0A2X2JYA8
E	586	SER	-	expression tag	UNP A0A2X2JYA8
E	587	GLY	-	expression tag	UNP A0A2X2JYA8
E	588	GLY	-	expression tag	UNP A0A2X2JYA8
E	589	GLY	-	expression tag	UNP A0A2X2JYA8
E	590	SER	-	expression tag	UNP A0A2X2JYA8
E	591	GLY	-	expression tag	UNP A0A2X2JYA8
E	592	GLY	-	expression tag	UNP A0A2X2JYA8
E	593	SER	-	expression tag	UNP A0A2X2JYA8
E	594	ALA	-	expression tag	UNP A0A2X2JYA8
E	595	TRP	-	expression tag	UNP A0A2X2JYA8
E	596	SER	-	expression tag	UNP A0A2X2JYA8
E	597	HIS	-	expression tag	UNP A0A2X2JYA8
E	598	PRO	-	expression tag	UNP A0A2X2JYA8

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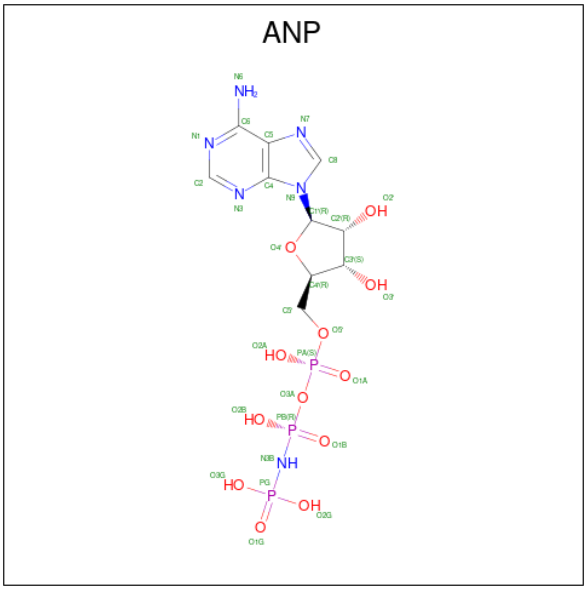
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Chain	Residue	Modelled	Actual	Comment	Reference
E	599	GLN	-	expression tag	UNP A0A2X2JYA8
E	600	PHE	-	expression tag	UNP A0A2X2JYA8
E	601	GLU	-	expression tag	UNP A0A2X2JYA8
E	602	LYS	-	expression tag	UNP A0A2X2JYA8
C	350	PRO	GLN	conflict	UNP A0A2X2JYA8
C	462	LEU	ILE	conflict	UNP A0A2X2JYA8
C	474	ALA	VAL	conflict	UNP A0A2X2JYA8
C	548	LYS	ARG	conflict	UNP A0A2X2JYA8
C	555	LEU	PHE	conflict	UNP A0A2X2JYA8
C	570	GLY	-	expression tag	UNP A0A2X2JYA8
C	571	SER	-	expression tag	UNP A0A2X2JYA8
C	572	GLY	-	expression tag	UNP A0A2X2JYA8
C	573	SER	-	expression tag	UNP A0A2X2JYA8
C	574	GLY	-	expression tag	UNP A0A2X2JYA8
C	575	TRP	-	expression tag	UNP A0A2X2JYA8
C	576	SER	-	expression tag	UNP A0A2X2JYA8
C	577	HIS	-	expression tag	UNP A0A2X2JYA8
C	578	PRO	-	expression tag	UNP A0A2X2JYA8
C	579	GLN	-	expression tag	UNP A0A2X2JYA8
C	580	PHE	-	expression tag	UNP A0A2X2JYA8
C	581	GLU	-	expression tag	UNP A0A2X2JYA8
C	582	LYS	-	expression tag	UNP A0A2X2JYA8
C	583	GLY	-	expression tag	UNP A0A2X2JYA8
C	584	GLY	-	expression tag	UNP A0A2X2JYA8
C	585	GLY	-	expression tag	UNP A0A2X2JYA8
C	586	SER	-	expression tag	UNP A0A2X2JYA8
C	587	GLY	-	expression tag	UNP A0A2X2JYA8
C	588	GLY	-	expression tag	UNP A0A2X2JYA8
C	589	GLY	-	expression tag	UNP A0A2X2JYA8
C	590	SER	-	expression tag	UNP A0A2X2JYA8
C	591	GLY	-	expression tag	UNP A0A2X2JYA8
C	592	GLY	-	expression tag	UNP A0A2X2JYA8
C	593	SER	-	expression tag	UNP A0A2X2JYA8
C	594	ALA	-	expression tag	UNP A0A2X2JYA8
C	595	TRP	-	expression tag	UNP A0A2X2JYA8
C	596	SER	-	expression tag	UNP A0A2X2JYA8
C	597	HIS	-	expression tag	UNP A0A2X2JYA8
C	598	PRO	-	expression tag	UNP A0A2X2JYA8
C	599	GLN	-	expression tag	UNP A0A2X2JYA8
C	600	PHE	-	expression tag	UNP A0A2X2JYA8
C	601	GLU	-	expression tag	UNP A0A2X2JYA8
C	602	LYS	-	expression tag	UNP A0A2X2JYA8

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	10	Total	C	H	N	O	P	0	0
			318	98	114	34	62	10		
2	H	10	Total	C	H	N	O	P	0	0
			318	98	114	34	62	10		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
3	D	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
3	C	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

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

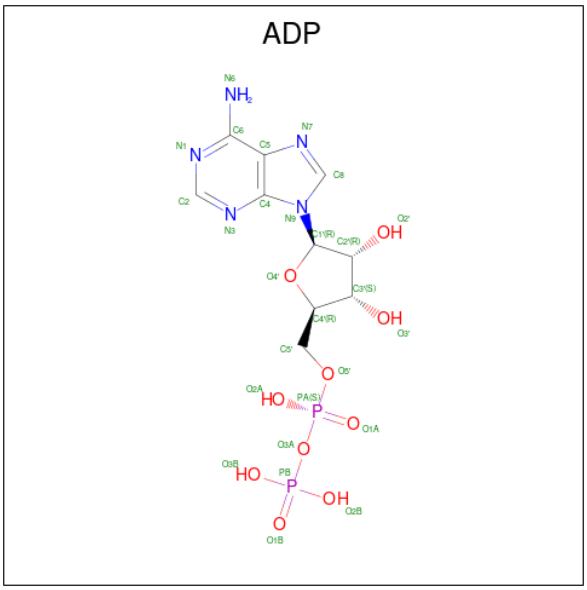
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Mg	0
			1	1	

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



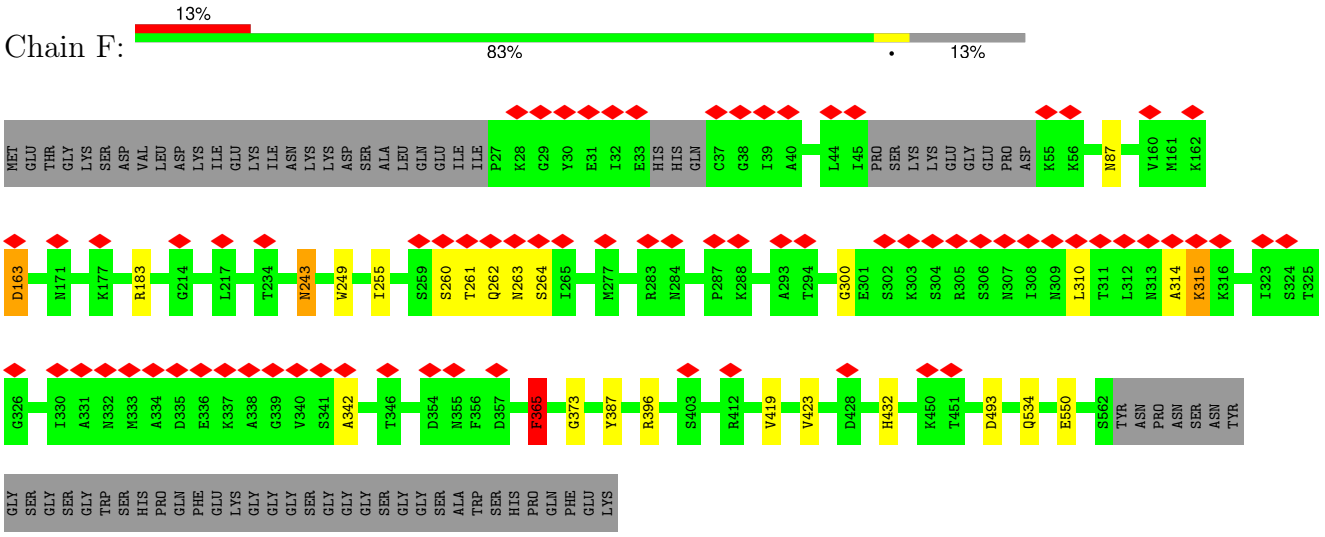
Mol	Chain	Residues	Atoms						AltConf
5	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

3 Residue-property plots

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

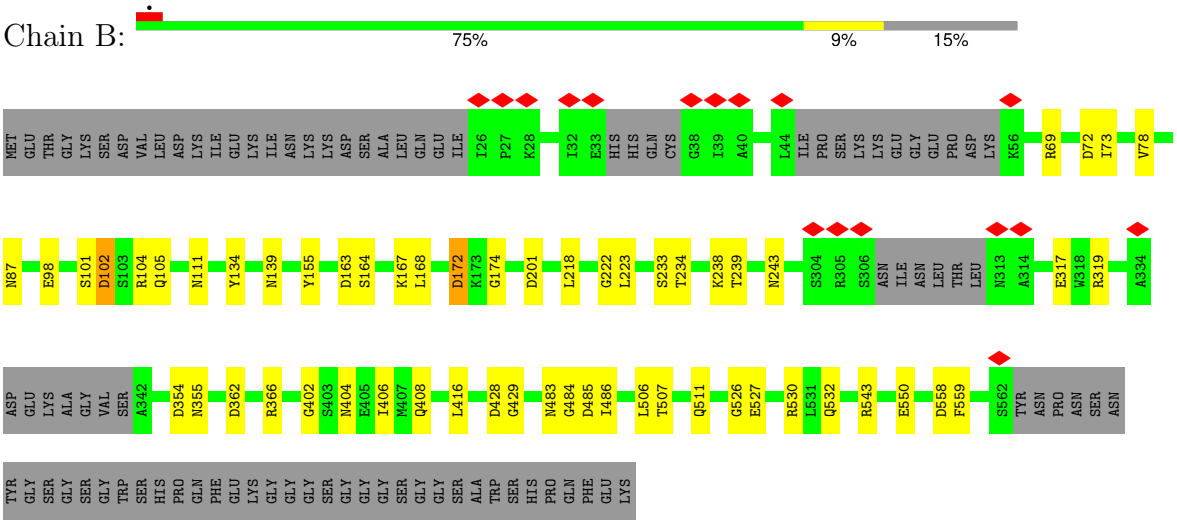
• Molecule 1: Pathogenicity island protein

Chain F:



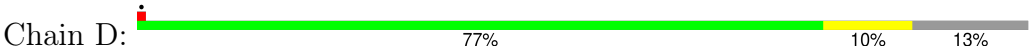
• Molecule 1: Pathogenicity island protein

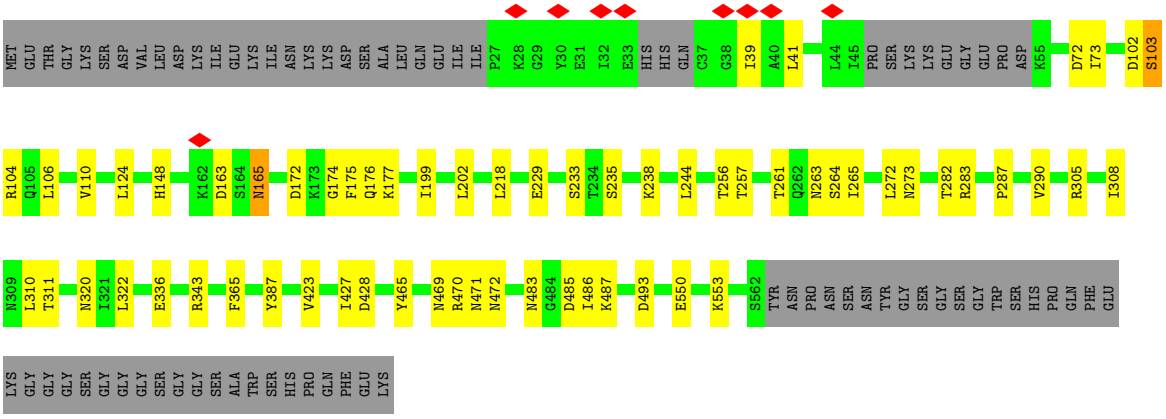
Chain B:



• Molecule 1: Pathogenicity island protein

Chain D:

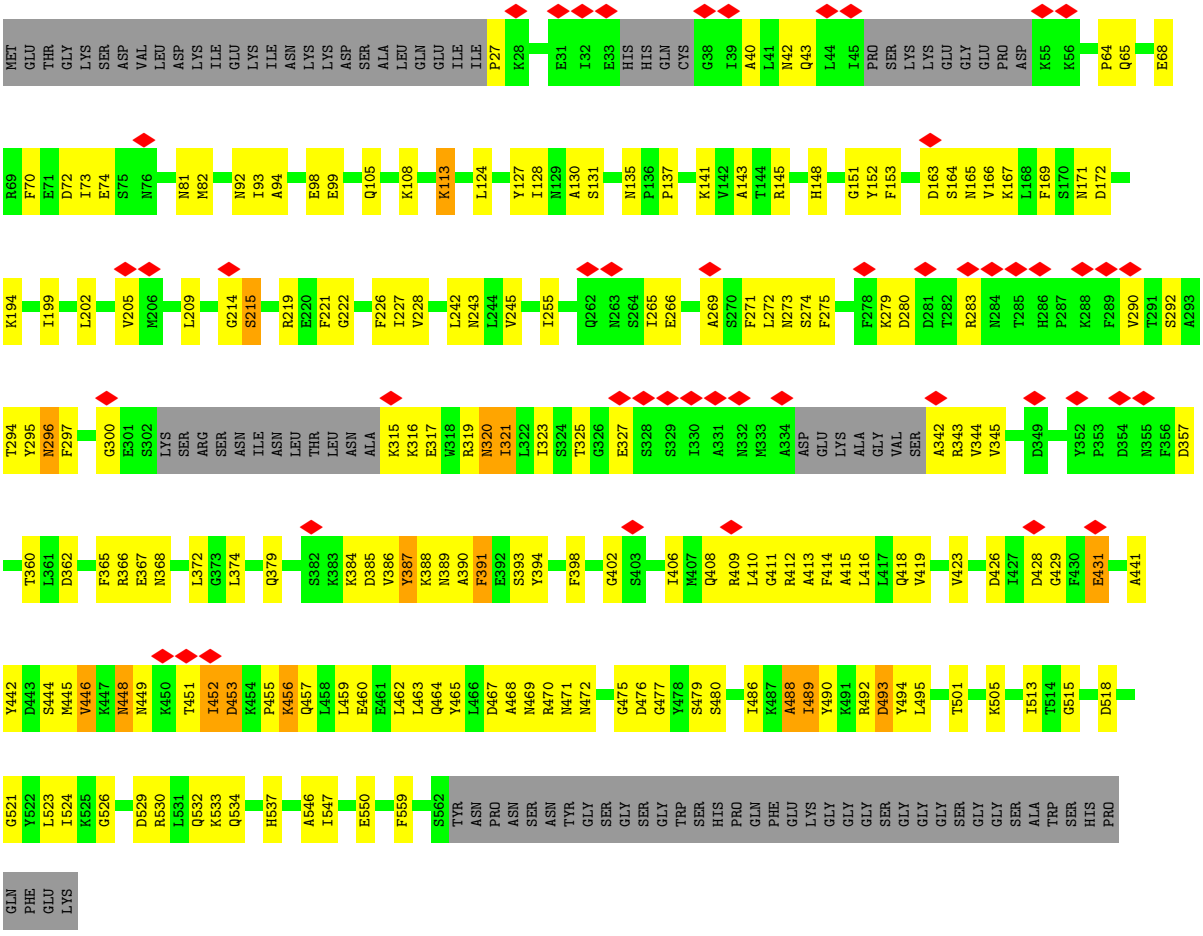




• Molecule 1: Pathogenicity island protein

Chain A:

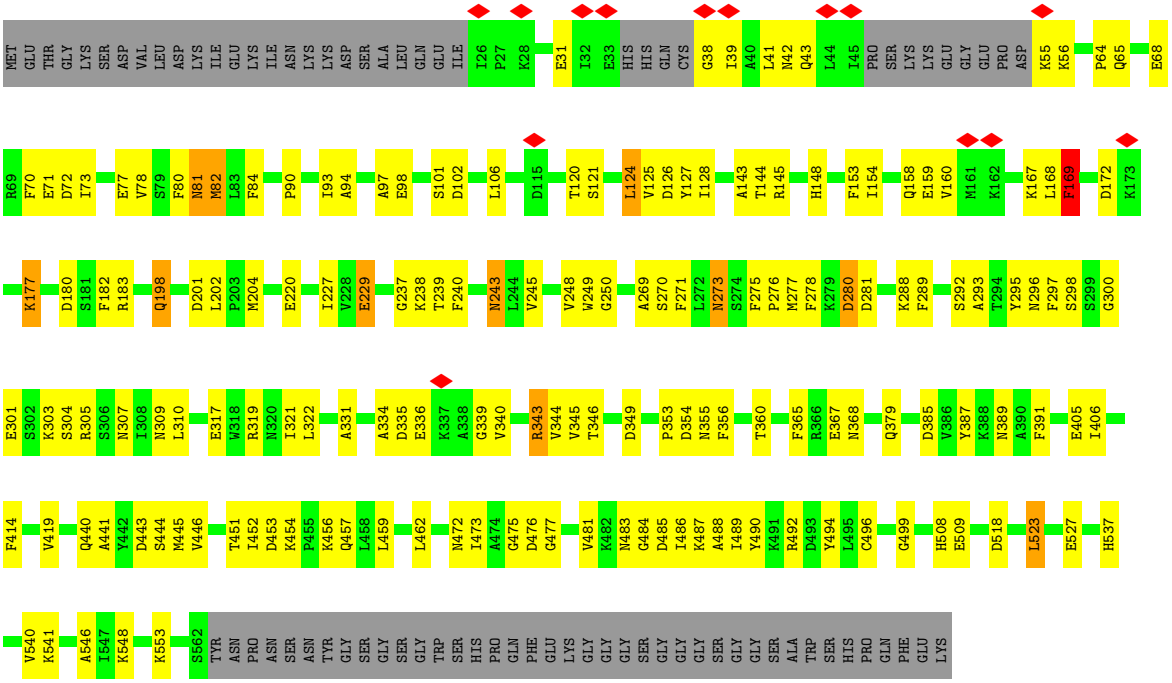




• Molecule 1: Pathogenicity island protein

Chain E:

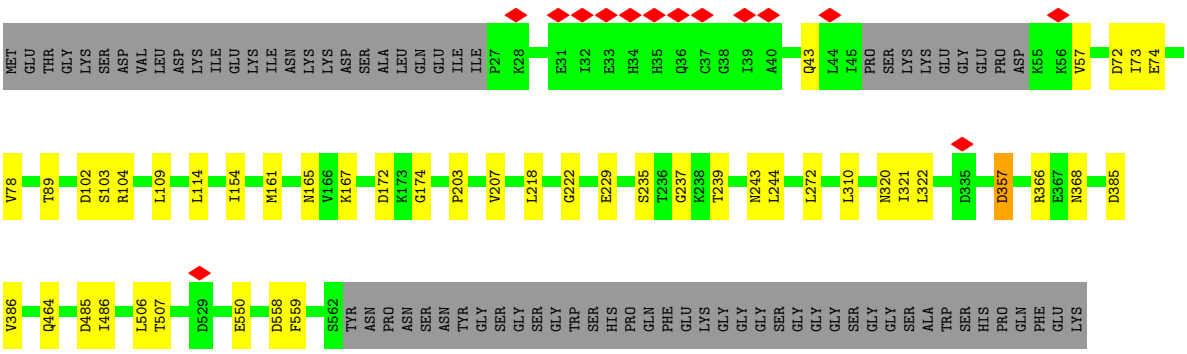




• Molecule 1: Pathogenicity island protein

Chain C:

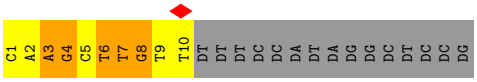




• Molecule 2: DNA (25-MER)

Chain G:

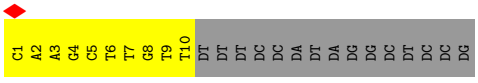




• Molecule 2: DNA (25-MER)

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.246	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	349.76, 349.76, 349.76	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	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, ANP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.87	49/4127 (1.2%)	1.90	222/5555 (4.0%)
1	B	0.39	5/4163 (0.1%)	0.46	6/5604 (0.1%)
1	C	0.28	3/4307 (0.1%)	0.36	2/5802 (0.0%)
1	D	0.74	13/4274 (0.3%)	0.74	23/5756 (0.4%)
1	E	2.04	49/4277 (1.1%)	2.05	217/5761 (3.8%)
1	F	0.70	0/4274	1.26	20/5756 (0.3%)
2	G	3.35	31/227 (13.7%)	3.18	42/348 (12.1%)
2	H	4.06	46/227 (20.3%)	3.63	55/348 (15.8%)
All	All	1.30	196/25876 (0.8%)	1.38	587/34930 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	DA	C6-N6	-13.08	1.23	1.33
2	G	2	DA	C6-N6	-13.02	1.23	1.33
2	H	3	DA	C6-N6	-12.63	1.23	1.33
2	H	2	DA	C6-N6	-11.85	1.24	1.33
2	H	8	DG	C2-N2	-10.72	1.23	1.34
2	H	1	DC	C4-N4	-10.60	1.24	1.33
2	H	5	DC	C4-N4	-10.21	1.24	1.33
2	H	5	DC	C5-C6	-10.04	1.26	1.34
2	G	1	DC	C5-C6	-10.02	1.26	1.34
2	H	8	DG	C3'-C2'	-9.73	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	DC	C5-C6	-9.72	1.26	1.34
2	H	4	DG	C2-N2	-9.62	1.25	1.34
2	G	8	DG	C2-N2	-9.61	1.25	1.34
2	G	1	DC	C4-N4	-9.34	1.25	1.33
1	A	148	HIS	CE1-NE2	-8.83	1.23	1.32
1	E	508	HIS	CE1-NE2	-8.81	1.23	1.32
1	E	145	ARG	CZ-NH2	-8.78	1.22	1.33
1	E	537	HIS	CE1-NE2	-8.78	1.23	1.32
1	A	537	HIS	CE1-NE2	-8.76	1.23	1.32
1	E	334	ALA	CA-CB	-8.76	1.41	1.52
1	E	183	ARG	CZ-NH2	-8.68	1.22	1.33
2	H	10	DT	C5'-C4'	-8.62	1.45	1.51
2	H	5	DC	C5'-C4'	-8.59	1.45	1.51
1	A	145	ARG	CZ-NH2	-8.55	1.22	1.33
2	G	3	DA	C5'-C4'	-8.53	1.45	1.51
1	C	104	ARG	CZ-NH2	-8.49	1.22	1.33
1	E	492	ARG	CZ-NH2	-8.49	1.22	1.33
1	A	409	ARG	CZ-NH2	-8.47	1.22	1.33
1	A	412	ARG	CZ-NH2	-8.46	1.22	1.33
1	B	104	ARG	CZ-NH2	-8.46	1.22	1.33
2	H	3	DA	C3'-C2'	-8.40	1.45	1.52
1	A	94	ALA	CA-CB	-8.35	1.42	1.53
2	H	5	DC	C3'-C2'	-8.32	1.45	1.52
1	A	470	ARG	CZ-NH2	-8.31	1.22	1.33
2	G	8	DG	C8-N7	-8.26	1.25	1.30
1	E	319	ARG	CZ-NH2	-8.25	1.22	1.33
1	A	492	ARG	CZ-NH2	-8.17	1.22	1.33
2	G	10	DT	C5'-C4'	-8.15	1.46	1.51
1	E	94	ALA	CA-CB	-8.13	1.41	1.53
1	A	537	HIS	CD2-NE2	-8.07	1.28	1.37
1	E	508	HIS	CD2-NE2	-8.02	1.29	1.37
1	A	148	HIS	CD2-NE2	-7.98	1.29	1.37
1	E	537	HIS	CD2-NE2	-7.97	1.29	1.37
2	H	3	DA	C5'-C4'	-7.96	1.46	1.51
2	H	2	DA	C3'-C2'	-7.93	1.45	1.52
2	G	2	DA	C5'-C4'	-7.92	1.46	1.51
2	H	6	DT	C3'-C2'	-7.91	1.45	1.52
2	H	2	DA	C5'-C4'	-7.89	1.46	1.51
2	G	10	DT	C3'-C2'	-7.79	1.45	1.52
2	H	6	DT	C5'-C4'	-7.74	1.46	1.51
1	E	269	ALA	CA-CB	-7.73	1.41	1.53
2	H	8	DG	C5'-C4'	-7.73	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7	DT	C5'-C4'	-7.71	1.46	1.51
2	G	1	DC	C3'-C2'	-7.70	1.45	1.52
2	H	8	DG	C2'-C1'	-7.65	1.44	1.52
2	H	4	DG	C8-N7	-7.63	1.26	1.30
2	H	9	DT	C2'-C1'	-7.63	1.44	1.52
2	G	8	DG	C3'-C2'	-7.62	1.46	1.52
2	G	8	DG	C5'-C4'	-7.58	1.46	1.51
1	A	475	GLY	N-CA	-7.51	1.37	1.45
2	H	4	DG	C5'-C4'	-7.50	1.46	1.51
1	E	441	ALA	CA-CB	-7.49	1.41	1.53
2	H	1	DC	C5'-C4'	-7.48	1.46	1.51
2	G	1	DC	C5'-C4'	-7.47	1.46	1.51
1	E	331	ALA	CA-CB	-7.42	1.41	1.53
1	A	546	ALA	CA-CB	-7.40	1.42	1.53
2	H	5	DC	N1-C6	-7.40	1.32	1.37
1	E	293	ALA	CA-CB	-7.39	1.41	1.53
2	H	4	DG	C3'-C2'	-7.38	1.46	1.52
2	H	9	DT	C5'-C4'	-7.35	1.46	1.51
1	A	413	ALA	CA-CB	-7.31	1.41	1.53
1	A	415	ALA	CA-CB	-7.31	1.42	1.53
1	A	130	ALA	CA-CB	-7.28	1.42	1.53
1	A	390	ALA	CA-CB	-7.25	1.42	1.53
1	D	470	ARG	CZ-NH2	-7.24	1.24	1.33
1	D	305	ARG	CZ-NH2	-7.22	1.24	1.33
1	E	343	ARG	CZ-NH2	-7.20	1.24	1.33
2	H	9	DT	C3'-C2'	-7.17	1.46	1.52
1	E	145	ARG	CZ-NH1	-7.15	1.22	1.32
1	A	219	ARG	CZ-NH2	-7.15	1.24	1.33
1	D	283	ARG	CZ-NH2	-7.14	1.24	1.33
1	E	183	ARG	CZ-NH1	-7.13	1.22	1.32
1	A	468	ALA	CA-CB	-7.13	1.42	1.53
1	D	104	ARG	CZ-NH2	-7.11	1.24	1.33
1	A	343	ARG	CZ-NH2	-7.09	1.24	1.33
2	G	7	DT	C2'-C1'	-7.04	1.45	1.52
2	H	4	DG	C2'-C1'	-7.02	1.45	1.52
2	G	7	DT	C3'-C2'	-6.99	1.46	1.52
1	E	488	ALA	CA-CB	-6.96	1.42	1.53
1	A	143	ALA	CA-CB	-6.95	1.42	1.53
1	E	484	GLY	N-CA	-6.95	1.38	1.45
1	A	145	ARG	CZ-NH1	-6.93	1.23	1.32
1	E	492	ARG	CZ-NH1	-6.91	1.23	1.32
1	A	409	ARG	CZ-NH1	-6.91	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	8	DG	N9-C8	-6.89	1.33	1.37
2	H	10	DT	C3'-C2'	-6.89	1.46	1.52
1	E	143	ALA	CA-CB	-6.88	1.41	1.53
1	C	104	ARG	CZ-NH1	-6.88	1.23	1.32
1	A	412	ARG	CZ-NH1	-6.88	1.23	1.32
1	B	104	ARG	CZ-NH1	-6.85	1.23	1.32
1	A	488	ALA	CA-CB	-6.84	1.42	1.53
1	A	470	ARG	CZ-NH1	-6.72	1.23	1.32
1	E	319	ARG	CZ-NH1	-6.72	1.23	1.32
1	A	492	ARG	CZ-NH1	-6.67	1.23	1.32
2	H	2	DA	N9-C8	-6.65	1.32	1.37
2	H	10	DT	C2'-C1'	-6.65	1.45	1.52
2	G	3	DA	C3'-C2'	-6.61	1.46	1.52
2	H	1	DC	C3'-C2'	-6.61	1.46	1.52
1	A	64	PRO	CA-CB	-6.59	1.46	1.54
1	E	64	PRO	CA-CB	-6.55	1.46	1.54
2	G	3	DA	C2'-C1'	-6.54	1.45	1.52
2	H	8	DG	C8-N7	-6.51	1.27	1.30
2	H	3	DA	C2'-C1'	-6.50	1.45	1.52
2	H	6	DT	C2'-C1'	-6.48	1.45	1.52
2	G	1	DC	C2'-C1'	-6.47	1.45	1.52
2	G	8	DG	C2'-C1'	-6.43	1.45	1.52
2	H	1	DC	N1-C6	-6.39	1.33	1.37
2	H	4	DG	N9-C8	-6.36	1.33	1.37
2	H	5	DC	C2'-C1'	-6.36	1.45	1.52
2	G	1	DC	N1-C6	-6.34	1.33	1.37
2	H	2	DA	C2'-C1'	-6.31	1.46	1.52
2	H	2	DA	C8-N7	-6.30	1.27	1.31
1	A	515	GLY	N-CA	-6.22	1.37	1.45
1	E	202	LEU	CA-CB	-6.22	1.47	1.53
2	H	3	DA	N9-C8	-6.17	1.32	1.37
2	G	2	DA	C3'-C2'	-6.09	1.47	1.52
2	H	3	DA	C8-N7	-6.08	1.27	1.31
2	G	3	DA	N9-C8	-6.06	1.32	1.37
1	A	300	GLY	N-CA	-6.03	1.38	1.45
1	E	202	LEU	N-CA	-6.02	1.41	1.46
2	G	2	DA	C8-N7	-5.96	1.27	1.31
2	H	8	DG	N9-C8	-5.96	1.33	1.37
2	G	2	DA	C2'-C1'	-5.91	1.46	1.52
2	G	2	DA	N9-C8	-5.91	1.33	1.37
2	H	1	DC	C2'-C1'	-5.79	1.46	1.52
2	H	6	DT	N1-C6	-5.77	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	DA	C8-N7	-5.73	1.27	1.31
1	D	305	ARG	CZ-NH1	-5.67	1.24	1.32
1	E	343	ARG	CZ-NH1	-5.66	1.24	1.32
1	D	174	GLY	N-CA	-5.64	1.38	1.45
1	A	343	ARG	CZ-NH1	-5.64	1.24	1.32
1	D	104	ARG	CZ-NH1	-5.63	1.24	1.32
1	E	492	ARG	CD-NE	-5.63	1.38	1.46
1	E	183	ARG	CD-NE	-5.63	1.38	1.46
1	A	470	ARG	CD-NE	-5.62	1.38	1.46
2	G	10	DT	C2'-C1'	-5.62	1.46	1.52
1	A	219	ARG	CZ-NH1	-5.60	1.25	1.32
1	D	470	ARG	CZ-NH1	-5.59	1.25	1.32
1	D	283	ARG	CZ-NH1	-5.58	1.25	1.32
1	E	319	ARG	CD-NE	-5.57	1.38	1.46
2	G	8	DG	C6-N1	-5.50	1.35	1.39
1	E	145	ARG	CD-NE	-5.48	1.38	1.46
1	B	485	ASP	CA-CB	-5.48	1.46	1.53
1	E	300	GLY	N-CA	-5.46	1.37	1.45
1	D	104	ARG	CD-NE	-5.45	1.38	1.46
1	A	72	ASP	CA-CB	-5.41	1.46	1.52
1	A	137	PRO	CA-CB	-5.40	1.46	1.53
1	E	477	GLY	N-CA	-5.38	1.37	1.45
1	A	145	ARG	CD-NE	-5.38	1.38	1.46
1	C	104	ARG	CD-NE	-5.37	1.38	1.46
1	A	411	GLY	N-CA	-5.37	1.37	1.45
1	D	305	ARG	CD-NE	-5.35	1.38	1.46
1	B	104	ARG	CD-NE	-5.32	1.38	1.46
1	E	276	PRO	CA-CB	-5.32	1.46	1.53
1	A	492	ARG	CD-NE	-5.32	1.38	1.46
1	A	521	GLY	N-CA	-5.30	1.37	1.45
1	E	250	GLY	N-CA	-5.28	1.38	1.45
1	A	412	ARG	CD-NE	-5.26	1.38	1.46
1	A	219	ARG	CD-NE	-5.25	1.38	1.46
1	A	409	ARG	CD-NE	-5.25	1.39	1.46
1	E	90	PRO	CA-CB	-5.24	1.46	1.53
1	A	343	ARG	CD-NE	-5.23	1.39	1.46
1	A	526	GLY	N-CA	-5.22	1.37	1.45
1	E	454	LYS	CA-CB	-5.22	1.47	1.53
1	D	470	ARG	CD-NE	-5.19	1.39	1.46
1	E	243	ASN	CG-ND2	-5.18	1.22	1.33
1	E	343	ARG	CD-NE	-5.16	1.39	1.46
1	A	222	GLY	N-CA	-5.16	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	304	SER	CA-CB	-5.15	1.46	1.53
1	E	158	GLN	CD-NE2	-5.13	1.22	1.33
1	D	283	ARG	CD-NE	-5.13	1.39	1.46
1	E	499	GLY	N-CA	-5.11	1.38	1.45
1	A	27	PRO	N-CD	-5.11	1.40	1.47
1	E	81	ASN	CG-ND2	-5.09	1.22	1.33
1	E	457	GLN	CD-NE2	-5.07	1.22	1.33
1	E	472	ASN	CG-ND2	-5.06	1.22	1.33
1	A	135	ASN	CA-CB	-5.05	1.46	1.53
1	E	237	GLY	N-CA	-5.05	1.38	1.45
1	A	81	ASN	CG-ND2	-5.04	1.22	1.33
1	A	402	GLY	N-CA	-5.03	1.38	1.45
1	E	440	GLN	CD-NE2	-5.02	1.22	1.33
1	E	355	ASN	CG-ND2	-5.01	1.22	1.33
1	E	65	GLN	CD-NE2	-5.00	1.22	1.33
1	B	484	GLY	N-CA	-5.00	1.37	1.45
1	A	105	GLN	CD-NE2	-5.00	1.22	1.33
1	E	475	GLY	N-CA	-5.00	1.37	1.45

All (587) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	4	DG	N7-C8-N9	12.31	119.25	113.10
2	G	8	DG	N7-C8-N9	12.27	119.24	113.10
2	H	2	DA	N7-C8-N9	11.77	119.69	113.80
2	H	8	DG	N7-C8-N9	11.41	118.81	113.10
2	H	3	DA	N7-C8-N9	11.40	119.50	113.80
2	H	3	DA	N1-C2-N3	11.38	134.99	129.30
2	G	3	DA	N1-C2-N3	11.30	134.95	129.30
2	G	10	DT	O5'-C5'-C4'	11.13	118.31	109.40
2	H	2	DA	N1-C2-N3	11.11	134.85	129.30
2	G	2	DA	N7-C8-N9	11.08	119.34	113.80
2	G	2	DA	N1-C2-N3	11.04	134.82	129.30
2	H	1	DC	O5'-C5'-C4'	10.95	118.16	109.40
2	G	3	DA	N7-C8-N9	10.68	119.14	113.80
2	H	4	DG	O5'-C5'-C4'	10.54	117.83	109.40
2	H	6	DT	N3-C4-O4	9.96	125.88	119.90
2	G	1	DC	O5'-C5'-C4'	9.56	117.05	109.40
2	G	10	DT	C2-N3-C4	9.54	132.93	127.20
2	H	9	DT	C2-N3-C4	9.54	132.93	127.20
2	H	6	DT	C5-C6-N1	9.44	129.37	123.70
2	G	8	DG	C6-N1-C2	9.44	130.76	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	10	DT	C2-N3-C4	9.39	132.84	127.20
2	G	7	DT	C2-N3-C4	9.21	132.73	127.20
2	G	7	DT	N3-C4-O4	9.16	125.39	119.90
2	H	6	DT	C2-N3-C4	9.11	132.66	127.20
2	H	10	DT	C5-C6-N1	8.99	129.10	123.70
2	G	10	DT	C5-C6-N1	8.89	129.03	123.70
2	G	7	DT	C5-C6-N1	8.84	129.00	123.70
2	G	10	DT	N3-C4-O4	8.80	125.18	119.90
2	H	8	DG	C6-N1-C2	8.79	130.37	125.10
2	H	10	DT	N3-C4-O4	8.78	125.17	119.90
2	H	9	DT	C5-C6-N1	8.75	128.95	123.70
2	H	9	DT	N3-C4-O4	8.71	125.13	119.90
2	H	4	DG	C6-N1-C2	8.64	130.28	125.10
2	H	4	DG	C8-N9-C4	-8.13	103.15	106.40
2	H	9	DT	O5'-C5'-C4'	7.85	115.68	109.40
2	G	8	DG	C8-N9-C4	-7.76	103.30	106.40
1	F	260	SER	CA-C-N	7.73	136.50	121.66
1	F	260	SER	C-N-CA	7.73	136.50	121.66
2	H	7	DT	O4'-C1'-N1	7.61	113.33	108.00
1	A	475	GLY	N-CA-C	7.58	119.88	111.85
1	E	356	PHE	CA-CB-CG	7.41	121.21	113.80
1	E	169	PHE	CA-CB-CG	7.41	121.21	113.80
2	G	2	DA	O5'-C5'-C4'	7.40	115.32	109.40
2	H	8	DG	C8-N9-C4	-7.26	103.50	106.40
1	A	414	PHE	CA-CB-CG	7.21	121.02	113.80
1	E	182	PHE	CA-CB-CG	7.14	120.94	113.80
1	F	264	SER	N-CA-C	7.14	120.19	110.55
1	E	243	ASN	CA-CB-CG	7.04	119.64	112.60
1	E	72	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	398	PHE	CA-CB-CG	7.02	120.82	113.80
1	E	201	ASP	CA-C-N	7.02	129.98	122.26
1	E	201	ASP	C-N-CA	7.02	129.98	122.26
1	E	275	PHE	CA-CB-CG	6.92	120.72	113.80
2	G	3	DA	O5'-C5'-C4'	6.92	114.93	109.40
1	E	278	PHE	CA-CB-CG	6.89	120.69	113.80
1	A	453	ASP	CA-CB-CG	6.87	119.47	112.60
2	G	1	DC	N3-C4-C5	-6.87	119.15	121.90
2	H	5	DC	N3-C4-C5	-6.87	119.15	121.90
1	A	148	HIS	CA-CB-CG	6.84	120.64	113.80
2	H	8	DG	O5'-C5'-C4'	6.84	114.87	109.40
1	A	449	ASN	CA-CB-CG	6.84	119.44	112.60
2	H	1	DC	N3-C4-C5	-6.82	119.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	309	ASN	CA-CB-CG	6.81	119.41	112.60
2	H	2	DA	C8-N9-C4	-6.81	103.08	105.80
1	E	102	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	70	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	221	PHE	CA-CB-CG	6.74	120.54	113.80
2	H	1	DC	C6-N1-C2	-6.73	117.61	120.30
1	E	271	PHE	CA-CB-CG	6.73	120.53	113.80
2	H	3	DA	C8-N9-C4	-6.70	103.12	105.80
1	B	102	ASP	CA-CB-CG	6.68	119.28	112.60
1	E	443	ASP	CA-CB-CG	6.68	119.28	112.60
2	G	1	DC	C6-N1-C2	-6.67	117.63	120.30
1	A	534	GLN	CA-C-N	6.65	130.69	122.37
1	A	534	GLN	C-N-CA	6.65	130.69	122.37
1	E	452	ILE	CA-C-N	6.64	131.88	122.05
1	E	452	ILE	C-N-CA	6.64	131.88	122.05
2	H	8	DG	O4'-C1'-N9	6.64	112.65	108.00
1	E	355	ASN	CA-CB-CG	6.64	119.24	112.60
2	H	2	DA	O5'-C5'-C4'	6.64	114.71	109.40
1	E	273	ASN	CA-CB-CG	6.63	119.23	112.60
1	E	414	PHE	CA-CB-CG	6.63	120.43	113.80
1	A	523	LEU	CA-C-N	6.62	130.91	122.37
1	A	523	LEU	C-N-CA	6.62	130.91	122.37
1	A	165	ASN	CA-CB-CG	6.62	119.22	112.60
2	H	3	DA	O5'-C5'-C4'	6.61	114.69	109.40
1	E	354	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	559	PHE	CA-CB-CG	6.59	120.39	113.80
2	G	8	DG	O5'-C5'-C4'	6.57	114.66	109.40
1	E	249	TRP	CA-C-N	6.57	129.70	120.57
1	E	249	TRP	C-N-CA	6.57	129.70	120.57
2	H	6	DT	O5'-C5'-C4'	6.55	114.64	109.40
1	E	476	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	467	ASP	CA-CB-CG	6.54	119.14	112.60
1	E	70	PHE	CA-CB-CG	6.54	120.34	113.80
1	E	289	PHE	CA-CB-CG	6.54	120.33	113.80
2	G	2	DA	C8-N9-C4	-6.53	103.19	105.80
1	E	349	ASP	CA-CB-CG	6.51	119.11	112.60
1	E	31	GLU	CA-C-N	6.51	131.26	123.19
1	E	31	GLU	C-N-CA	6.51	131.26	123.19
1	A	271	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	296	ASN	CA-CB-CG	6.50	119.10	112.60
1	E	296	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	489	ILE	CA-C-N	6.48	131.38	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	489	ILE	C-N-CA	6.48	131.38	122.77
1	E	297	PHE	CA-CB-CG	6.46	120.26	113.80
1	F	315	LYS	N-CA-C	6.44	120.41	110.42
1	E	250	GLY	N-CA-C	6.44	122.09	111.59
1	D	172	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	280	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	42	ASN	CA-CB-CG	6.43	119.03	112.60
1	E	472	ASN	CA-CB-CG	6.42	119.02	112.60
1	B	483	ASN	CA-CB-CG	6.42	119.02	112.60
2	H	5	DC	C6-N1-C2	-6.40	117.74	120.30
1	E	453	ASP	N-CA-CB	6.39	118.33	110.53
1	A	529	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	72	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	385	ASP	CA-CB-CG	6.37	118.97	112.60
2	H	4	DG	N1-C6-O6	6.37	123.72	119.90
1	A	469	ASN	CA-CB-CG	6.37	118.97	112.60
1	A	471	ASN	CA-CB-CG	6.36	118.96	112.60
2	H	5	DC	O5'-C5'-C4'	6.33	114.46	109.40
1	E	180	ASP	CA-CB-CG	6.33	118.92	112.60
2	H	10	DT	O5'-C5'-C4'	6.33	114.46	109.40
1	A	537	HIS	CA-CB-CG	6.32	120.12	113.80
1	E	198	GLN	CA-C-N	6.32	130.09	122.26
1	E	198	GLN	C-N-CA	6.32	130.09	122.26
1	D	472	ASN	CA-CB-CG	6.31	118.91	112.60
1	A	389	ASN	CA-CB-CG	6.30	118.90	112.60
1	E	322	LEU	CA-C-N	6.30	130.97	122.90
1	E	322	LEU	C-N-CA	6.30	130.97	122.90
1	A	153	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	135	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	81	ASN	CA-CB-CG	6.27	118.87	112.60
1	E	240	PHE	CA-CB-CG	6.27	120.07	113.80
1	E	453	ASP	CA-CB-CG	6.26	118.86	112.60
1	D	471	ASN	CA-CB-CG	6.25	118.85	112.60
1	E	475	GLY	N-CA-C	6.24	118.37	110.38
1	E	227	ILE	CA-C-N	6.24	131.23	123.12
1	E	227	ILE	C-N-CA	6.24	131.23	123.12
2	G	7	DT	O5'-C5'-C4'	6.23	114.38	109.40
1	A	412	ARG	CD-NE-CZ	6.22	133.12	124.40
1	F	163	ASP	CA-CB-CG	6.22	118.82	112.60
1	E	537	HIS	CA-CB-CG	6.21	120.01	113.80
1	C	104	ARG	CD-NE-CZ	6.21	133.09	124.40
1	A	472	ASN	CA-CB-CG	6.20	118.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	ARG	CD-NE-CZ	6.19	133.07	124.40
1	A	518	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	145	ARG	CD-NE-CZ	6.16	133.02	124.40
1	A	93	ILE	CA-C-N	6.15	130.61	122.30
1	A	93	ILE	C-N-CA	6.15	130.61	122.30
1	A	297	PHE	CA-CB-CG	6.13	119.93	113.80
1	E	81	ASN	CA-CB-CG	6.12	118.72	112.60
1	E	126	ASP	CA-CB-CG	6.12	118.72	112.60
1	E	346	THR	CA-C-N	6.10	131.53	122.86
1	E	346	THR	C-N-CA	6.10	131.53	122.86
2	H	3	DA	C5-N7-C8	-6.10	100.85	103.90
1	A	493	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	275	PHE	CA-CB-CG	6.07	119.87	113.80
1	E	368	ASN	CA-CB-CG	6.07	118.67	112.60
2	H	8	DG	C5-N7-C8	-6.06	101.27	104.30
1	E	65	GLN	CA-C-N	6.05	130.65	122.90
1	E	65	GLN	C-N-CA	6.05	130.65	122.90
1	A	273	ASN	CA-CB-CG	6.05	118.65	112.60
1	E	494	TYR	CA-C-N	6.05	131.52	123.05
1	E	494	TYR	C-N-CA	6.05	131.52	123.05
1	A	169	PHE	CA-CB-CG	6.05	119.85	113.80
1	B	104	ARG	CD-NE-CZ	6.04	132.86	124.40
1	E	343	ARG	CD-NE-CZ	6.01	132.81	124.40
2	G	3	DA	C5-N7-C8	-6.01	100.90	103.90
1	D	470	ARG	CD-NE-CZ	5.96	132.75	124.40
1	E	80	PHE	CA-C-N	5.96	131.92	122.62
1	E	80	PHE	C-N-CA	5.96	131.92	122.62
1	E	496	CYS	CA-C-N	5.96	129.93	122.43
1	E	496	CYS	C-N-CA	5.96	129.93	122.43
1	A	449	ASN	CA-C-N	5.94	131.37	122.99
1	A	449	ASN	C-N-CA	5.94	131.37	122.99
1	E	335	ASP	CA-C-N	5.94	129.96	121.71
1	E	335	ASP	C-N-CA	5.94	129.96	121.71
2	G	7	DT	C6-N1-C2	-5.94	118.33	121.30
1	D	283	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	42	ASN	CA-C-N	5.93	130.90	122.72
1	A	42	ASN	C-N-CA	5.93	130.90	122.72
2	G	3	DA	C8-N9-C4	-5.93	103.43	105.80
1	A	226	PHE	CA-C-N	5.92	130.90	123.14
1	A	226	PHE	C-N-CA	5.92	130.90	123.14
1	E	344	VAL	CA-C-N	5.92	129.76	122.37
1	E	344	VAL	C-N-CA	5.92	129.76	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	469	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	391	PHE	CA-CB-CG	5.91	119.71	113.80
2	H	3	DA	C2-N3-C4	-5.91	107.65	110.60
2	H	4	DG	C5-N7-C8	-5.91	101.35	104.30
1	F	315	LYS	CB-CA-C	5.90	119.54	109.80
1	E	43	GLN	CA-C-N	5.90	130.86	122.72
1	E	43	GLN	C-N-CA	5.90	130.86	122.72
1	A	137	PRO	CA-C-N	5.88	130.48	122.84
1	A	137	PRO	C-N-CA	5.88	130.48	122.84
2	H	5	DC	C5-C6-N1	5.87	123.94	121.00
1	E	546	ALA	CA-C-N	5.87	130.83	123.14
1	E	546	ALA	C-N-CA	5.87	130.83	123.14
1	A	153	PHE	CA-C-N	5.87	130.41	122.90
1	A	153	PHE	C-N-CA	5.87	130.41	122.90
1	D	483	ASN	CA-CB-CG	5.85	118.45	112.60
1	D	175	PHE	CA-CB-CG	5.84	119.64	113.80
2	H	5	DC	C4-C5-C6	5.84	120.32	117.40
1	E	71	GLU	CA-C-N	5.83	130.16	122.30
1	E	71	GLU	C-N-CA	5.83	130.16	122.30
1	E	483	ASN	CA-C-N	5.82	126.81	121.86
1	E	483	ASN	C-N-CA	5.82	126.81	121.86
1	D	263	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	319	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	E	101	SER	CA-C-N	5.81	131.11	122.86
1	E	101	SER	C-N-CA	5.81	131.11	122.86
1	E	276	PRO	CA-C-N	5.81	131.02	123.00
1	E	276	PRO	C-N-CA	5.81	131.02	123.00
1	A	40	ALA	CA-C-N	5.81	131.01	123.00
1	A	40	ALA	C-N-CA	5.81	131.01	123.00
2	G	1	DC	C5-C6-N1	5.80	123.90	121.00
2	H	2	DA	C2-N3-C4	-5.79	107.70	110.60
1	E	56	LYS	CA-C-N	5.76	130.94	123.11
1	E	56	LYS	C-N-CA	5.76	130.94	123.11
1	E	509	GLU	CA-C-N	5.75	128.30	120.54
1	E	509	GLU	C-N-CA	5.75	128.30	120.54
1	E	229	GLU	CA-C-N	5.74	130.97	122.99
1	E	229	GLU	C-N-CA	5.74	130.97	122.99
2	G	3	DA	C2-N3-C4	-5.73	107.73	110.60
1	A	494	TYR	CA-C-N	5.73	131.07	123.05
1	A	494	TYR	C-N-CA	5.73	131.07	123.05
1	A	505	LYS	CA-C-N	5.73	130.39	122.77
1	A	505	LYS	C-N-CA	5.73	130.39	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	307	ASN	CA-C-N	5.73	127.78	120.56
1	E	307	ASN	C-N-CA	5.73	127.78	120.56
1	E	84	PHE	CA-C-N	5.72	130.62	122.72
1	E	84	PHE	C-N-CA	5.72	130.62	122.72
1	E	321	ILE	CA-C-N	5.72	130.37	122.77
1	E	321	ILE	C-N-CA	5.72	130.37	122.77
2	H	1	DC	C5-C6-N1	5.71	123.86	121.00
2	G	1	DC	C4-C5-C6	5.70	120.25	117.40
1	E	488	ALA	CA-C-N	5.69	131.06	122.98
1	E	488	ALA	C-N-CA	5.69	131.06	122.98
1	A	315	LYS	CA-C-N	5.68	131.00	122.99
1	A	315	LYS	C-N-CA	5.68	131.00	122.99
2	H	6	DT	C6-N1-C2	-5.67	118.46	121.30
2	H	2	DA	C5-N7-C8	-5.67	101.06	103.90
2	G	2	DA	C5-N7-C8	-5.66	101.07	103.90
2	H	1	DC	O4'-C1'-N1	5.66	111.96	108.00
1	F	365	PHE	CA-CB-CG	5.66	119.46	113.80
1	E	93	ILE	CA-C-N	5.65	130.16	122.19
1	E	93	ILE	C-N-CA	5.65	130.16	122.19
1	A	98	GLU	CA-C-N	5.64	127.83	120.28
1	A	98	GLU	C-N-CA	5.64	127.83	120.28
1	A	271	PHE	CA-C-N	5.63	130.61	122.16
1	A	271	PHE	C-N-CA	5.63	130.61	122.16
1	A	321	ILE	CA-C-N	5.63	131.10	123.11
1	A	321	ILE	C-N-CA	5.63	131.10	123.11
1	E	172	ASP	CA-CB-CG	-5.63	106.97	112.60
1	A	475	GLY	CA-C-O	-5.62	117.78	122.33
1	E	38	GLY	CA-C-N	5.62	129.41	121.66
1	E	38	GLY	C-N-CA	5.62	129.41	121.66
1	E	548	LYS	CA-C-N	5.62	127.74	120.44
1	E	548	LYS	C-N-CA	5.62	127.74	120.44
2	H	9	DT	C6-N1-C2	-5.61	118.50	121.30
1	A	477	GLY	CA-C-N	5.60	130.73	123.00
1	A	477	GLY	C-N-CA	5.60	130.73	123.00
2	G	8	DG	C5-N7-C8	-5.59	101.50	104.30
1	E	301	GLU	CA-C-N	5.58	130.71	123.00
1	E	301	GLU	C-N-CA	5.58	130.71	123.00
1	A	65	GLN	CA-C-N	5.58	129.62	121.80
1	A	65	GLN	C-N-CA	5.58	129.62	121.80
1	A	530	ARG	CA-C-N	5.57	128.01	120.44
1	A	530	ARG	C-N-CA	5.57	128.01	120.44
1	A	165	ASN	CA-C-N	5.57	128.55	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	ASN	C-N-CA	5.57	128.55	120.98
1	E	39	ILE	N-CA-CB	5.57	116.60	110.53
1	F	261	THR	CA-C-N	5.56	132.16	121.54
1	F	261	THR	C-N-CA	5.56	132.16	121.54
1	A	94	ALA	CA-C-N	5.56	130.72	122.99
1	A	94	ALA	C-N-CA	5.56	130.72	122.99
1	A	495	LEU	CA-C-N	5.56	130.07	122.84
1	A	495	LEU	C-N-CA	5.56	130.07	122.84
1	E	94	ALA	CA-C-N	5.56	130.66	122.94
1	E	94	ALA	C-N-CA	5.56	130.66	122.94
1	E	441	ALA	CA-C-N	5.54	127.64	120.44
1	E	441	ALA	C-N-CA	5.54	127.64	120.44
1	E	354	ASP	CA-C-N	5.53	130.63	123.00
1	E	354	ASP	C-N-CA	5.53	130.63	123.00
1	A	92	ASN	CA-C-N	5.53	129.75	122.51
1	A	92	ASN	C-N-CA	5.53	129.75	122.51
1	F	263	ASN	N-CA-C	-5.53	100.10	108.67
2	H	1	DC	C4-C5-C6	5.52	120.16	117.40
1	F	243	ASN	CA-CB-CG	5.52	118.12	112.60
2	G	4	DG	O4'-C1'-N9	5.51	111.86	108.00
2	H	7	DT	N3-C2-O2	-5.51	119.00	122.30
2	G	2	DA	C2-N3-C4	-5.50	107.85	110.60
1	A	472	ASN	CA-C-N	5.50	130.63	122.99
1	A	472	ASN	C-N-CA	5.50	130.63	122.99
1	A	128	ILE	N-CA-CB	5.50	116.98	110.55
1	E	456	LYS	N-CA-CB	5.49	117.97	110.01
1	E	271	PHE	N-CA-CB	5.49	117.97	110.01
1	A	471	ASN	CA-C-N	5.48	131.25	122.86
1	A	471	ASN	C-N-CA	5.48	131.25	122.86
1	A	152	TYR	CA-C-N	5.48	130.73	123.05
1	A	152	TYR	C-N-CA	5.48	130.73	123.05
1	A	479	SER	N-CA-CB	5.47	118.05	110.17
1	E	120	THR	CA-C-N	5.47	127.55	120.44
1	E	120	THR	C-N-CA	5.47	127.55	120.44
2	H	10	DT	C6-N1-C2	-5.46	118.57	121.30
2	G	10	DT	C6-N1-C2	-5.45	118.57	121.30
1	E	336	GLU	CA-C-N	5.44	128.44	120.71
1	E	336	GLU	C-N-CA	5.44	128.44	120.71
1	F	315	LYS	CA-C-N	5.43	131.01	122.21
1	F	315	LYS	C-N-CA	5.43	131.01	122.21
1	A	64	PRO	CA-C-N	5.43	130.43	122.77
1	A	64	PRO	C-N-CA	5.43	130.43	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	445	MET	N-CA-CB	5.43	117.89	110.01
1	E	367	GLU	CA-C-N	5.42	130.64	122.99
1	E	367	GLU	C-N-CA	5.42	130.64	122.99
2	G	6	DT	O4'-C1'-N1	5.42	111.79	108.00
1	A	414	PHE	CA-C-N	5.41	127.47	120.44
1	A	414	PHE	C-N-CA	5.41	127.47	120.44
1	A	43	GLN	CA-C-N	5.40	129.80	122.19
1	A	43	GLN	C-N-CA	5.40	129.80	122.19
1	A	384	LYS	CA-C-N	5.40	127.46	120.44
1	A	384	LYS	C-N-CA	5.40	127.46	120.44
1	A	215	SER	CA-C-N	5.40	127.36	120.56
1	A	215	SER	C-N-CA	5.40	127.36	120.56
1	A	441	ALA	CA-C-N	5.40	127.46	120.44
1	A	441	ALA	C-N-CA	5.40	127.46	120.44
1	A	459	LEU	N-CA-CB	5.39	117.83	110.01
1	A	389	ASN	CA-C-N	5.39	127.50	120.28
1	A	389	ASN	C-N-CA	5.39	127.50	120.28
1	E	144	THR	CA-C-N	5.39	131.26	122.81
1	E	144	THR	C-N-CA	5.39	131.26	122.81
1	E	277	MET	CA-C-N	5.38	130.67	122.65
1	E	277	MET	C-N-CA	5.38	130.67	122.65
1	A	166	VAL	CA-C-N	5.38	130.59	123.00
1	A	166	VAL	C-N-CA	5.38	130.59	123.00
1	F	314	ALA	N-CA-C	5.37	118.10	110.10
1	E	489	ILE	CA-C-N	5.37	130.13	122.72
1	E	489	ILE	C-N-CA	5.37	130.13	122.72
1	E	128	ILE	N-CA-CB	5.36	116.82	110.55
1	A	151	GLY	CA-C-N	5.36	130.54	122.99
1	A	151	GLY	C-N-CA	5.36	130.54	122.99
1	A	459	LEU	CA-C-N	5.36	127.40	120.44
1	A	459	LEU	C-N-CA	5.36	127.40	120.44
1	E	167	LYS	CA-C-N	5.36	130.97	122.62
1	E	167	LYS	C-N-CA	5.36	130.97	122.62
1	A	72	ASP	N-CA-CB	5.35	118.33	109.88
1	F	432	HIS	CB-CG-CD2	-5.34	124.25	131.20
1	A	81	ASN	CA-C-N	5.34	130.67	122.93
1	A	81	ASN	C-N-CA	5.34	130.67	122.93
1	A	113	LYS	CA-C-N	5.34	130.52	123.05
1	A	113	LYS	C-N-CA	5.34	130.52	123.05
1	A	418	GLN	CA-C-N	5.33	127.28	120.56
1	A	418	GLN	C-N-CA	5.33	127.28	120.56
1	E	204	MET	CA-C-N	5.33	127.28	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	204	MET	C-N-CA	5.33	127.28	120.56
1	E	270	SER	N-CA-CB	5.33	117.74	110.01
2	G	3	DA	O4'-C1'-N9	5.33	111.73	108.00
1	E	298	SER	CA-C-N	5.32	130.50	123.00
1	E	298	SER	C-N-CA	5.32	130.50	123.00
1	E	472	ASN	CA-C-N	5.31	130.36	122.71
1	E	472	ASN	C-N-CA	5.31	130.36	122.71
1	A	222	GLY	CA-C-N	5.31	130.56	122.65
1	A	222	GLY	C-N-CA	5.31	130.56	122.65
1	E	127	TYR	CA-C-N	5.31	127.25	120.56
1	E	127	TYR	C-N-CA	5.31	127.25	120.56
1	A	393	SER	CA-C-N	5.30	127.39	120.28
1	A	393	SER	C-N-CA	5.30	127.39	120.28
1	A	127	TYR	N-CA-CB	5.30	117.70	110.01
1	F	183	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	E	486	ILE	N-CA-CB	5.29	116.30	110.53
1	A	518	ASP	N-CA-CB	5.29	117.68	110.01
1	E	82	MET	CA-C-N	5.28	131.29	122.73
1	E	82	MET	C-N-CA	5.28	131.29	122.73
1	E	289	PHE	CA-C-N	5.28	127.21	120.56
1	E	289	PHE	C-N-CA	5.28	127.21	120.56
1	A	490	TYR	CA-C-N	5.27	131.09	122.81
1	A	490	TYR	C-N-CA	5.27	131.09	122.81
1	E	310	LEU	CA-C-N	5.27	130.86	122.59
1	E	310	LEU	C-N-CA	5.27	130.86	122.59
1	E	289	PHE	N-CA-CB	5.26	117.64	110.01
1	A	402	GLY	CA-C-N	5.26	127.60	120.44
1	A	402	GLY	C-N-CA	5.26	127.60	120.44
1	F	342	ALA	N-CA-C	5.25	119.19	111.04
1	E	459	LEU	N-CA-CB	5.25	117.63	110.01
1	A	297	PHE	N-CA-CB	5.25	117.84	110.12
1	A	446	VAL	N-CA-CB	5.25	116.34	110.51
1	A	546	ALA	CA-C-N	5.25	130.24	122.94
1	A	546	ALA	C-N-CA	5.25	130.24	122.94
1	E	237	GLY	CA-C-N	5.25	127.27	120.44
1	E	237	GLY	C-N-CA	5.25	127.27	120.44
1	E	477	GLY	CA-C-N	5.25	130.82	122.94
1	E	477	GLY	C-N-CA	5.25	130.82	122.94
1	D	471	ASN	CA-C-N	5.25	130.91	122.83
1	D	471	ASN	C-N-CA	5.25	130.91	122.83
1	A	448	ASN	CA-C-N	5.24	129.38	122.30
1	A	448	ASN	C-N-CA	5.24	129.38	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	VAL	N-CA-CB	5.24	116.76	110.31
1	A	82	MET	CA-C-N	5.24	130.81	122.74
1	A	82	MET	C-N-CA	5.24	130.81	122.74
1	E	490	TYR	CA-C-N	5.24	130.81	122.59
1	E	490	TYR	C-N-CA	5.24	130.81	122.59
1	A	547	ILE	CA-C-N	5.24	128.20	120.82
1	A	547	ILE	C-N-CA	5.24	128.20	120.82
2	G	5	DC	N3-C2-O2	-5.23	118.24	121.90
2	H	8	DG	C5-C6-N1	-5.23	108.89	111.50
1	A	320	ASN	CA-C-N	5.23	129.98	121.62
1	A	320	ASN	C-N-CA	5.23	129.98	121.62
1	E	345	VAL	CA-C-N	5.23	130.51	122.93
1	E	345	VAL	C-N-CA	5.23	130.51	122.93
1	A	390	ALA	CA-C-N	5.22	127.22	120.44
1	A	390	ALA	C-N-CA	5.22	127.22	120.44
1	A	532	GLN	CA-C-N	5.22	128.28	120.87
1	A	532	GLN	C-N-CA	5.22	128.28	120.87
1	E	55	LYS	CA-C-N	5.22	129.76	121.99
1	E	55	LYS	C-N-CA	5.22	129.76	121.99
1	A	143	ALA	CA-C-N	5.21	130.38	122.56
1	A	143	ALA	C-N-CA	5.21	130.38	122.56
1	A	131	SER	N-CA-CB	5.20	117.56	110.01
1	A	394	TYR	CA-C-N	5.20	127.20	120.44
1	A	394	TYR	C-N-CA	5.20	127.20	120.44
1	E	98	GLU	CA-C-N	5.20	127.77	120.28
1	E	98	GLU	C-N-CA	5.20	127.77	120.28
1	A	456	LYS	N-CA-CB	5.20	117.55	110.01
1	A	480	SER	N-CA-CB	5.20	117.68	109.83
1	D	172	ASP	N-CA-CB	5.20	117.64	109.69
1	A	167	LYS	CB-CG-CD	5.20	123.25	111.30
1	E	303	LYS	N-CA-CB	5.19	117.18	109.19
1	D	261	THR	CA-C-N	5.18	127.53	120.54
1	D	261	THR	C-N-CA	5.18	127.53	120.54
1	A	214	GLY	CA-C-N	5.18	127.17	120.44
1	A	214	GLY	C-N-CA	5.18	127.17	120.44
1	A	265	ILE	CA-C-N	5.18	127.22	120.28
1	A	265	ILE	C-N-CA	5.18	127.22	120.28
1	F	300	GLY	CA-C-N	5.18	131.12	122.73
1	F	300	GLY	C-N-CA	5.18	131.12	122.73
1	A	416	LEU	N-CA-CB	5.18	117.52	110.01
1	E	462	LEU	N-CA-CB	5.18	117.52	110.01
1	E	481	VAL	CA-C-N	5.17	127.17	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	481	VAL	C-N-CA	5.17	127.17	120.44
1	A	127	TYR	CA-C-N	5.17	127.07	120.56
1	A	127	TYR	C-N-CA	5.17	127.07	120.56
1	E	240	PHE	N-CA-CB	5.17	117.51	110.01
2	H	1	DC	C3'-C2'-C1'	5.17	108.70	102.50
1	A	533	LYS	N-CA-CB	5.16	117.56	109.97
1	E	125	VAL	N-CA-CB	5.16	116.58	110.55
1	E	444	SER	N-CA-CB	5.16	117.48	110.01
1	A	141	LYS	CA-C-N	5.15	130.23	123.17
1	A	141	LYS	C-N-CA	5.15	130.23	123.17
1	A	74	GLU	N-CA-CB	5.15	117.48	110.01
1	E	238	LYS	CA-C-N	5.15	127.18	120.28
1	E	238	LYS	C-N-CA	5.15	127.18	120.28
1	E	292	SER	CA-C-N	5.15	127.14	120.44
1	E	292	SER	C-N-CA	5.15	127.14	120.44
1	E	485	ASP	CA-C-N	5.15	128.77	121.66
1	E	485	ASP	C-N-CA	5.15	128.77	121.66
1	A	456	LYS	CA-C-N	5.15	127.14	120.44
1	A	456	LYS	C-N-CA	5.15	127.14	120.44
1	A	465	TYR	N-CA-CB	5.15	117.61	109.94
1	E	457	GLN	N-CA-CB	5.14	117.47	110.01
1	E	42	ASN	CA-C-N	5.14	128.77	121.42
1	E	42	ASN	C-N-CA	5.14	128.77	121.42
1	A	124	LEU	N-CA-CB	5.14	117.46	110.01
1	A	524	ILE	N-CA-CB	5.14	116.32	110.72
1	E	339	GLY	CA-C-N	5.13	127.03	120.56
1	E	339	GLY	C-N-CA	5.13	127.03	120.56
1	E	340	VAL	N-CA-CB	5.13	116.56	110.55
1	D	177	LYS	N-CA-CB	5.13	117.45	110.01
1	D	176	GLN	N-CA-CB	5.13	117.44	110.01
1	E	456	LYS	CB-CG-CD	5.13	123.09	111.30
1	A	445	MET	N-CA-CB	5.12	117.65	110.12
1	A	391	PHE	N-CA-CB	5.12	117.43	110.01
1	A	295	TYR	CA-C-N	5.12	127.09	120.44
1	A	295	TYR	C-N-CA	5.12	127.09	120.44
1	E	124	LEU	N-CA-CB	5.12	117.43	110.01
1	E	145	ARG	CD-NE-CZ	5.12	131.56	124.40
1	E	278	PHE	CA-C-N	5.12	130.76	122.53
1	E	278	PHE	C-N-CA	5.12	130.76	122.53
1	A	219	ARG	N-CA-CB	5.11	117.64	110.12
1	E	451	THR	CA-C-N	5.11	127.00	120.56
1	E	451	THR	C-N-CA	5.11	127.00	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	445	MET	CA-C-N	5.11	127.19	120.60
1	A	445	MET	C-N-CA	5.11	127.19	120.60
1	E	102	ASP	CA-C-N	5.11	127.08	120.44
1	E	102	ASP	C-N-CA	5.11	127.08	120.44
2	G	6	DT	N3-C2-O2	-5.11	119.23	122.30
1	A	451	THR	CA-C-N	5.11	130.67	122.50
1	A	451	THR	C-N-CA	5.11	130.67	122.50
2	G	5	DC	O5'-C5'-C4'	5.10	113.48	109.40
1	E	121	SER	N-CA-CB	5.10	117.40	110.01
2	G	7	DT	O4'-C1'-N1	5.10	111.57	108.00
1	A	460	GLU	N-CA-CB	5.10	117.40	110.01
1	A	130	ALA	CA-C-N	5.09	127.06	120.44
1	A	130	ALA	C-N-CA	5.09	127.06	120.44
1	D	172	ASP	CA-C-N	5.09	127.10	120.28
1	D	172	ASP	C-N-CA	5.09	127.10	120.28
1	D	264	SER	CA-C-N	5.09	126.97	120.56
1	D	264	SER	C-N-CA	5.09	126.97	120.56
1	D	265	ILE	N-CA-CB	5.09	116.50	110.55
1	A	457	GLN	CA-C-N	5.09	127.06	120.44
1	A	457	GLN	C-N-CA	5.09	127.06	120.44
1	A	501	THR	CA-C-N	5.09	126.97	120.56
1	A	501	THR	C-N-CA	5.09	126.97	120.56
1	C	104	ARG	CG-CD-NE	5.09	123.20	112.00
1	A	164	SER	CA-C-N	5.09	129.12	120.88
1	A	164	SER	C-N-CA	5.09	129.12	120.88
1	A	387	TYR	CA-C-N	5.09	127.06	120.44
1	A	387	TYR	C-N-CA	5.09	127.06	120.44
1	E	121	SER	CA-C-N	5.09	127.05	120.44
1	E	121	SER	C-N-CA	5.09	127.05	120.44
1	E	360	THR	CA-C-N	5.09	127.09	120.28
1	E	360	THR	C-N-CA	5.09	127.09	120.28
2	G	2	DA	O4'-C1'-N9	5.09	111.56	108.00
2	G	8	DG	C5-C6-N1	-5.09	108.96	111.50
1	E	182	PHE	CA-C-N	5.08	128.69	121.42
1	E	182	PHE	C-N-CA	5.08	128.69	121.42
1	E	288	LYS	CA-C-N	5.08	127.04	120.44
1	E	288	LYS	C-N-CA	5.08	127.04	120.44
2	G	2	DA	C3'-C2'-C1'	5.08	108.59	102.50
1	E	354	ASP	N-CA-CB	5.08	117.37	110.01
1	A	412	ARG	CG-CD-NE	5.07	123.16	112.00
1	E	296	ASN	CA-C-N	5.07	127.58	120.28
1	E	296	ASN	C-N-CA	5.07	127.58	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	73	ILE	CA-C-N	5.07	127.03	120.44
1	E	73	ILE	C-N-CA	5.07	127.03	120.44
1	D	103	SER	CA-C-N	5.06	127.02	120.44
1	D	103	SER	C-N-CA	5.06	127.02	120.44
1	E	127	TYR	N-CA-CB	5.06	117.35	110.01
1	E	353	PRO	CA-C-N	5.06	127.02	120.44
1	E	353	PRO	C-N-CA	5.06	127.02	120.44
1	A	463	LEU	CA-C-N	5.06	127.37	120.54
1	A	463	LEU	C-N-CA	5.06	127.37	120.54
2	H	4	DG	C5-C6-N1	-5.06	108.97	111.50
1	A	269	ALA	CA-C-N	5.06	127.33	120.65
1	A	269	ALA	C-N-CA	5.06	127.33	120.65
1	A	408	GLN	CA-C-N	5.06	127.02	120.44
1	A	408	GLN	C-N-CA	5.06	127.02	120.44
1	A	108	LYS	CB-CG-CD	5.06	122.93	111.30
1	A	467	ASP	N-CA-CB	5.05	117.34	110.01
1	A	533	LYS	CA-CB-CG	5.05	124.21	114.10
1	E	446	VAL	N-CA-CB	5.05	116.46	110.55
1	E	553	LYS	CA-CB-CG	5.05	124.20	114.10
1	A	68	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	513	ILE	CA-C-N	5.05	127.00	120.44
1	A	513	ILE	C-N-CA	5.05	127.00	120.44
1	E	473	ILE	CA-C-N	5.05	130.49	122.62
1	E	473	ILE	C-N-CA	5.05	130.49	122.62
1	A	412	ARG	CA-CB-CG	5.04	124.19	114.10
1	F	365	PHE	CB-CG-CD2	-5.04	112.13	120.70
1	A	412	ARG	CA-C-N	5.04	127.03	120.28
1	A	412	ARG	C-N-CA	5.04	127.03	120.28
1	E	31	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	99	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	388	LYS	N-CA-CB	5.04	117.32	110.01
1	A	521	GLY	CA-C-N	5.04	126.99	120.44
1	A	521	GLY	C-N-CA	5.04	126.99	120.44
1	E	456	LYS	CA-C-N	5.04	126.99	120.44
1	E	456	LYS	C-N-CA	5.04	126.99	120.44
1	E	41	LEU	CA-C-N	5.03	130.49	122.74
1	E	41	LEU	C-N-CA	5.03	130.49	122.74
1	E	343	ARG	CA-C-N	5.03	130.40	122.70
1	E	343	ARG	C-N-CA	5.03	130.40	122.70
1	E	305	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	A	73	ILE	CA-C-N	5.02	126.97	120.44
1	A	73	ILE	C-N-CA	5.02	126.97	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	SER	CA-C-N	5.02	130.00	122.47
1	B	101	SER	C-N-CA	5.02	130.00	122.47
1	B	98	GLU	N-CA-CB	5.02	117.28	110.01
1	A	316	LYS	CB-CG-CD	5.02	122.84	111.30
1	E	68	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	386	VAL	CA-C-N	5.01	126.95	120.44
1	A	386	VAL	C-N-CA	5.01	126.95	120.44
1	A	455	PRO	CA-C-N	5.01	126.95	120.44
1	A	455	PRO	C-N-CA	5.01	126.95	120.44
1	E	43	GLN	N-CA-CB	5.01	117.63	110.06
1	A	462	LEU	N-CA-CB	5.01	117.27	110.01
1	A	464	GLN	CA-CB-CG	5.01	124.12	114.10
1	A	406	ILE	CA-C-N	5.01	126.95	120.44
1	A	406	ILE	C-N-CA	5.01	126.95	120.44
1	E	124	LEU	CA-C-N	5.01	126.87	120.56
1	E	124	LEU	C-N-CA	5.01	126.87	120.56
1	A	342	ALA	CA-C-N	5.00	130.66	122.65
1	A	342	ALA	C-N-CA	5.00	130.66	122.65
1	E	406	ILE	CA-C-N	5.00	126.95	120.44
1	E	406	ILE	C-N-CA	5.00	126.95	120.44
1	E	487	LYS	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	365	PHE	Sidechain
1	F	396	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4052	4060	4056	41	0
1	B	4088	4094	4088	31	0
1	C	4227	4231	4229	30	0
1	D	4197	4208	4203	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4200	4215	4211	26	0
1	F	4197	4208	4204	7	0
2	G	204	114	104	7	0
2	H	204	114	98	0	0
3	B	31	13	13	2	0
3	C	31	13	13	3	0
3	D	31	13	13	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	E	27	12	12	0	0
All	All	25493	25295	25244	164	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 3.

All (164) 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:D:550:GLU:N	1:D:550:GLU:OE1	2.13	0.82
1:C:550:GLU:N	1:C:550:GLU:OE1	2.12	0.82
1:B:550:GLU:N	1:B:550:GLU:OE1	2.15	0.80
1:A:280:ASP:OD1	1:A:325:THR:OG1	1.99	0.80
1:D:72:ASP:OD1	1:D:73:ILE:N	2.16	0.79
2:G:6:DT:C6	2:G:7:DT:H72	2.18	0.78
1:B:402:GLY:O	1:B:408:GLN:NE2	2.17	0.77
1:C:172:ASP:OD1	1:C:174:GLY:N	2.18	0.77
1:C:72:ASP:OD1	1:C:73:ILE:N	2.19	0.75
1:A:194:LYS:NZ	1:A:367:GLU:OE1	2.18	0.75
1:A:272:LEU:O	1:A:320:ASN:ND2	2.20	0.74
1:A:431:GLU:N	1:A:431:GLU:OE1	2.23	0.72
2:G:6:DT:C5	2:G:7:DT:H72	2.25	0.71
1:C:239:THR:O	1:C:243:ASN:ND2	2.23	0.71
1:B:511:GLN:N	1:B:511:GLN:OE1	2.25	0.70
1:C:237:GLY:N	3:C:701:ANP:O1A	2.26	0.69
1:A:550:GLU:N	1:A:550:GLU:OE1	2.26	0.68
1:D:336:GLU:N	1:D:336:GLU:OE1	2.27	0.68
1:E:317:GLU:N	1:E:317:GLU:OE1	2.27	0.67
1:F:387:TYR:CE1	1:F:423:VAL:HG22	2.30	0.67
2:G:7:DT:N3	2:G:8:DG:O6	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:OD1	1:B:73:ILE:N	2.29	0.66
1:A:387:TYR:CE1	1:A:423:VAL:HG12	2.31	0.65
1:B:69:ARG:NH1	1:B:139:ASN:OD1	2.30	0.64
1:A:362:ASP:OD1	1:A:366:ARG:NH2	2.30	0.64
1:B:527:GLU:N	1:B:527:GLU:OE1	2.30	0.63
1:B:558:ASP:OD1	1:B:559:PHE:N	2.31	0.63
3:D:701:ANP:O2G	1:E:343:ARG:NH1	2.32	0.63
1:D:110:VAL:HG12	1:E:97:ALA:HB1	1.81	0.63
1:C:161:MET:O	1:C:167:LYS:NZ	2.30	0.61
1:E:220:GLU:N	1:E:220:GLU:OE1	2.33	0.61
1:A:215:SER:OG	1:A:274:SER:O	2.09	0.60
1:D:465:TYR:OH	1:D:487:LYS:NZ	2.33	0.60
1:A:292:SER:O	1:A:296:ASN:ND2	2.35	0.60
1:E:148:HIS:O	1:E:273:ASN:ND2	2.35	0.59
1:D:102:ASP:OD1	1:D:103:SER:N	2.35	0.59
1:A:228:VAL:HG23	1:A:345:VAL:HG13	1.85	0.58
1:E:385:ASP:O	1:E:389:ASN:ND2	2.37	0.58
1:C:385:ASP:OD1	1:C:386:VAL:N	2.37	0.57
1:B:317:GLU:OE2	1:B:319:ARG:NH2	2.35	0.56
1:E:245:VAL:O	1:E:248:VAL:HG12	2.05	0.56
1:B:222:GLY:C	1:B:223:LEU:HD12	2.31	0.56
1:B:532:GLN:OE1	1:B:543:ARG:NH1	2.40	0.55
1:A:444:SER:O	1:A:448:ASN:ND2	2.40	0.55
1:B:172:ASP:OD1	1:B:174:GLY:N	2.39	0.55
1:B:506:LEU:O	1:B:507:THR:OG1	2.19	0.55
1:B:362:ASP:OD2	3:B:701:ANP:N6	2.40	0.54
1:D:199:ILE:O	1:D:199:ILE:HD12	2.07	0.54
1:B:201:ASP:N	1:B:201:ASP:OD1	2.40	0.53
1:E:239:THR:O	1:E:243:ASN:ND2	2.41	0.53
1:C:357:ASP:N	1:C:357:ASP:OD1	2.41	0.53
1:D:235:SER:N	3:D:701:ANP:O1B	2.42	0.53
1:C:235:SER:H	3:C:701:ANP:HNB1	1.57	0.53
1:B:428:ASP:OD1	1:B:429:GLY:N	2.42	0.53
1:A:453:ASP:O	1:A:456:LYS:N	2.42	0.52
1:D:322:LEU:C	1:D:322:LEU:HD23	2.34	0.52
1:E:81:ASN:OD1	1:E:82:MET:N	2.43	0.52
1:A:283:ARG:NE	1:A:327:GLU:OE1	2.43	0.51
1:E:77:GLU:OE1	1:E:78:VAL:N	2.43	0.51
1:A:357:ASP:CG	1:A:360:THR:HG22	2.36	0.51
1:A:266:GLU:OE1	1:A:266:GLU:N	2.41	0.51
1:D:272:LEU:O	1:D:320:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HG22	1:A:202:LEU:HD12	1.93	0.50
1:A:442:TYR:O	1:A:446:VAL:HG23	2.11	0.50
1:C:43:GLN:N	1:C:57:VAL:O	2.43	0.50
1:D:485:ASP:N	1:D:485:ASP:OD1	2.45	0.50
1:E:280:ASP:OD1	1:E:281:ASP:N	2.45	0.50
1:A:320:ASN:N	1:A:320:ASN:OD1	2.44	0.50
1:A:387:TYR:CD1	1:A:423:VAL:HG12	2.47	0.50
1:C:72:ASP:OD1	1:C:74:GLU:N	2.42	0.49
1:A:317:GLU:OE1	1:A:317:GLU:N	2.44	0.48
1:B:234:THR:O	3:B:701:ANP:N3B	2.45	0.48
1:C:109:LEU:HB2	1:C:114:LEU:HD23	1.95	0.48
1:B:111:ASN:O	1:C:78:VAL:HG22	2.13	0.48
1:D:106:LEU:HD21	1:D:124:LEU:HD23	1.94	0.48
1:A:209:LEU:HD22	1:A:245:VAL:HG12	1.95	0.48
1:C:486:ILE:HD12	1:C:486:ILE:N	2.28	0.48
1:B:486:ILE:HD12	1:B:486:ILE:N	2.28	0.48
1:B:354:ASP:OD1	1:B:355:ASN:N	2.44	0.48
1:C:244:LEU:C	1:C:244:LEU:HD23	2.38	0.48
1:A:227:ILE:HB	1:A:344:VAL:HG13	1.96	0.48
1:C:322:LEU:C	1:C:322:LEU:HD23	2.39	0.48
1:B:102:ASP:OD2	1:B:105:GLN:NE2	2.46	0.48
1:D:148:HIS:O	1:D:273:ASN:ND2	2.47	0.47
1:A:452:ILE:HD12	1:A:452:ILE:N	2.30	0.47
1:F:387:TYR:CD1	1:F:423:VAL:HG22	2.49	0.47
1:F:419:VAL:O	1:F:423:VAL:HG23	2.14	0.47
1:A:488:ALA:C	1:A:489:ILE:HD12	2.40	0.47
1:C:485:ASP:OD1	1:C:485:ASP:N	2.47	0.47
1:E:168:LEU:HD12	1:E:169:PHE:H	1.80	0.46
1:D:486:ILE:N	1:D:486:ILE:HD12	2.30	0.46
1:B:164:SER:O	1:B:167:LYS:NZ	2.46	0.46
1:D:311:THR:OG1	1:C:172:ASP:OD2	2.31	0.46
2:G:7:DT:O2	2:G:8:DG:N7	2.48	0.46
1:B:218:LEU:HD12	1:B:416:LEU:HD11	1.97	0.46
1:B:233:SER:O	1:B:238:LYS:NZ	2.42	0.46
1:C:218:LEU:O	1:C:222:GLY:N	2.49	0.46
1:F:243:ASN:HB3	1:F:365:PHE:CE2	2.51	0.45
1:E:198:GLN:OE1	1:E:198:GLN:N	2.46	0.45
2:G:7:DT:C2	2:G:8:DG:N7	2.85	0.45
1:D:244:LEU:C	1:D:244:LEU:HD23	2.42	0.45
1:D:233:SER:O	1:D:238:LYS:NZ	2.50	0.45
1:A:365:PHE:C	1:A:365:PHE:CD1	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ILE:HG22	1:C:322:LEU:N	2.33	0.45
1:D:387:TYR:CE1	1:D:423:VAL:HG22	2.51	0.44
1:B:155:TYR:O	1:B:168:LEU:HD11	2.17	0.44
1:B:404:ASN:OD1	1:B:406:ILE:N	2.50	0.44
1:A:205:VAL:O	1:A:209:LEU:HD23	2.17	0.44
1:A:242:LEU:HD21	1:A:255:ILE:HG23	2.00	0.44
1:A:279:LYS:N	1:A:323:ILE:O	2.48	0.44
1:E:523:LEU:HD12	1:E:523:LEU:O	2.18	0.44
1:C:310:LEU:HD22	1:C:310:LEU:N	2.32	0.44
1:B:163:ASP:OD1	1:B:164:SER:N	2.51	0.44
1:B:406:ILE:N	1:B:406:ILE:HD12	2.32	0.44
1:E:153:PHE:C	1:E:154:ILE:HD12	2.43	0.44
1:E:391:PHE:HB2	1:E:419:VAL:HG21	1.99	0.44
1:B:239:THR:O	1:B:243:ASN:ND2	2.51	0.43
1:F:249:TRP:CZ3	1:F:373:GLY:HA3	2.53	0.43
1:E:160:VAL:HG22	1:E:160:VAL:O	2.18	0.43
1:E:365:PHE:CD1	1:E:365:PHE:C	2.96	0.43
1:A:428:ASP:OD1	1:A:429:GLY:N	2.51	0.43
1:A:243:ASN:HA	1:A:255:ILE:HD11	2.01	0.43
1:D:343:ARG:NH1	3:C:701:ANP:O3G	2.48	0.43
1:A:227:ILE:HB	1:A:344:VAL:HG22	2.01	0.43
1:B:362:ASP:O	1:B:366:ARG:HG2	2.19	0.42
1:C:102:ASP:OD1	1:C:103:SER:N	2.52	0.42
1:D:365:PHE:CD1	1:D:365:PHE:C	2.98	0.42
1:E:527:GLU:OE1	1:E:527:GLU:N	2.49	0.42
1:C:558:ASP:OD1	1:C:559:PHE:N	2.53	0.42
1:B:526:GLY:N	1:B:530:ARG:O	2.46	0.42
1:C:506:LEU:O	1:C:507:THR:OG1	2.21	0.42
1:A:391:PHE:HB2	1:A:419:VAL:HG21	2.01	0.42
1:A:488:ALA:O	1:A:489:ILE:HD12	2.19	0.42
1:D:199:ILE:HG22	1:D:202:LEU:HD12	2.01	0.42
1:D:427:ILE:HG22	1:D:428:ASP:N	2.35	0.42
1:A:486:ILE:H	1:A:486:ILE:HD12	1.83	0.42
1:D:311:THR:HG21	1:C:172:ASP:OD2	2.20	0.42
1:D:39:ILE:O	1:D:39:ILE:HG23	2.19	0.41
1:B:78:VAL:HG11	1:A:113:LYS:HG2	2.02	0.41
1:E:518:ASP:HA	1:E:523:LEU:HD11	2.02	0.41
1:C:322:LEU:HD23	1:C:322:LEU:O	2.20	0.41
1:F:243:ASN:HA	1:F:255:ILE:HD11	2.02	0.41
1:D:165:ASN:OD1	1:D:165:ASN:N	2.51	0.41
1:D:310:LEU:HD22	1:D:310:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLN:NE2	1:A:426:ASP:OD2	2.52	0.41
1:C:154:ILE:HD12	1:C:154:ILE:N	2.36	0.41
2:G:3:DA:C2	2:G:4:DG:C4	3.09	0.41
1:C:244:LEU:HD23	1:C:244:LEU:O	2.21	0.41
1:A:362:ASP:HA	1:A:365:PHE:CE2	2.56	0.41
1:C:272:LEU:O	1:C:320:ASN:ND2	2.53	0.41
1:D:256:THR:HG22	1:D:257:THR:N	2.36	0.41
1:A:171:ASN:OD1	1:A:172:ASP:N	2.53	0.41
1:A:476:ASP:N	1:A:476:ASP:OD1	2.53	0.41
1:E:106:LEU:HD21	1:E:124:LEU:HD23	2.03	0.41
1:E:154:ILE:HD12	1:E:154:ILE:N	2.35	0.41
1:C:203:PRO:O	1:C:207:VAL:HG23	2.20	0.41
1:E:379:GLN:NE2	1:E:387:TYR:OH	2.52	0.41
2:G:8:DG:N1	2:G:9:DT:O4	2.54	0.41
1:F:315:LYS:HD3	1:E:177:LYS:HD2	2.02	0.40
1:A:290:VAL:O	1:A:294:THR:HG23	2.21	0.40
1:E:540:VAL:HG12	1:E:541:LYS:N	2.36	0.40
1:D:287:PRO:HA	1:D:290:VAL:HG22	2.03	0.40
1:A:374:LEU:HD22	1:A:374:LEU:N	2.36	0.40
1:E:159:GLU:OE1	1:E:159:GLU:N	2.54	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	494/602 (82%)	465 (94%)	29 (6%)	0	100	100
1	B	499/602 (83%)	471 (94%)	27 (5%)	1 (0%)	43	74
1	C	523/602 (87%)	490 (94%)	33 (6%)	0	100	100
1	D	518/602 (86%)	493 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	518/602 (86%)	491 (95%)	27 (5%)	0	100 100
1	F	518/602 (86%)	490 (95%)	26 (5%)	2 (0%)	30 62
All	All	3070/3612 (85%)	2900 (94%)	167 (5%)	3 (0%)	49 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	262	GLN
1	F	87	ASN
1	B	87	ASN

5.3.2 Protein sidechains (i)

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	454/534 (85%)	446 (98%)	8 (2%)	51 70
1	B	458/534 (86%)	456 (100%)	2 (0%)	84 81
1	C	474/534 (89%)	467 (98%)	7 (2%)	57 72
1	D	470/534 (88%)	461 (98%)	9 (2%)	50 68
1	E	471/534 (88%)	465 (99%)	6 (1%)	61 73
1	F	470/534 (88%)	464 (99%)	6 (1%)	61 73
All	All	2797/3204 (87%)	2759 (99%)	38 (1%)	57 72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	163	ASP
1	F	310	LEU
1	F	365	PHE
1	F	493	ASP
1	F	534	GLN
1	F	550	GLU
1	B	134	TYR

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Mol	Chain	Res	Type
1	B	172	ASP
1	D	41	LEU
1	D	163	ASP
1	D	165	ASN
1	D	218	LEU
1	D	229	GLU
1	D	282	THR
1	D	308	ILE
1	D	493	ASP
1	D	553	LYS
1	A	163	ASP
1	A	321	ILE
1	A	368	ASN
1	A	372	LEU
1	A	410	LEU
1	A	431	GLU
1	A	452	ILE
1	A	493	ASP
1	E	169	PHE
1	E	177	LYS
1	E	229	GLU
1	E	295	TYR
1	E	405	GLU
1	E	523	LEU
1	C	89	THR
1	C	165	ASN
1	C	229	GLU
1	C	357	ASP
1	C	366	ARG
1	C	368	ASN
1	C	464	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	135	ASN
1	F	165	ASN
1	F	284	ASN
1	F	511	GLN
1	B	262	GLN
1	B	448	ASN
1	D	176	GLN

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Mol	Chain	Res	Type
1	D	404	ASN
1	D	511	GLN
1	A	42	ASN
1	E	111	ASN
1	E	332	ASN
1	C	139	ASN
1	C	286	HIS
1	C	399	ASN
1	C	448	ASN
1	C	472	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	B	701	4	33,33,33	2.32	6 (18%)	45,52,52	1.18	3 (6%)
5	ADP	E	701	4	28,29,29	1.08	1 (3%)	43,45,45	1.33	8 (18%)
3	ANP	D	701	4	33,33,33	2.22	5 (15%)	45,52,52	1.30	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ANP	C	701	4	33,33,33	2.20	5 (15%)	45,52,52	1.19	3 (6%)

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	B	701	4	-	4/18/38/38	0/3/3/3
5	ADP	E	701	4	-	5/16/32/32	0/3/3/3
3	ANP	D	701	4	-	5/18/38/38	0/3/3/3
3	ANP	C	701	4	-	5/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	ANP	PB-O3A	9.03	1.70	1.59
3	D	701	ANP	PB-O3A	8.61	1.69	1.59
3	C	701	ANP	PB-O3A	8.40	1.69	1.59
3	B	701	ANP	PG-N3B	6.19	1.79	1.63
3	D	701	ANP	PG-N3B	6.02	1.79	1.63
3	C	701	ANP	PG-N3B	6.02	1.79	1.63
3	B	701	ANP	PG-O1G	4.70	1.53	1.46
3	C	701	ANP	PG-O1G	4.62	1.53	1.46
3	D	701	ANP	PG-O1G	4.45	1.52	1.46
3	B	701	ANP	PB-O1B	2.79	1.50	1.46
3	D	701	ANP	PB-O1B	2.59	1.50	1.46
3	C	701	ANP	PB-O1B	2.50	1.50	1.46
5	E	701	ADP	PA-O3A	-2.47	1.56	1.59
3	D	701	ANP	PB-O2B	-2.28	1.50	1.56
3	C	701	ANP	PB-O2B	-2.26	1.50	1.56
3	B	701	ANP	PB-O2B	-2.26	1.50	1.56
3	B	701	ANP	PA-O3A	2.23	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	701	ANP	O1G-PG-N3B	-5.24	104.05	111.77
3	C	701	ANP	O2B-PB-O1B	5.09	120.78	109.87
3	D	701	ANP	O2B-PB-O1B	4.93	120.45	109.87
3	B	701	ANP	O2B-PB-O1B	4.68	119.90	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	701	ANP	O1G-PG-N3B	-3.95	105.96	111.77
3	C	701	ANP	O1G-PG-N3B	-3.77	106.22	111.77
5	E	701	ADP	C4-C5-N7	2.89	113.89	110.58
3	D	701	ANP	O2G-PG-O3G	2.89	115.36	107.59
5	E	701	ADP	C5-C4-N3	-2.89	122.74	126.72
5	E	701	ADP	O2A-PA-O3A	2.70	114.57	107.27
5	E	701	ADP	O3B-PB-O3A	2.59	113.33	104.64
5	E	701	ADP	N3-C4-N9	2.38	131.21	127.17
3	C	701	ANP	O2G-PG-O3G	2.32	113.82	107.59
5	E	701	ADP	O3B-PB-O2B	-2.26	99.31	107.80
3	B	701	ANP	O2G-PG-O3G	2.24	113.61	107.59
5	E	701	ADP	C2-N1-C6	-2.02	115.41	118.73
5	E	701	ADP	C5-C6-N1	2.01	122.61	117.51

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	ANP	PB-N3B-PG-O1G
3	B	701	ANP	PG-N3B-PB-O1B
3	B	701	ANP	PA-O3A-PB-O2B
3	D	701	ANP	PB-N3B-PG-O1G
3	D	701	ANP	PG-N3B-PB-O1B
3	D	701	ANP	C5'-O5'-PA-O1A
3	D	701	ANP	C5'-O5'-PA-O3A
3	C	701	ANP	PB-N3B-PG-O1G
3	C	701	ANP	PG-N3B-PB-O1B
5	E	701	ADP	C5'-O5'-PA-O1A
5	E	701	ADP	C5'-O5'-PA-O2A
5	E	701	ADP	C5'-O5'-PA-O3A
5	E	701	ADP	O4'-C4'-C5'-O5'
5	E	701	ADP	C3'-C4'-C5'-O5'
3	D	701	ANP	C5'-O5'-PA-O2A
3	C	701	ANP	PB-O3A-PA-O2A
3	C	701	ANP	C4'-C5'-O5'-PA
3	B	701	ANP	PA-O3A-PB-O1B
3	C	701	ANP	PB-O3A-PA-O1A

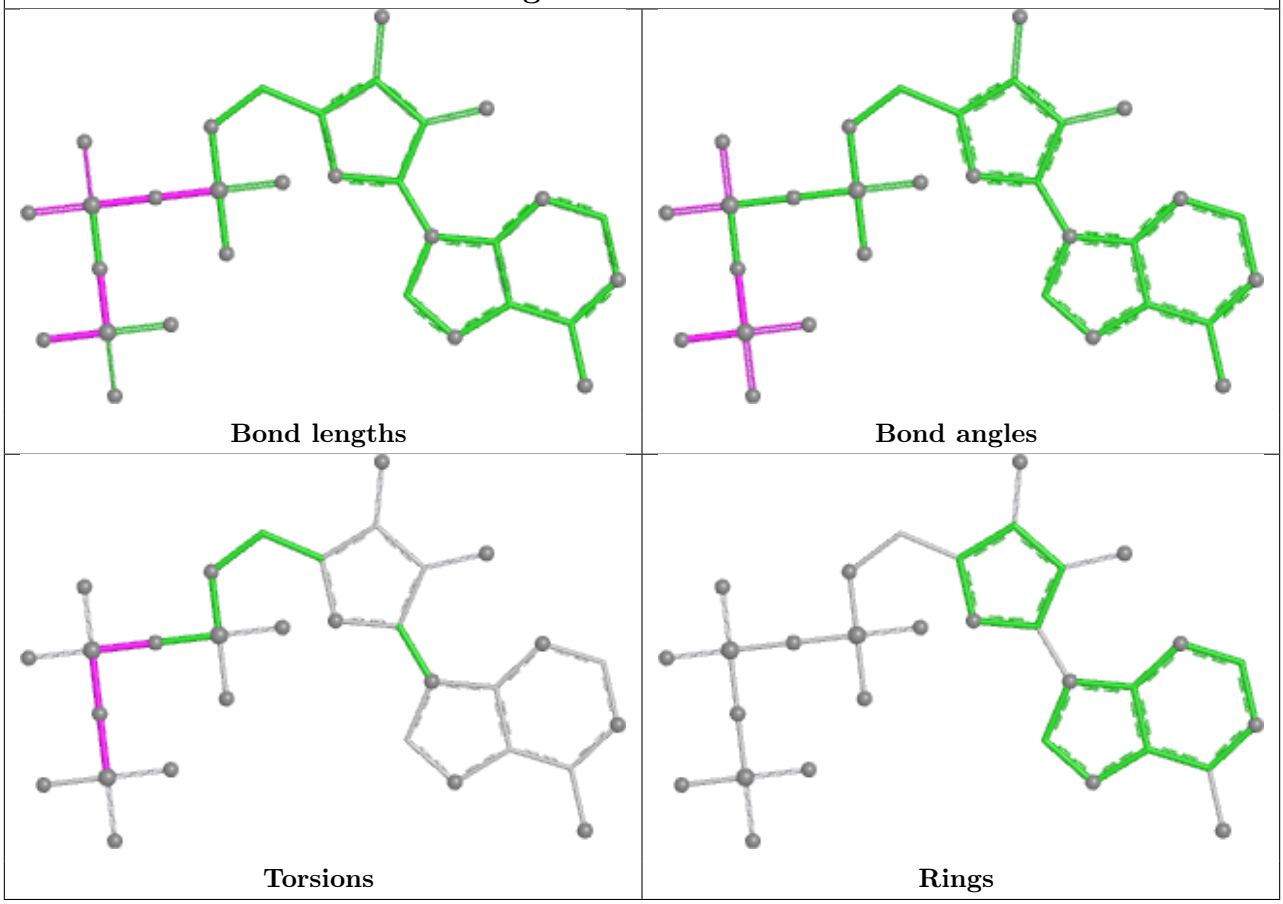
There are no ring outliers.

3 monomers are involved in 7 short contacts:

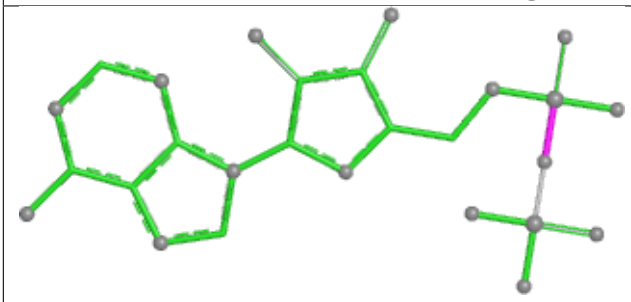
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	ANP	2	0
3	D	701	ANP	2	0
3	C	701	ANP	3	0

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

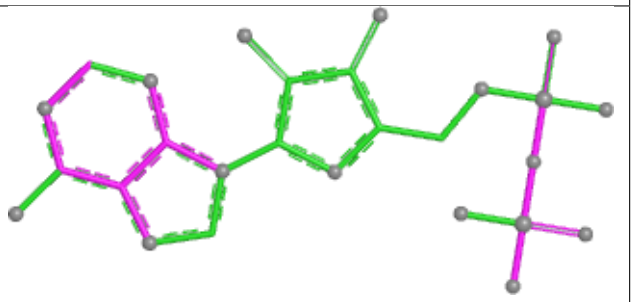
Ligand ANP B 701



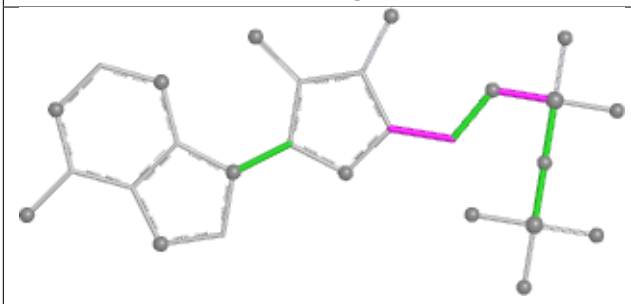
Ligand ADP E 701



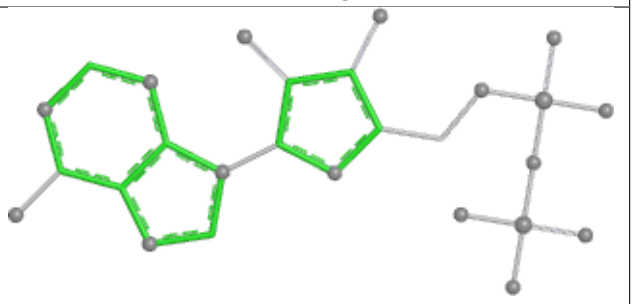
Bond lengths



Bond angles

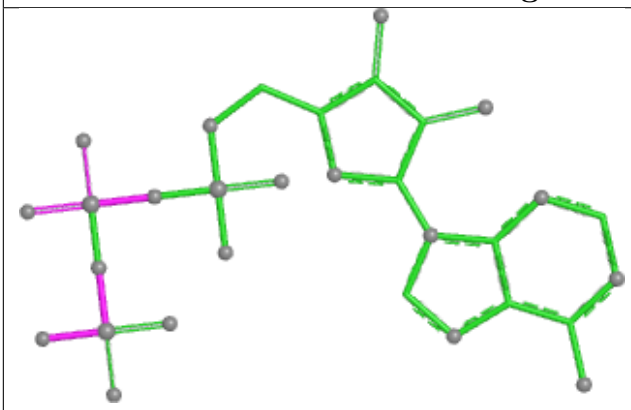


Torsions

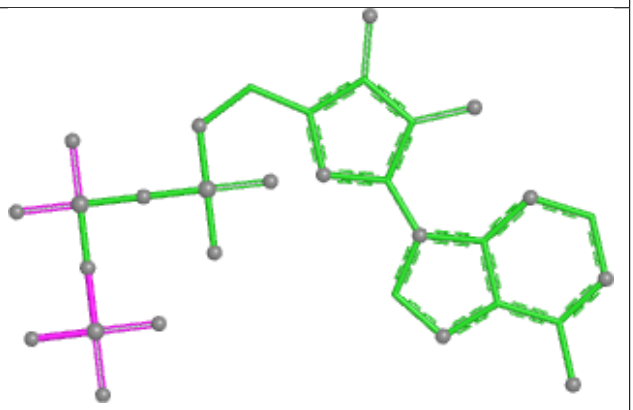


Rings

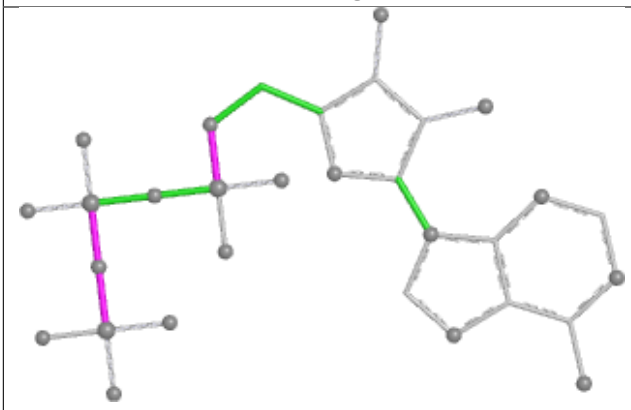
Ligand ANP D 701



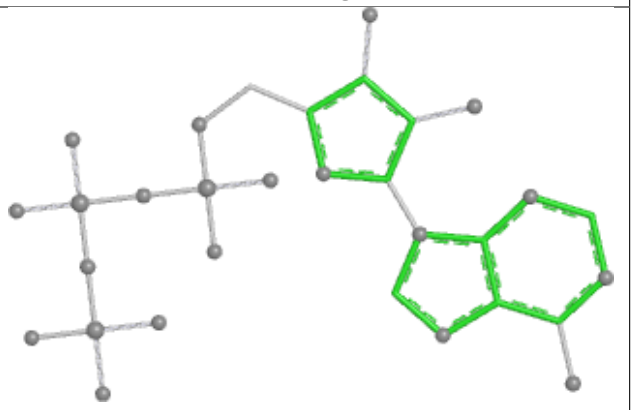
Bond lengths



Bond angles

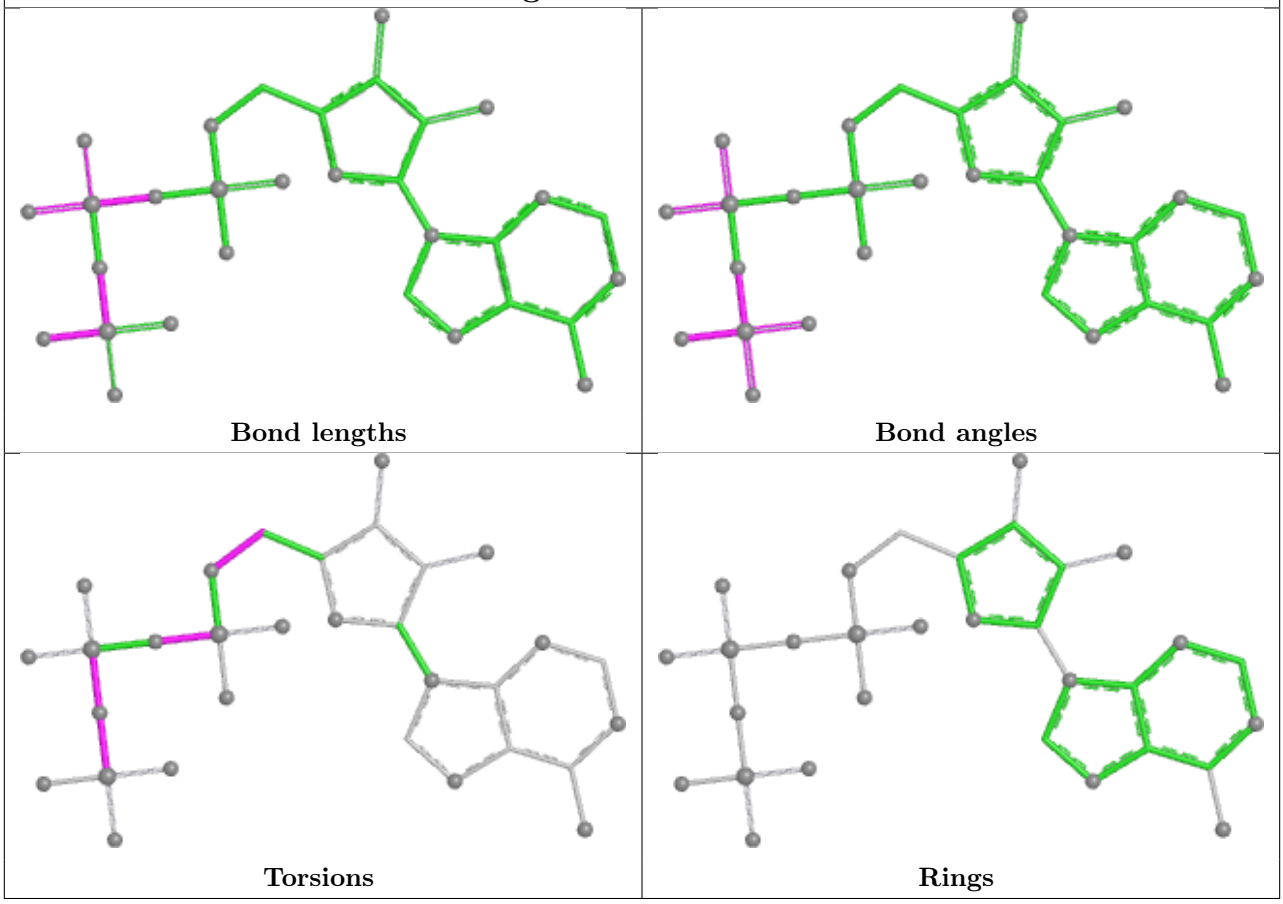


Torsions



Rings

Ligand ANP C 701



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.

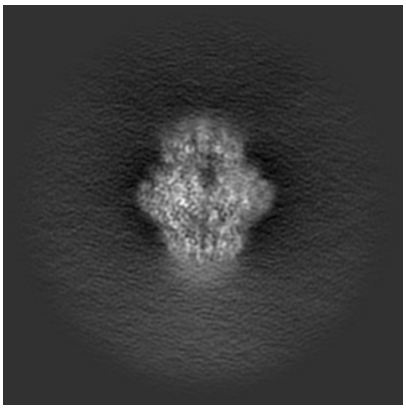
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-79708. These allow visual inspection of the internal detail of the map and identification of artifacts.

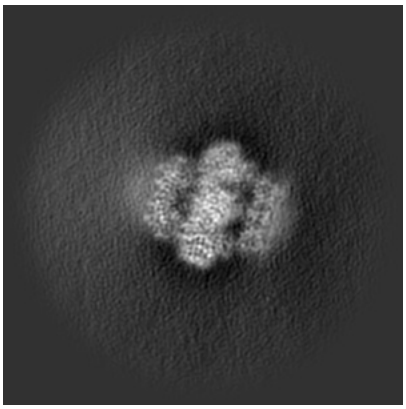
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

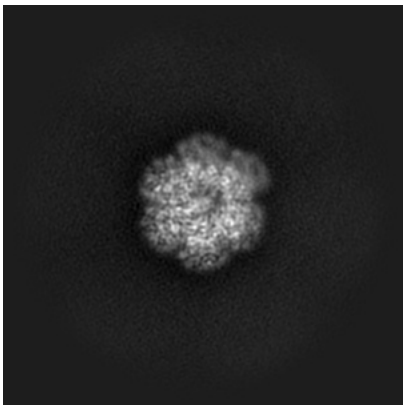
6.1.1 Primary map



X

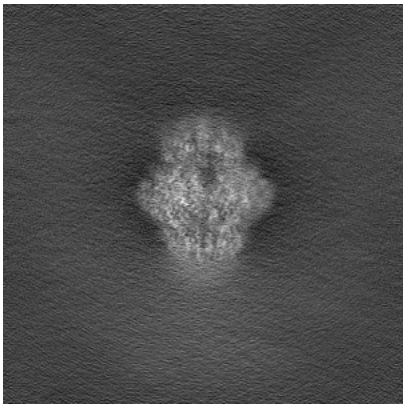


Y

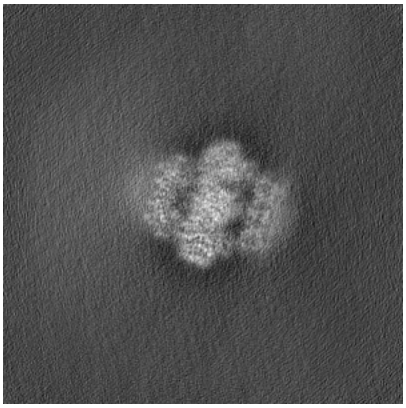


Z

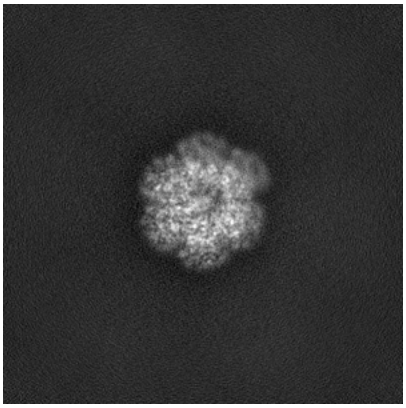
6.1.2 Raw map



X



Y

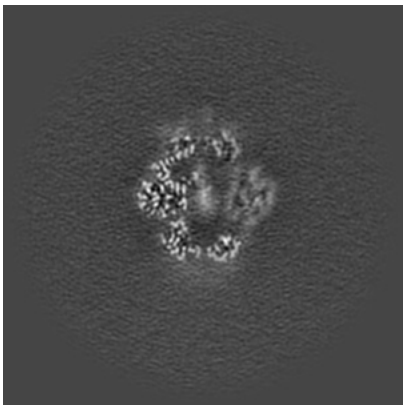


Z

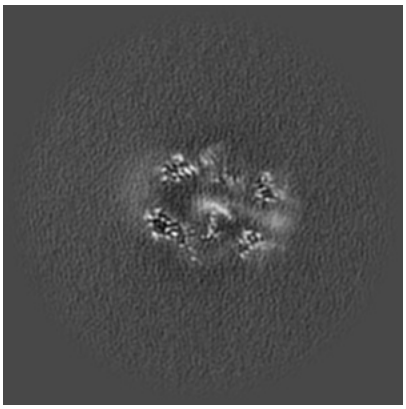
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

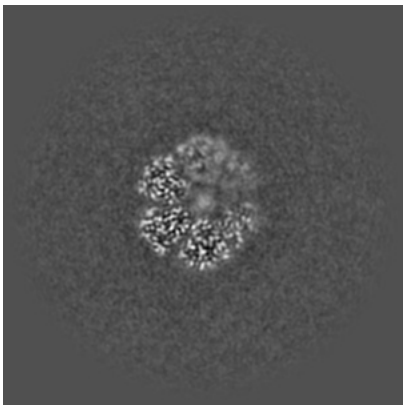
6.2.1 Primary map



X Index: 160

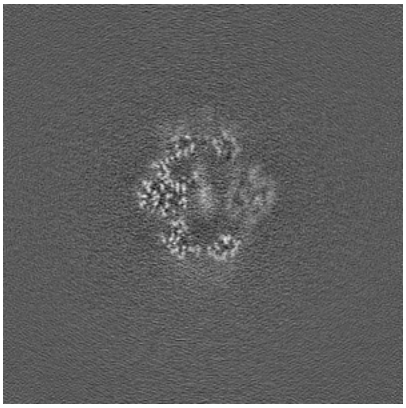


Y Index: 160

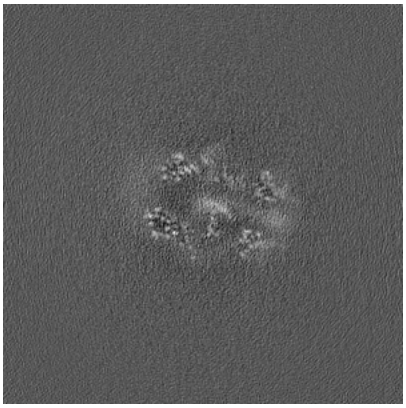


Z Index: 160

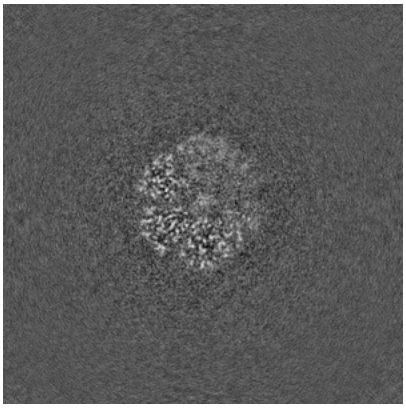
6.2.2 Raw map



X Index: 160



Y Index: 160

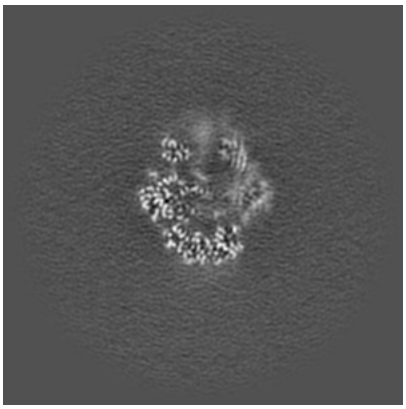


Z Index: 160

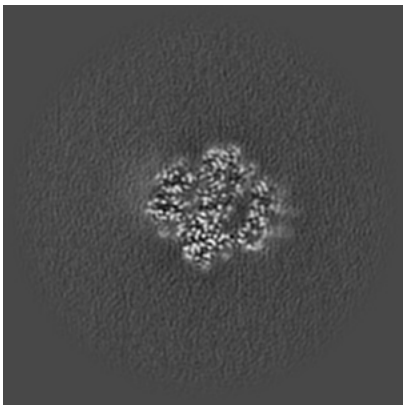
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

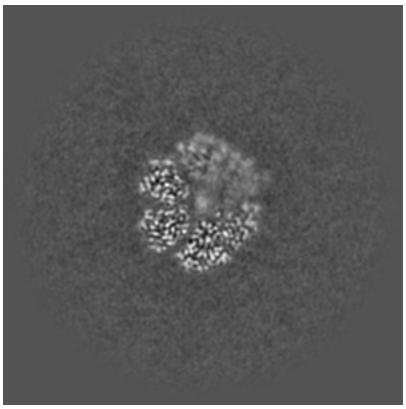
6.3.1 Primary map



X Index: 150

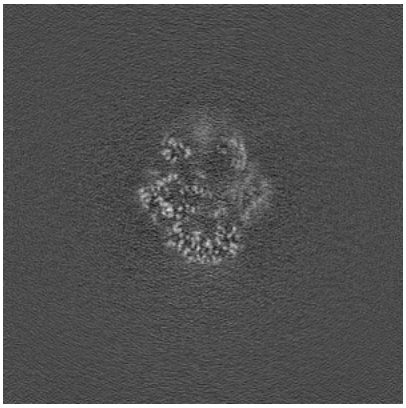


Y Index: 142

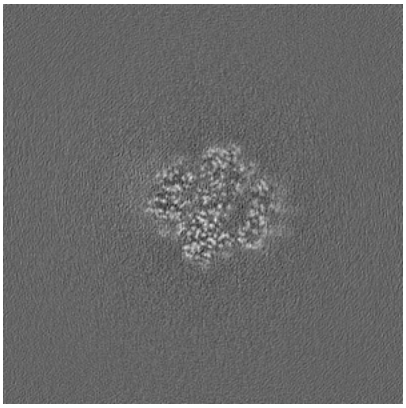


Z Index: 163

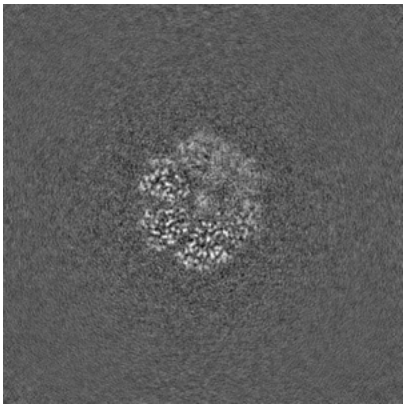
6.3.2 Raw map



X Index: 149



Y Index: 142

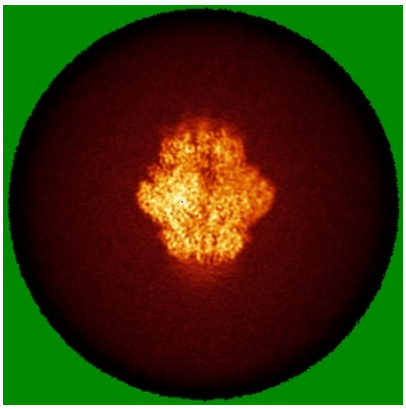


Z Index: 163

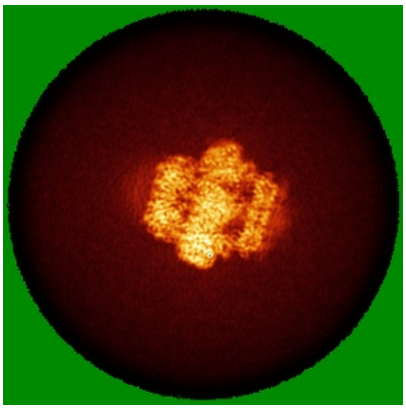
The images above show the largest variance slices of the map in three orthogonal directions.

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

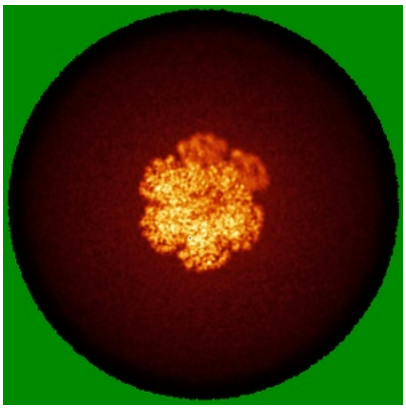
6.4.1 Primary map



X

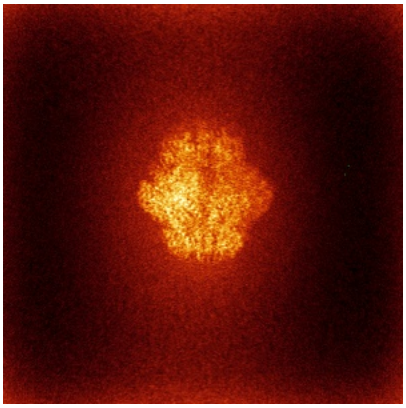


Y

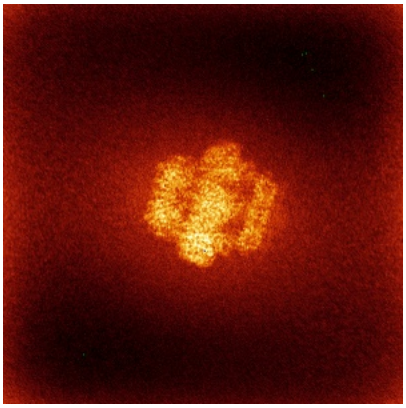


Z

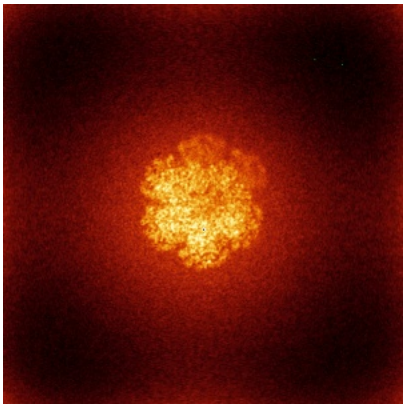
6.4.2 Raw map



X



Y

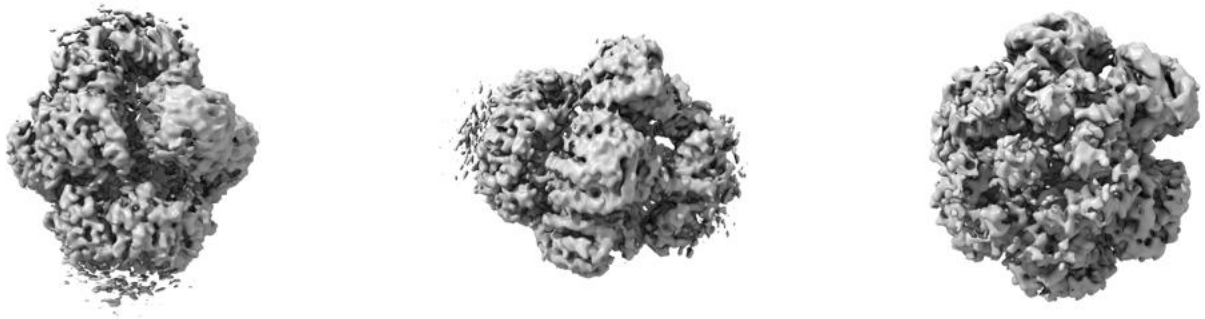


Z

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)

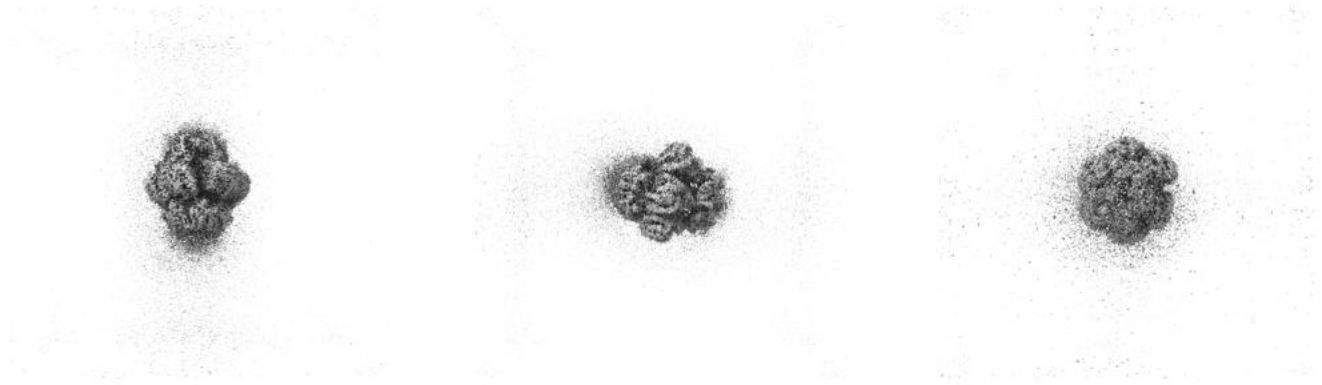
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

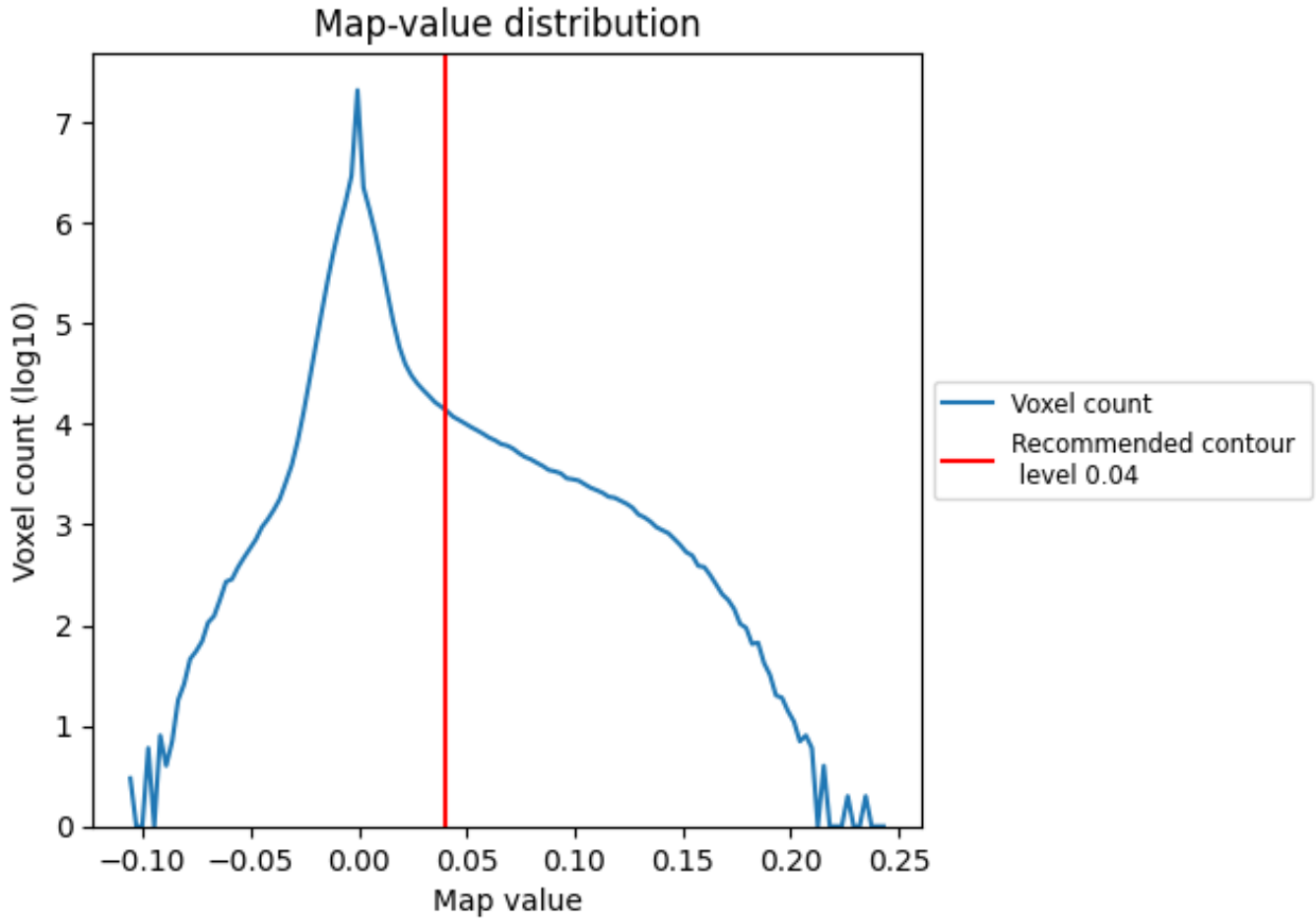
6.6 Mask visualisation (i)

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

7 Map analysis

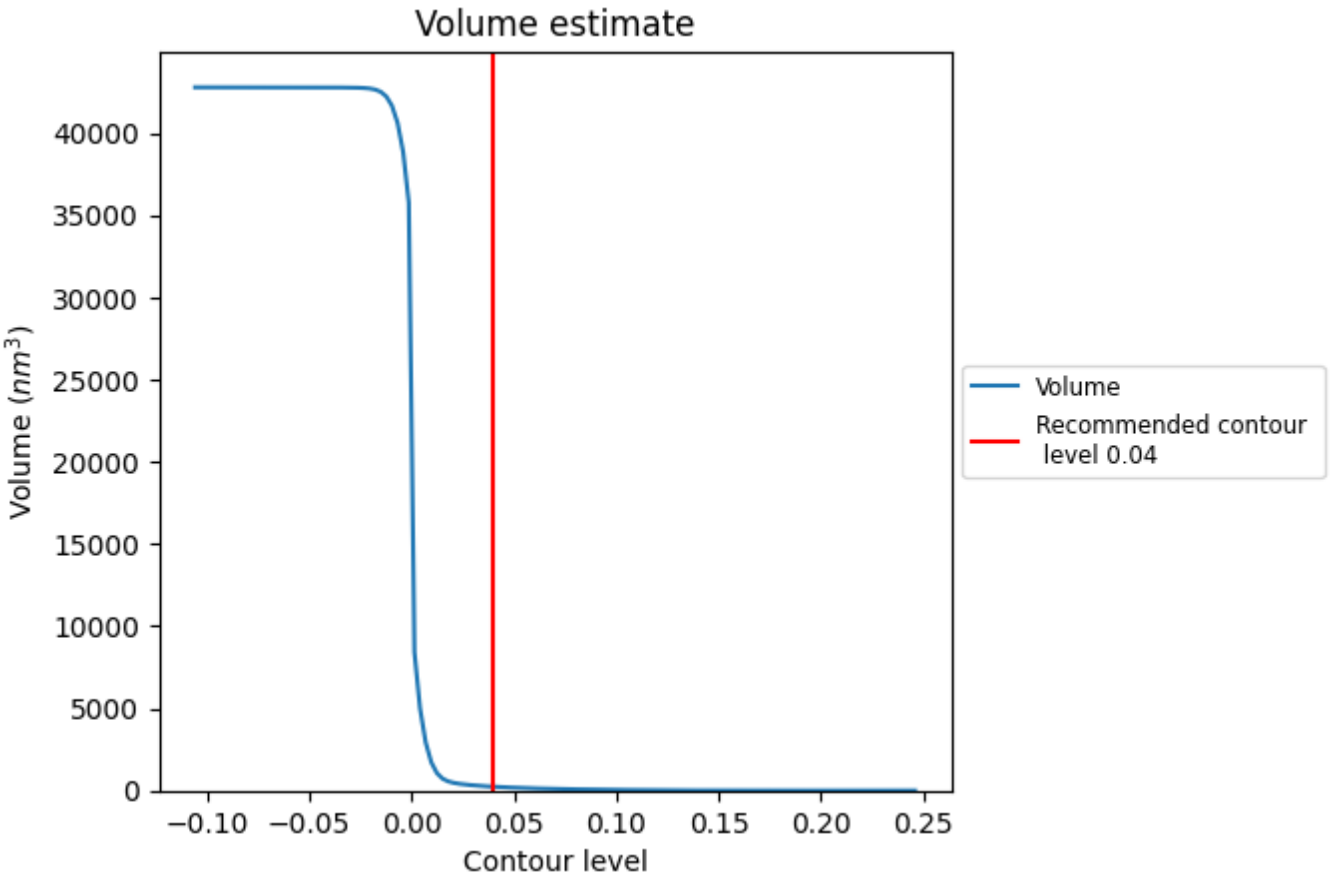
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

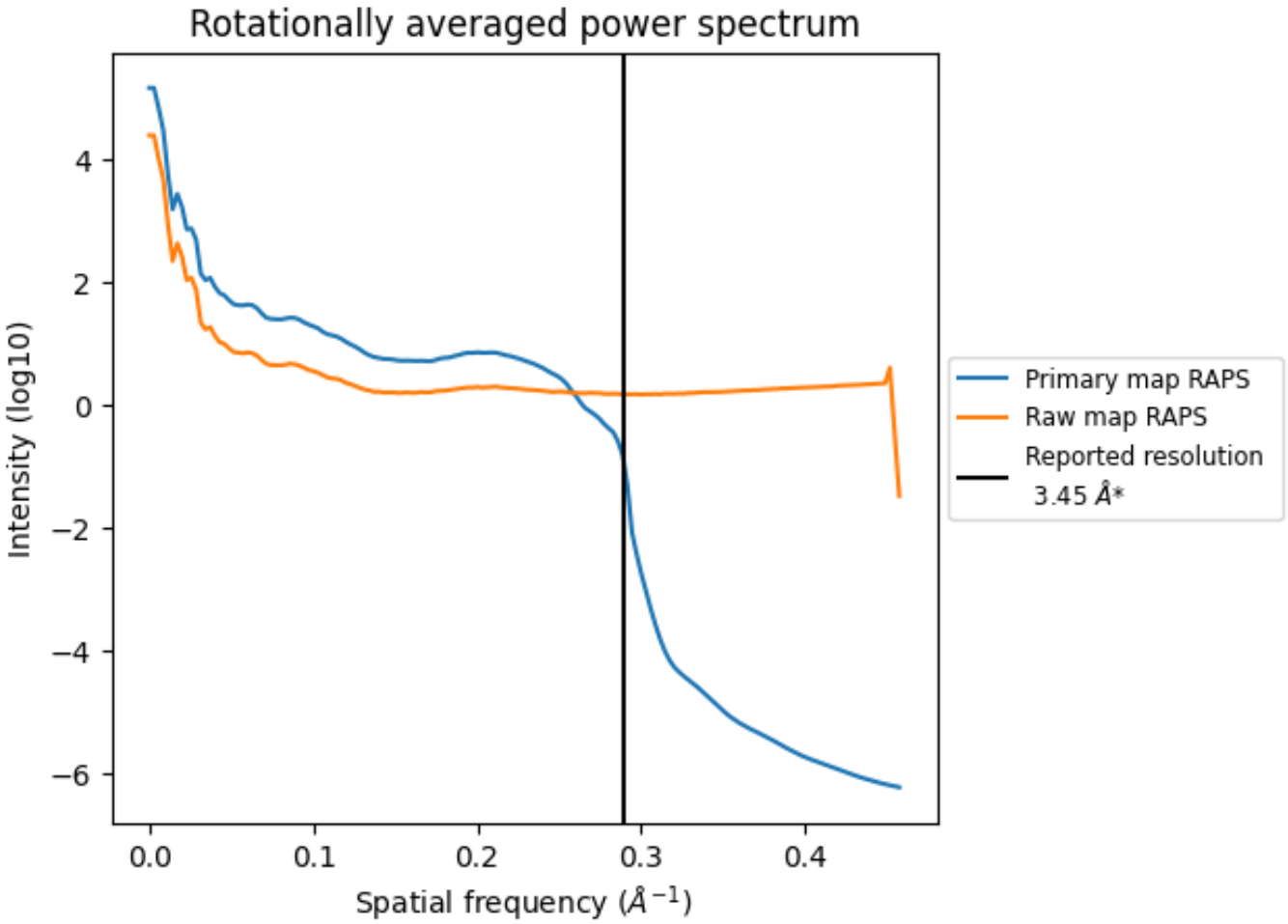
7.2 Volume estimate



The volume at the recommended contour level is 233 nm^3; this corresponds to an approximate mass of 211 kDa.

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

7.3 Rotationally averaged power spectrum (i)

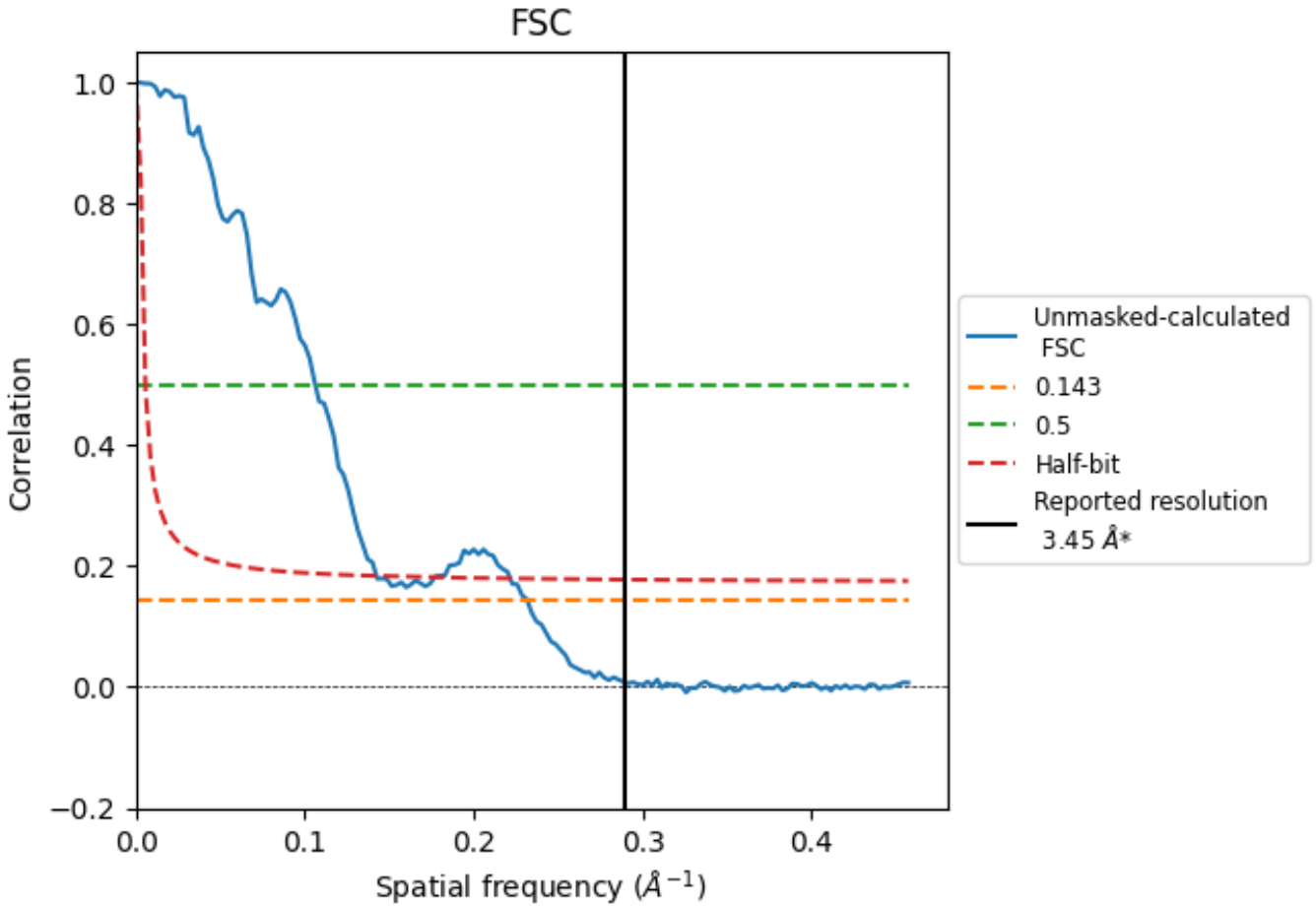


*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8.2 Resolution estimates (i)

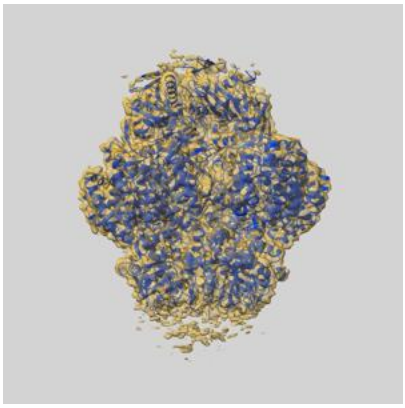
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	9.42	7.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.45 by more than 10 %

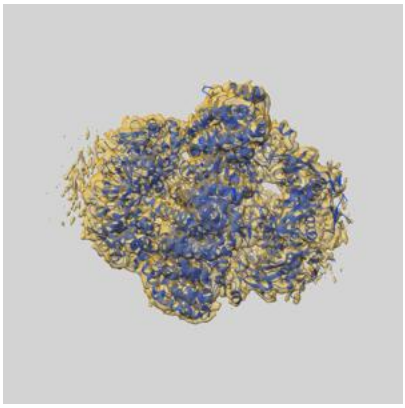
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-79708 and PDB model 39QW. Per-residue inclusion information can be found in section 3 on page 12.

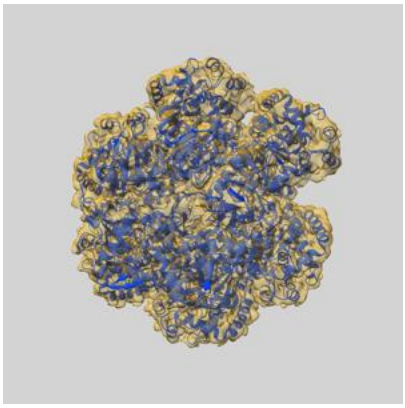
9.1 Map-model overlay



X



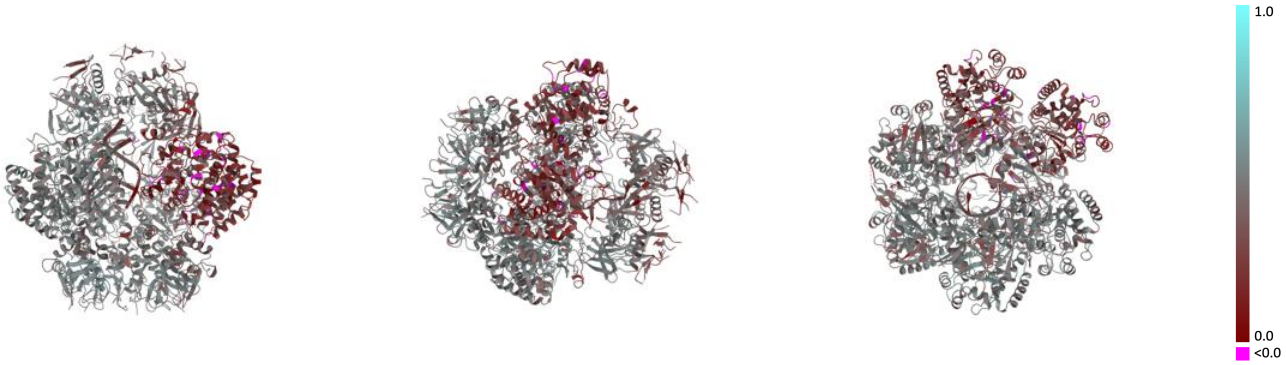
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

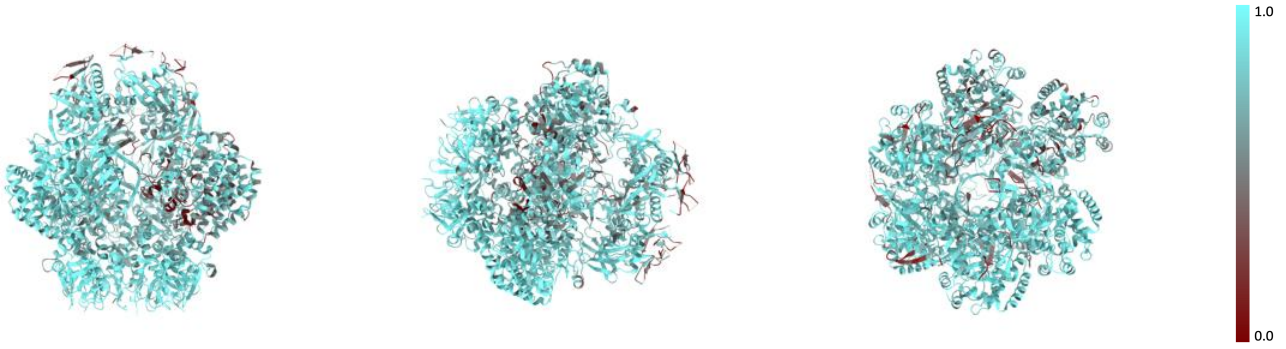
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

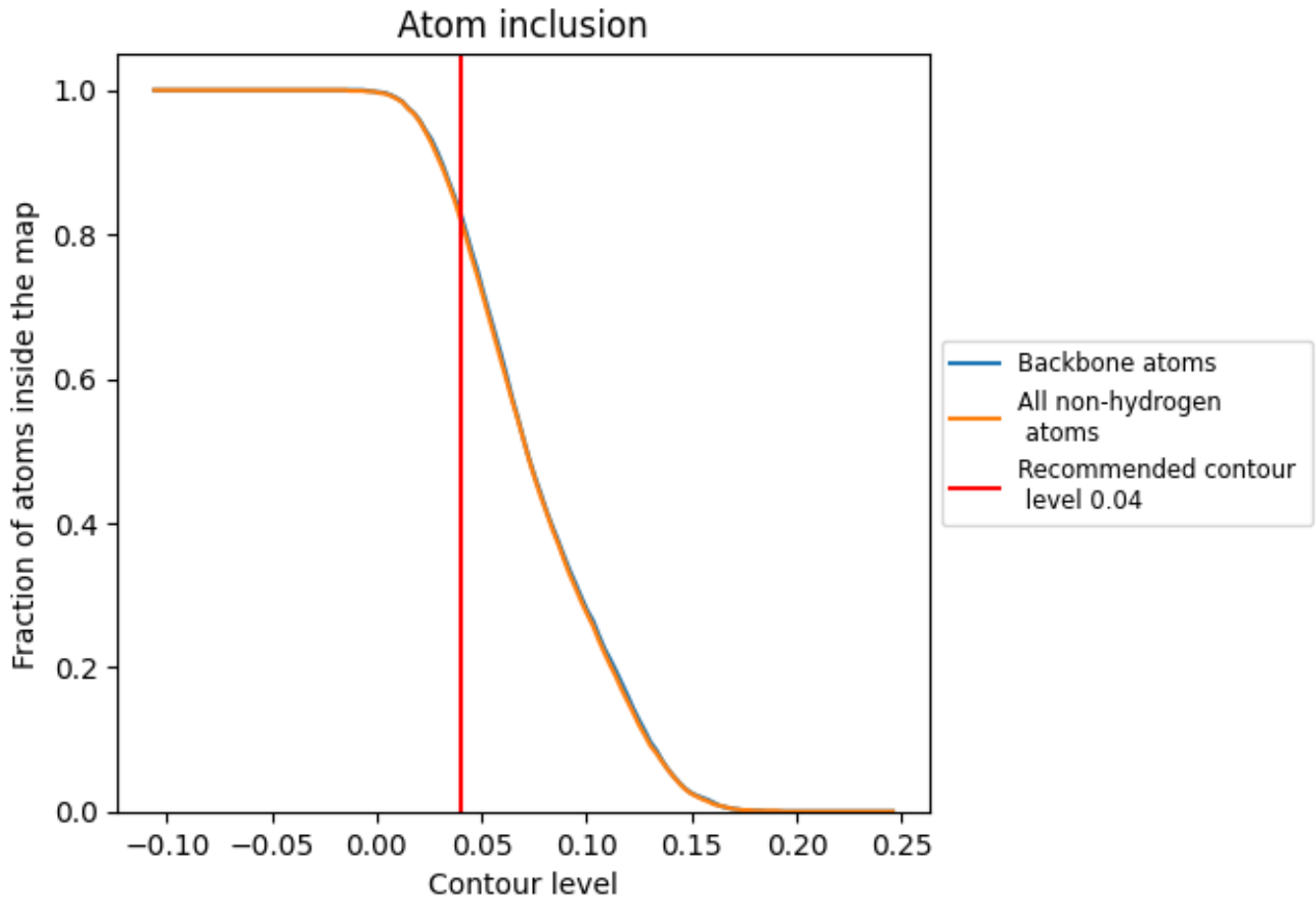
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.4180
A	0.7440	0.3170
B	0.8570	0.4630
C	0.8680	0.4820
D	0.8810	0.4840
E	0.8680	0.4680
F	0.7100	0.3050
G	0.8280	0.2410
H	0.8770	0.3420

