



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 03:20 PM JST

PDB ID : 7EMY  
EMDB ID : EMD-31198  
Title : Pyochelin synthetase, a dimeric nonribosomal peptide synthetase elongation module  
Authors : Wang, J.L.; Wang, Z.J.  
Deposited on : 2021-04-15  
Resolution : 2.97 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

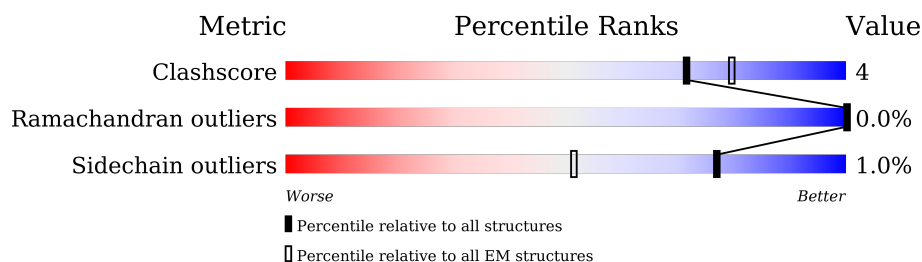
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1455	<div> <div>9%</div> <div>72%</div> <div>18%</div> <div>• 8%</div> </div>
1	B	1455	<div> <div>•</div> <div>72%</div> <div>18%</div> <div>• 8%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 41094 atoms, of which 20576 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 Dihydroaeruginosic acid synthetase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1334	Total	C	H	N	O	S	0	0
			20444	6431	10245	1881	1854	33		
1	B	1334	Total	C	H	N	O	S	0	0
			20444	6431	10245	1881	1854	33		

There are 34 discrepancies between the modelled and reference sequences:

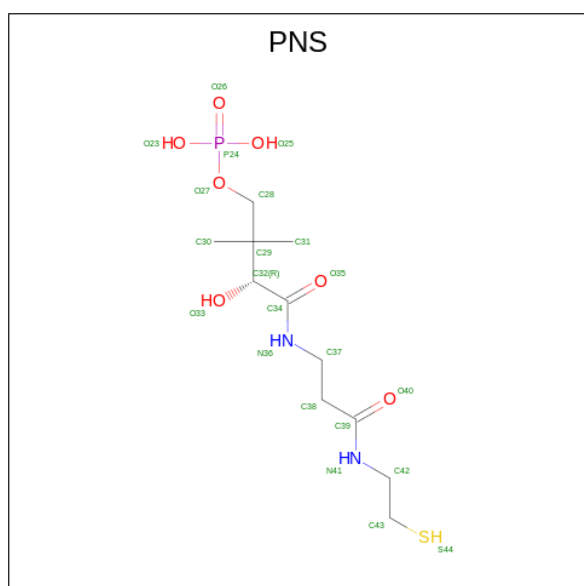
Chain	Residue	Modelled	Actual	Comment	Reference
A	1439	HIS	-	expression tag	UNP G3XCV2
A	1440	HIS	-	expression tag	UNP G3XCV2
A	1441	HIS	-	expression tag	UNP G3XCV2
A	1442	HIS	-	expression tag	UNP G3XCV2
A	1443	HIS	-	expression tag	UNP G3XCV2
A	1444	HIS	-	expression tag	UNP G3XCV2
A	1445	LEU	-	expression tag	UNP G3XCV2
A	1446	PRO	-	expression tag	UNP G3XCV2
A	1447	SER	-	expression tag	UNP G3XCV2
A	1448	TRP	-	expression tag	UNP G3XCV2
A	1449	SER	-	expression tag	UNP G3XCV2
A	1450	HIS	-	expression tag	UNP G3XCV2
A	1451	PRO	-	expression tag	UNP G3XCV2
A	1452	GLN	-	expression tag	UNP G3XCV2
A	1453	PHE	-	expression tag	UNP G3XCV2
A	1454	GLU	-	expression tag	UNP G3XCV2
A	1455	LYS	-	expression tag	UNP G3XCV2
B	1439	HIS	-	expression tag	UNP G3XCV2
B	1440	HIS	-	expression tag	UNP G3XCV2
B	1441	HIS	-	expression tag	UNP G3XCV2
B	1442	HIS	-	expression tag	UNP G3XCV2
B	1443	HIS	-	expression tag	UNP G3XCV2
B	1444	HIS	-	expression tag	UNP G3XCV2
B	1445	LEU	-	expression tag	UNP G3XCV2
B	1446	PRO	-	expression tag	UNP G3XCV2
B	1447	SER	-	expression tag	UNP G3XCV2

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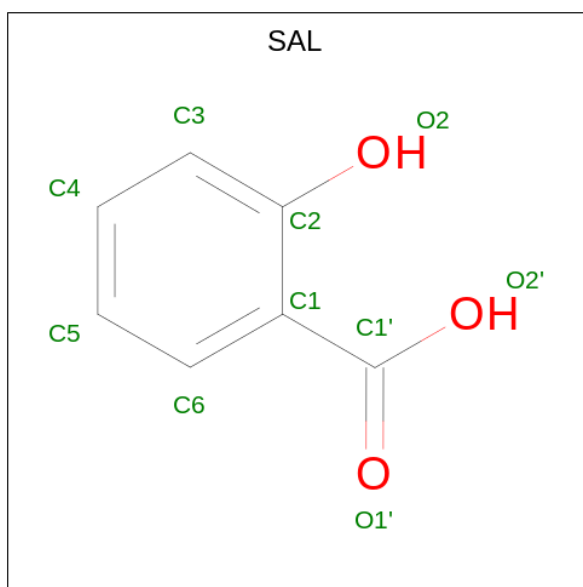
Chain	Residue	Modelled	Actual	Comment	Reference
B	1448	TRP	-	expression tag	UNP G3XCV2
B	1449	SER	-	expression tag	UNP G3XCV2
B	1450	HIS	-	expression tag	UNP G3XCV2
B	1451	PRO	-	expression tag	UNP G3XCV2
B	1452	GLN	-	expression tag	UNP G3XCV2
B	1453	PHE	-	expression tag	UNP G3XCV2
B	1454	GLU	-	expression tag	UNP G3XCV2
B	1455	LYS	-	expression tag	UNP G3XCV2

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula:  $C_{11}H_{23}N_2O_7PS$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total	C	H	N	O	P	S	0
			41	11	20	2	6	1	1	
2	B	1	Total	C	H	N	O	P	S	0
			41	11	20	2	6	1	1	

- Molecule 3 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula:  $C_7H_6O_3$ ).

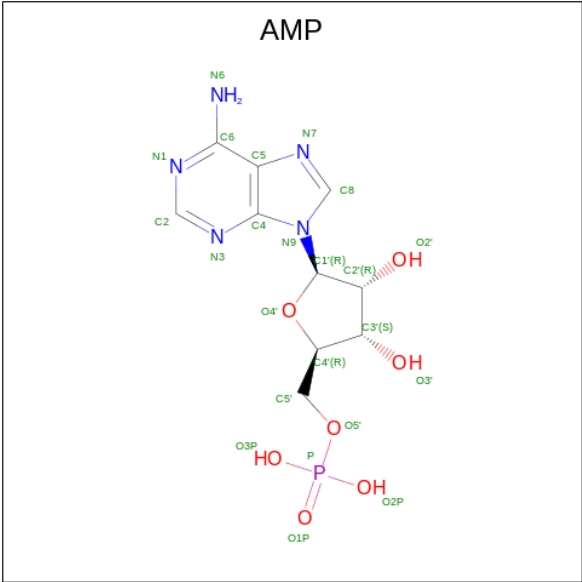


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			14	7	5	2	
3	B	1	Total	C	H	O	0
			14	7	5	2	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

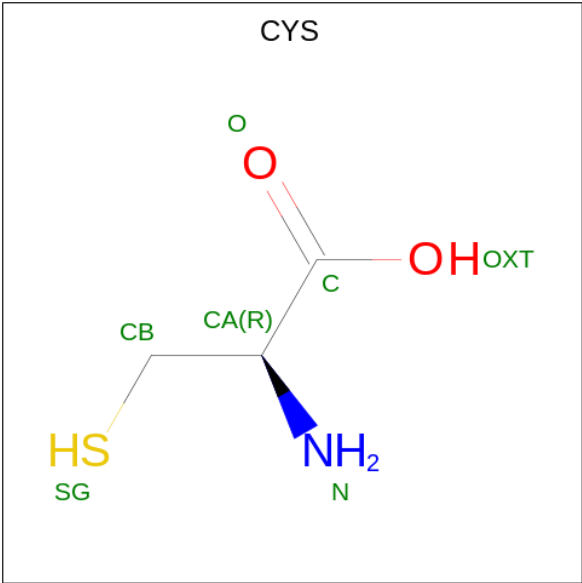
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	
5	B	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	

- Molecule 6 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	S	0
			12	3	6	1	1	1	
6	B	1	Total	C	H	N	O	S	0
			12	3	6	1	1	1	

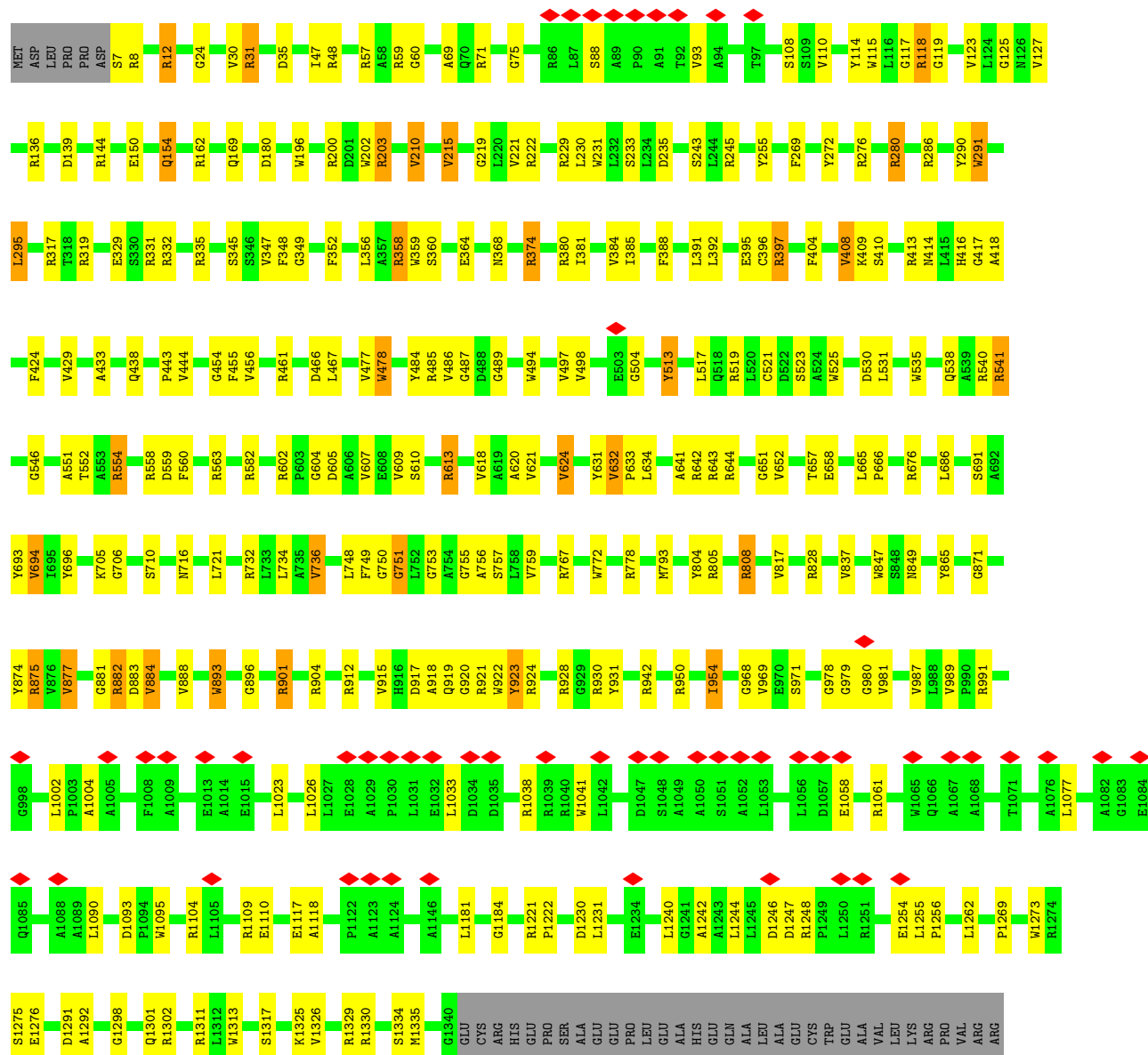
### 3 Residue-property plots

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: Dihydroaeruginosic acid synthetase



- Molecule 1: Dihydroaeruginosic acid synthetase





GLU	GLU	GLY	VAL	LEU	HIS	HIS	HIS	HIS	HIS	LEU	PRO	PRO	GLN	PHE	GLU	LYS	ARG	GLU	ALA	SER	PHE	PHE	SER	LEU	GLY	GLY	ASP	SER	LEU	LEU	ALA	THR	THR	LEU	ARG	GLU	ARG	GLY	VAL	ARG	LEU	GLY	MET	ALA	ASP	PHE	THR	ARG	GLN	PRO	THR	THR	LEU	ALA	GLY	LEU	ARG	ALA	HIS	LEU	GLN	VAL	GLN	GLN	THR	VAL	GLU	ILE	GLU	GLU	THR	THR	LEU
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219049	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size ( $\text{\AA}$ )	250.0, 250.0, 250.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0, 1.0, 1.0	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, AMP, SAL, PNS

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	1.81	258/10412 (2.5%)	1.49	74/14189 (0.5%)
1	B	1.78	243/10412 (2.3%)	1.47	70/14189 (0.5%)
All	All	1.79	501/20824 (2.4%)	1.48	144/28378 (0.5%)

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	A	0	3
1	B	0	4
All	All	0	7

All (501) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	ARG	CZ-NH1	-7.87	1.22	1.33
1	A	541	ARG	CZ-NH1	-7.86	1.22	1.33
1	B	229	ARG	CZ-NH1	-7.86	1.22	1.33
1	B	332	ARG	CZ-NH1	-7.86	1.22	1.33
1	B	901	ARG	CZ-NH1	-7.85	1.22	1.33
1	A	229	ARG	CZ-NH1	-7.83	1.22	1.33
1	A	554	ARG	CZ-NH1	-7.83	1.22	1.33
1	B	331	ARG	CZ-NH1	-7.83	1.22	1.33
1	B	317	ARG	CZ-NH1	-7.82	1.22	1.33
1	B	358	ARG	CZ-NH1	-7.82	1.22	1.33
1	B	71	ARG	CZ-NH1	-7.81	1.22	1.33
1	A	875	ARG	CZ-NH1	-7.81	1.22	1.33
1	A	245	ARG	CZ-NH1	-7.81	1.22	1.33
1	B	31	ARG	CZ-NH1	-7.81	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	519	ARG	CZ-NH1	-7.81	1.22	1.33
1	B	245	ARG	CZ-NH1	-7.80	1.23	1.33
1	A	332	ARG	CZ-NH1	-7.80	1.23	1.33
1	B	882	ARG	CZ-NH1	-7.80	1.23	1.33
1	A	1311	ARG	CZ-NH1	-7.80	1.23	1.33
1	B	461	ARG	CZ-NH1	-7.80	1.23	1.33
1	A	331	ARG	CZ-NH1	-7.80	1.23	1.33
1	B	118	ARG	CZ-NH1	-7.79	1.23	1.33
1	A	317	ARG	CZ-NH1	-7.79	1.23	1.33
1	A	991	ARG	CZ-NH1	-7.79	1.23	1.33
1	B	380	ARG	CZ-NH1	-7.79	1.23	1.33
1	A	563	ARG	CZ-NH1	-7.79	1.23	1.33
1	A	1329	ARG	CZ-NH1	-7.79	1.23	1.33
1	B	200	ARG	CZ-NH1	-7.79	1.23	1.33
1	B	554	ARG	CZ-NH1	-7.78	1.23	1.33
1	A	901	ARG	CZ-NH1	-7.77	1.23	1.33
1	A	1330	ARG	CZ-NH1	-7.77	1.23	1.33
1	B	136	ARG	CZ-NH1	-7.76	1.23	1.33
1	B	558	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	668	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	431	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	461	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	778	ARG	CZ-NH1	-7.76	1.23	1.33
1	B	203	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	8	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	582	ARG	CZ-NH1	-7.76	1.23	1.33
1	B	1311	ARG	CZ-NH1	-7.75	1.23	1.33
1	A	71	ARG	CZ-NH1	-7.75	1.23	1.33
1	A	588	ARG	CZ-NH1	-7.75	1.23	1.33
1	A	912	ARG	CZ-NH1	-7.75	1.23	1.33
1	A	118	ARG	CZ-NH1	-7.75	1.23	1.33
1	A	643	ARG	CZ-NH1	-7.75	1.23	1.33
1	B	319	ARG	CZ-NH1	-7.75	1.23	1.33
1	A	558	ARG	CZ-NH1	-7.75	1.23	1.33
1	B	828	ARG	CZ-NH1	-7.75	1.23	1.33
1	B	413	ARG	CZ-NH1	-7.74	1.23	1.33
1	A	413	ARG	CZ-NH1	-7.74	1.23	1.33
1	B	541	ARG	CZ-NH1	-7.74	1.23	1.33
1	A	200	ARG	CZ-NH1	-7.74	1.23	1.33
1	A	930	ARG	CZ-NH1	-7.73	1.23	1.33
1	A	380	ARG	CZ-NH1	-7.73	1.23	1.33
1	B	12	ARG	CZ-NH1	-7.73	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1329	ARG	CZ-NH1	-7.73	1.23	1.33
1	A	519	ARG	CZ-NH1	-7.73	1.23	1.33
1	A	31	ARG	CZ-NH1	-7.72	1.23	1.33
1	A	485	ARG	CZ-NH1	-7.72	1.23	1.33
1	B	59	ARG	CZ-NH1	-7.72	1.23	1.33
1	B	991	ARG	CZ-NH1	-7.72	1.23	1.33
1	A	12	ARG	CZ-NH1	-7.72	1.23	1.33
1	B	276	ARG	CZ-NH1	-7.72	1.23	1.33
1	B	286	ARG	CZ-NH1	-7.71	1.23	1.33
1	B	1330	ARG	CZ-NH1	-7.71	1.23	1.33
1	A	579	ARG	CZ-NH1	-7.71	1.23	1.33
1	A	673	ARG	CZ-NH1	-7.71	1.23	1.33
1	B	8	ARG	CZ-NH1	-7.71	1.23	1.33
1	A	319	ARG	CZ-NH1	-7.71	1.23	1.33
1	B	335	ARG	CZ-NH1	-7.71	1.23	1.33
1	B	397	ARG	CZ-NH1	-7.71	1.23	1.33
1	A	644	ARG	CZ-NH1	-7.70	1.23	1.33
1	A	732	ARG	CZ-NH1	-7.70	1.23	1.33
1	B	805	ARG	CZ-NH1	-7.70	1.23	1.33
1	B	540	ARG	CZ-NH1	-7.70	1.23	1.33
1	B	875	ARG	CZ-NH1	-7.69	1.23	1.33
1	A	576	ARG	CZ-NH1	-7.69	1.23	1.33
1	A	59	ARG	CZ-NH1	-7.69	1.23	1.33
1	A	286	ARG	CZ-NH1	-7.69	1.23	1.33
1	B	582	ARG	CZ-NH1	-7.68	1.23	1.33
1	A	136	ARG	CZ-NH1	-7.68	1.23	1.33
1	B	280	ARG	CZ-NH1	-7.68	1.23	1.33
1	A	203	ARG	CZ-NH1	-7.68	1.23	1.33
1	A	397	ARG	CZ-NH1	-7.67	1.23	1.33
1	B	613	ARG	CZ-NH1	-7.67	1.23	1.33
1	B	643	ARG	CZ-NH1	-7.67	1.23	1.33
1	A	280	ARG	CZ-NH1	-7.66	1.23	1.33
1	B	644	ARG	CZ-NH1	-7.66	1.23	1.33
1	B	563	ARG	CZ-NH1	-7.65	1.23	1.33
1	A	335	ARG	CZ-NH1	-7.64	1.23	1.33
1	B	778	ARG	CZ-NH1	-7.64	1.23	1.33
1	B	732	ARG	CZ-NH1	-7.62	1.23	1.33
1	B	904	ARG	CZ-NH1	-7.62	1.23	1.33
1	B	912	ARG	CZ-NH1	-7.61	1.23	1.33
1	A	276	ARG	CZ-NH1	-7.61	1.23	1.33
1	B	921	ARG	CZ-NH1	-7.58	1.23	1.33
1	A	921	ARG	CZ-NH1	-7.57	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	924	ARG	CZ-NH1	-7.57	1.23	1.33
1	A	924	ARG	CZ-NH1	-7.53	1.23	1.33
1	A	904	ARG	CZ-NH1	-7.52	1.23	1.33
1	B	332	ARG	CZ-NH2	-7.49	1.23	1.33
1	A	828	ARG	CZ-NH1	-7.47	1.23	1.33
1	A	805	ARG	CZ-NH1	-7.46	1.23	1.33
1	A	540	ARG	CZ-NH1	-7.46	1.23	1.33
1	A	332	ARG	CZ-NH2	-7.43	1.23	1.33
1	A	826	ARG	CZ-NH1	-7.41	1.23	1.33
1	B	245	ARG	CZ-NH2	-7.37	1.23	1.33
1	B	358	ARG	CZ-NH2	-7.37	1.23	1.33
1	A	554	ARG	CZ-NH2	-7.36	1.23	1.33
1	A	541	ARG	CZ-NH2	-7.34	1.23	1.33
1	B	118	ARG	CZ-NH2	-7.33	1.23	1.33
1	B	319	ARG	CZ-NH2	-7.32	1.23	1.33
1	A	229	ARG	CZ-NH2	-7.31	1.23	1.33
1	B	200	ARG	CZ-NH2	-7.31	1.23	1.33
1	B	229	ARG	CZ-NH2	-7.31	1.23	1.33
1	B	136	ARG	CZ-NH2	-7.31	1.23	1.33
1	A	901	ARG	CZ-NH2	-7.30	1.23	1.33
1	A	461	ARG	CZ-NH2	-7.30	1.23	1.33
1	A	930	ARG	CZ-NH2	-7.29	1.23	1.33
1	B	397	ARG	CZ-NH2	-7.29	1.23	1.33
1	B	1311	ARG	CZ-NH2	-7.28	1.23	1.33
1	B	991	ARG	CZ-NH2	-7.28	1.23	1.33
1	A	673	ARG	CZ-NH2	-7.28	1.23	1.33
1	A	778	ARG	CZ-NH2	-7.28	1.23	1.33
1	A	732	ARG	CZ-NH2	-7.27	1.23	1.33
1	B	203	ARG	CZ-NH2	-7.27	1.23	1.33
1	B	331	ARG	CZ-NH2	-7.27	1.23	1.33
1	B	1330	ARG	CZ-NH2	-7.26	1.23	1.33
1	A	8	ARG	CZ-NH2	-7.26	1.23	1.33
1	A	203	ARG	CZ-NH2	-7.26	1.23	1.33
1	B	485	ARG	CZ-NH2	-7.26	1.23	1.33
1	A	118	ARG	CZ-NH2	-7.25	1.23	1.33
1	B	901	ARG	CZ-NH2	-7.25	1.23	1.33
1	B	1329	ARG	CZ-NH2	-7.25	1.23	1.33
1	B	519	ARG	CZ-NH2	-7.25	1.23	1.33
1	B	413	ARG	CZ-NH2	-7.25	1.23	1.33
1	A	588	ARG	CZ-NH2	-7.24	1.23	1.33
1	A	200	ARG	CZ-NH2	-7.24	1.23	1.33
1	A	136	ARG	CZ-NH2	-7.24	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	ARG	CZ-NH2	-7.24	1.23	1.33
1	A	331	ARG	CZ-NH2	-7.23	1.23	1.33
1	B	317	ARG	CZ-NH2	-7.23	1.23	1.33
1	A	71	ARG	CZ-NH2	-7.23	1.23	1.33
1	A	413	ARG	CZ-NH2	-7.23	1.23	1.33
1	A	875	ARG	CZ-NH2	-7.23	1.23	1.33
1	B	8	ARG	CZ-NH2	-7.23	1.23	1.33
1	B	71	ARG	CZ-NH2	-7.23	1.23	1.33
1	A	563	ARG	CZ-NH2	-7.23	1.23	1.33
1	A	485	ARG	CZ-NH2	-7.23	1.23	1.33
1	A	317	ARG	CZ-NH2	-7.23	1.23	1.33
1	B	31	ARG	CZ-NH2	-7.23	1.23	1.33
1	B	461	ARG	CZ-NH2	-7.23	1.23	1.33
1	A	558	ARG	CZ-NH2	-7.22	1.23	1.33
1	A	912	ARG	CZ-NH2	-7.22	1.23	1.33
1	A	286	ARG	CZ-NH2	-7.22	1.23	1.33
1	A	59	ARG	CZ-NH2	-7.22	1.23	1.33
1	A	431	ARG	CZ-NH2	-7.22	1.23	1.33
1	B	59	ARG	CZ-NH2	-7.21	1.23	1.33
1	B	280	ARG	CZ-NH2	-7.21	1.23	1.33
1	A	245	ARG	CZ-NH2	-7.21	1.23	1.33
1	A	397	ARG	CZ-NH2	-7.21	1.23	1.33
1	B	882	ARG	CZ-NH2	-7.21	1.23	1.33
1	A	1329	ARG	CZ-NH2	-7.20	1.23	1.33
1	B	828	ARG	CZ-NH2	-7.20	1.23	1.33
1	A	31	ARG	CZ-NH2	-7.20	1.23	1.33
1	A	319	ARG	CZ-NH2	-7.19	1.23	1.33
1	B	380	ARG	CZ-NH2	-7.19	1.23	1.33
1	B	12	ARG	CZ-NH2	-7.19	1.23	1.33
1	B	732	ARG	CZ-NH2	-7.19	1.23	1.33
1	A	380	ARG	CZ-NH2	-7.18	1.23	1.33
1	A	576	ARG	CZ-NH2	-7.18	1.23	1.33
1	B	276	ARG	CZ-NH2	-7.18	1.23	1.33
1	A	12	ARG	CZ-NH2	-7.18	1.23	1.33
1	B	554	ARG	CZ-NH2	-7.17	1.23	1.33
1	B	778	ARG	CZ-NH2	-7.17	1.23	1.33
1	A	644	ARG	CZ-NH2	-7.17	1.23	1.33
1	A	643	ARG	CZ-NH2	-7.17	1.23	1.33
1	B	613	ARG	CZ-NH2	-7.17	1.23	1.33
1	A	668	ARG	CZ-NH2	-7.16	1.23	1.33
1	B	286	ARG	CZ-NH2	-7.16	1.23	1.33
1	B	541	ARG	CZ-NH2	-7.16	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	805	ARG	CZ-NH2	-7.16	1.23	1.33
1	A	1311	ARG	CZ-NH2	-7.16	1.23	1.33
1	B	875	ARG	CZ-NH2	-7.15	1.23	1.33
1	A	280	ARG	CZ-NH2	-7.15	1.23	1.33
1	B	563	ARG	CZ-NH2	-7.14	1.23	1.33
1	A	991	ARG	CZ-NH2	-7.14	1.23	1.33
1	B	540	ARG	CZ-NH2	-7.13	1.23	1.33
1	B	912	ARG	CZ-NH2	-7.12	1.23	1.33
1	B	582	ARG	CZ-NH2	-7.12	1.23	1.33
1	A	276	ARG	CZ-NH2	-7.12	1.23	1.33
1	B	643	ARG	CZ-NH2	-7.12	1.23	1.33
1	A	1330	ARG	CZ-NH2	-7.11	1.23	1.33
1	A	579	ARG	CZ-NH2	-7.11	1.23	1.33
1	A	921	ARG	CZ-NH2	-7.11	1.23	1.33
1	A	335	ARG	CZ-NH2	-7.11	1.23	1.33
1	A	519	ARG	CZ-NH2	-7.11	1.23	1.33
1	B	335	ARG	CZ-NH2	-7.09	1.23	1.33
1	B	644	ARG	CZ-NH2	-7.08	1.23	1.33
1	A	904	ARG	CZ-NH2	-7.07	1.23	1.33
1	B	558	ARG	CZ-NH2	-7.07	1.23	1.33
1	B	904	ARG	CZ-NH2	-7.04	1.23	1.33
1	B	921	ARG	CZ-NH2	-7.03	1.24	1.33
1	B	924	ARG	CZ-NH2	-7.00	1.24	1.33
1	A	540	ARG	CZ-NH2	-7.00	1.24	1.33
1	A	826	ARG	CZ-NH2	-6.98	1.24	1.33
1	A	805	ARG	CZ-NH2	-6.98	1.24	1.33
1	A	828	ARG	CZ-NH2	-6.97	1.24	1.33
1	A	924	ARG	CZ-NH2	-6.93	1.24	1.33
1	A	513	TYR	CD1-CE1	-5.98	1.30	1.39
1	B	513	TYR	CD1-CE1	-5.92	1.30	1.39
1	A	575	TYR	CD1-CE1	-5.90	1.30	1.39
1	A	628	GLY	N-CA	-5.86	1.37	1.46
1	B	750	GLY	N-CA	-5.80	1.37	1.46
1	A	804	TYR	CD2-CE2	-5.79	1.30	1.39
1	B	347	VAL	CB-CG2	-5.79	1.40	1.52
1	A	347	VAL	CB-CG2	-5.79	1.40	1.52
1	A	804	TYR	CD1-CE1	-5.79	1.30	1.39
1	B	513	TYR	CD2-CE2	-5.78	1.30	1.39
1	B	631	TYR	CD2-CE2	-5.77	1.30	1.39
1	B	804	TYR	CD1-CE1	-5.77	1.30	1.39
1	B	978	GLY	N-CA	-5.76	1.37	1.46
1	B	804	TYR	CD2-CE2	-5.75	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	884	VAL	CB-CG1	-5.75	1.40	1.52
1	A	896	GLY	N-CA	-5.75	1.37	1.46
1	A	575	TYR	CD2-CE2	-5.74	1.30	1.39
1	B	751	GLY	N-CA	-5.73	1.37	1.46
1	A	513	TYR	CD2-CE2	-5.71	1.30	1.39
1	A	487	GLY	N-CA	-5.71	1.37	1.46
1	A	978	GLY	N-CA	-5.70	1.37	1.46
1	A	979	GLY	N-CA	-5.69	1.37	1.46
1	B	444	VAL	CB-CG1	-5.68	1.41	1.52
1	A	884	VAL	CB-CG1	-5.67	1.41	1.52
1	A	989	VAL	CB-CG2	-5.67	1.41	1.52
1	B	272	TYR	CD2-CE2	-5.67	1.30	1.39
1	A	489	GLY	N-CA	-5.67	1.37	1.46
1	A	614	GLY	N-CA	-5.66	1.37	1.46
1	A	931	TYR	CD1-CE1	-5.66	1.30	1.39
1	B	487	GLY	N-CA	-5.66	1.37	1.46
1	B	408	VAL	CB-CG1	-5.65	1.41	1.52
1	A	607	VAL	CB-CG1	-5.64	1.41	1.52
1	B	896	GLY	N-CA	-5.64	1.37	1.46
1	B	489	GLY	N-CA	-5.63	1.37	1.46
1	A	444	VAL	CB-CG1	-5.63	1.41	1.52
1	A	272	TYR	CD2-CE2	-5.63	1.30	1.39
1	B	290	TYR	CD2-CE2	-5.63	1.30	1.39
1	B	607	VAL	CB-CG1	-5.62	1.41	1.52
1	A	290	TYR	CD2-CE2	-5.62	1.30	1.39
1	B	631	TYR	CD1-CE1	-5.61	1.30	1.39
1	A	408	VAL	CB-CG1	-5.61	1.41	1.52
1	B	979	GLY	N-CA	-5.61	1.37	1.46
1	B	290	TYR	CD1-CE1	-5.59	1.30	1.39
1	B	621	VAL	CB-CG2	-5.59	1.41	1.52
1	A	497	VAL	CB-CG1	-5.58	1.41	1.52
1	B	694	VAL	CB-CG2	-5.58	1.41	1.52
1	A	651	GLY	N-CA	-5.57	1.37	1.46
1	B	989	VAL	CB-CG2	-5.57	1.41	1.52
1	B	497	VAL	CB-CG1	-5.57	1.41	1.52
1	B	759	VAL	CB-CG1	-5.56	1.41	1.52
1	B	272	TYR	CD1-CE1	-5.56	1.31	1.39
1	B	888	VAL	CB-CG1	-5.56	1.41	1.52
1	A	408	VAL	CB-CG2	-5.54	1.41	1.52
1	B	125	GLY	N-CA	-5.54	1.37	1.46
1	A	210	VAL	CB-CG1	-5.54	1.41	1.52
1	B	408	VAL	CB-CG2	-5.54	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	931	TYR	CD2-CE2	-5.54	1.31	1.39
1	B	968	GLY	N-CA	-5.54	1.37	1.46
1	A	877	VAL	CB-CG1	-5.53	1.41	1.52
1	B	110	VAL	CB-CG2	-5.53	1.41	1.52
1	B	651	GLY	N-CA	-5.53	1.37	1.46
1	B	706	GLY	N-CA	-5.53	1.37	1.46
1	A	755	GLY	N-CA	-5.52	1.37	1.46
1	A	890	GLY	N-CA	-5.52	1.37	1.46
1	A	876	VAL	CB-CG2	-5.52	1.41	1.52
1	B	652	VAL	CB-CG2	-5.52	1.41	1.52
1	A	349	GLY	N-CA	-5.52	1.37	1.46
1	A	694	VAL	CB-CG2	-5.51	1.41	1.52
1	A	888	VAL	CB-CG1	-5.51	1.41	1.52
1	A	290	TYR	CD1-CE1	-5.50	1.31	1.39
1	B	755	GLY	N-CA	-5.50	1.37	1.46
1	A	429	VAL	CB-CG2	-5.50	1.41	1.52
1	A	968	GLY	N-CA	-5.50	1.37	1.46
1	A	652	VAL	CB-CG2	-5.49	1.41	1.52
1	A	935	GLY	N-CA	-5.49	1.37	1.46
1	B	877	VAL	CB-CG1	-5.49	1.41	1.52
1	B	210	VAL	CB-CG1	-5.49	1.41	1.52
1	A	546	GLY	N-CA	-5.48	1.37	1.46
1	A	24	GLY	N-CA	-5.48	1.37	1.46
1	A	125	GLY	N-CA	-5.47	1.37	1.46
1	B	349	GLY	N-CA	-5.47	1.37	1.46
1	B	456	VAL	CB-CG2	-5.47	1.41	1.52
1	A	119	GLY	N-CA	-5.47	1.37	1.46
1	A	272	TYR	CD1-CE1	-5.47	1.31	1.39
1	A	607	VAL	CB-CG2	-5.46	1.41	1.52
1	B	429	VAL	CB-CG2	-5.46	1.41	1.52
1	A	888	VAL	CB-CG2	-5.46	1.41	1.52
1	B	736	VAL	CB-CG1	-5.46	1.41	1.52
1	A	580	VAL	CB-CG1	-5.46	1.41	1.52
1	B	609	VAL	CB-CG2	-5.46	1.41	1.52
1	B	624	VAL	CB-CG2	-5.46	1.41	1.52
1	B	60	GLY	N-CA	-5.45	1.37	1.46
1	B	618	VAL	CB-CG2	-5.45	1.41	1.52
1	A	417	GLY	N-CA	-5.45	1.37	1.46
1	A	624	VAL	CB-CG1	-5.45	1.41	1.52
1	B	609	VAL	CB-CG1	-5.45	1.41	1.52
1	A	871	GLY	N-CA	-5.45	1.37	1.46
1	A	915	VAL	CB-CG2	-5.45	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	884	VAL	CB-CG2	-5.45	1.41	1.52
1	B	871	GLY	N-CA	-5.45	1.37	1.46
1	B	24	GLY	N-CA	-5.44	1.37	1.46
1	B	736	VAL	CB-CG2	-5.44	1.41	1.52
1	B	347	VAL	CB-CG1	-5.44	1.41	1.52
1	B	546	GLY	N-CA	-5.44	1.37	1.46
1	A	456	VAL	CB-CG2	-5.43	1.41	1.52
1	B	525	TRP	CD1-NE1	-5.43	1.28	1.38
1	A	601	VAL	CB-CG1	-5.43	1.41	1.52
1	A	987	VAL	CB-CG1	-5.43	1.41	1.52
1	A	671	VAL	CB-CG2	-5.43	1.41	1.52
1	A	604	GLY	N-CA	-5.42	1.38	1.46
1	B	477	VAL	CB-CG2	-5.42	1.41	1.52
1	B	604	GLY	N-CA	-5.42	1.38	1.46
1	B	417	GLY	N-CA	-5.42	1.38	1.46
1	B	915	VAL	CB-CG2	-5.42	1.41	1.52
1	A	60	GLY	N-CA	-5.41	1.38	1.46
1	A	525	TRP	CD1-NE1	-5.41	1.28	1.38
1	A	877	VAL	CB-CG2	-5.41	1.41	1.52
1	B	881	GLY	N-CA	-5.41	1.38	1.46
1	A	444	VAL	CB-CG2	-5.41	1.41	1.52
1	B	444	VAL	CB-CG2	-5.41	1.41	1.52
1	A	706	GLY	N-CA	-5.41	1.38	1.46
1	A	884	VAL	CB-CG2	-5.41	1.41	1.52
1	B	888	VAL	CB-CG2	-5.40	1.41	1.52
1	B	477	VAL	CB-CG1	-5.40	1.41	1.52
1	B	624	VAL	CB-CG1	-5.40	1.41	1.52
1	A	477	VAL	CB-CG1	-5.40	1.41	1.52
1	A	127	VAL	CB-CG1	-5.39	1.41	1.52
1	A	624	VAL	CB-CG2	-5.39	1.41	1.52
1	A	117	GLY	N-CA	-5.39	1.38	1.46
1	A	623	GLY	N-CA	-5.39	1.38	1.46
1	B	607	VAL	CB-CG2	-5.39	1.41	1.52
1	B	119	GLY	N-CA	-5.38	1.38	1.46
1	B	987	VAL	CB-CG1	-5.38	1.41	1.52
1	B	359	TRP	CD1-NE1	-5.38	1.28	1.38
1	A	889	VAL	CB-CG1	-5.38	1.41	1.52
1	B	117	GLY	N-CA	-5.37	1.38	1.46
1	B	632	VAL	CB-CG1	-5.37	1.41	1.52
1	B	915	VAL	CB-CG1	-5.37	1.41	1.52
1	A	876	VAL	CB-CG1	-5.37	1.41	1.52
1	A	477	VAL	CB-CG2	-5.37	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	753	GLY	N-CA	-5.37	1.38	1.46
1	B	877	VAL	CB-CG2	-5.37	1.41	1.52
1	B	127	VAL	CB-CG1	-5.36	1.41	1.52
1	A	969	VAL	CB-CG2	-5.36	1.41	1.52
1	B	221	VAL	CB-CG2	-5.36	1.41	1.52
1	B	504	GLY	N-CA	-5.36	1.38	1.46
1	A	881	GLY	N-CA	-5.35	1.38	1.46
1	B	384	VAL	CB-CG1	-5.35	1.41	1.52
1	B	497	VAL	CB-CG2	-5.35	1.41	1.52
1	A	347	VAL	CB-CG1	-5.35	1.41	1.52
1	B	291	TRP	CD1-NE1	-5.35	1.28	1.38
1	A	384	VAL	CB-CG1	-5.35	1.41	1.52
1	A	497	VAL	CB-CG2	-5.34	1.41	1.52
1	A	933	GLY	N-CA	-5.34	1.38	1.46
1	B	759	VAL	CB-CG2	-5.34	1.41	1.52
1	A	632	VAL	CB-CG1	-5.34	1.41	1.52
1	A	929	GLY	N-CA	-5.34	1.38	1.46
1	B	969	VAL	CB-CG2	-5.34	1.41	1.52
1	A	632	VAL	CB-CG2	-5.33	1.41	1.52
1	B	1334	SER	CB-OG	-5.33	1.35	1.42
1	A	233	SER	CB-OG	-5.33	1.35	1.42
1	B	691	SER	CB-OG	-5.32	1.35	1.42
1	A	902	GLY	N-CA	-5.32	1.38	1.46
1	A	221	VAL	CB-CG1	-5.32	1.41	1.52
1	A	1298	GLY	N-CA	-5.32	1.38	1.46
1	A	535	TRP	CD1-NE1	-5.32	1.28	1.38
1	A	922	TRP	CD1-NE1	-5.32	1.28	1.38
1	B	454	GLY	N-CA	-5.31	1.38	1.46
1	A	291	TRP	CD1-NE1	-5.31	1.28	1.38
1	B	233	SER	CB-OG	-5.31	1.35	1.42
1	B	30	VAL	CB-CG1	-5.31	1.41	1.52
1	A	219	GLY	N-CA	-5.31	1.38	1.46
1	A	580	VAL	CB-CG2	-5.31	1.41	1.52
1	A	969	VAL	CB-CG1	-5.31	1.41	1.52
1	B	219	GLY	N-CA	-5.31	1.38	1.46
1	A	494	TRP	CD1-NE1	-5.31	1.28	1.38
1	B	486	VAL	CB-CG2	-5.30	1.41	1.52
1	A	243	SER	CB-OG	-5.30	1.35	1.42
1	B	618	VAL	CB-CG1	-5.30	1.41	1.52
1	A	915	VAL	CB-CG1	-5.30	1.41	1.52
1	A	684	VAL	CB-CG1	-5.29	1.41	1.52
1	A	127	VAL	CB-CG2	-5.29	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	583	GLY	N-CA	-5.29	1.38	1.46
1	B	486	VAL	CB-CG1	-5.29	1.41	1.52
1	B	535	TRP	CD1-NE1	-5.29	1.28	1.38
1	A	971	SER	CB-OG	-5.29	1.35	1.42
1	B	498	VAL	CB-CG1	-5.29	1.41	1.52
1	B	632	VAL	CB-CG2	-5.29	1.41	1.52
1	A	30	VAL	CB-CG1	-5.29	1.41	1.52
1	A	202	TRP	CD1-NE1	-5.28	1.28	1.38
1	A	691	SER	CB-OG	-5.28	1.35	1.42
1	A	920	GLY	N-CA	-5.28	1.38	1.46
1	B	243	SER	CB-OG	-5.28	1.35	1.42
1	B	429	VAL	CB-CG1	-5.28	1.41	1.52
1	A	498	VAL	CB-CG1	-5.28	1.41	1.52
1	B	920	GLY	N-CA	-5.28	1.38	1.46
1	A	221	VAL	CB-CG2	-5.28	1.41	1.52
1	A	980	GLY	N-CA	-5.27	1.38	1.46
1	B	127	VAL	CB-CG2	-5.27	1.41	1.52
1	A	932	TRP	CD1-NE1	-5.27	1.28	1.38
1	A	478	TRP	CD1-NE1	-5.27	1.28	1.38
1	A	486	VAL	CB-CG1	-5.27	1.41	1.52
1	A	486	VAL	CB-CG2	-5.27	1.41	1.52
1	A	429	VAL	CB-CG1	-5.26	1.41	1.52
1	A	1313	TRP	CD1-NE1	-5.26	1.29	1.38
1	B	478	TRP	CD1-NE1	-5.26	1.29	1.38
1	B	922	TRP	CD1-NE1	-5.26	1.29	1.38
1	A	1317	SER	CB-OG	-5.26	1.35	1.42
1	B	123	VAL	CB-CG2	-5.26	1.41	1.52
1	B	410	SER	CB-OG	-5.26	1.35	1.42
1	B	409	LYS	CE-NZ	-5.26	1.35	1.49
1	A	123	VAL	CB-CG2	-5.25	1.41	1.52
1	A	1334	SER	CB-OG	-5.25	1.35	1.42
1	B	108	SER	CB-OG	-5.25	1.35	1.42
1	B	123	VAL	CB-CG1	-5.25	1.41	1.52
1	A	454	GLY	N-CA	-5.25	1.38	1.46
1	A	893	TRP	CD1-NE1	-5.25	1.29	1.38
1	B	231	TRP	CD1-NE1	-5.25	1.29	1.38
1	A	115	TRP	CD1-NE1	-5.24	1.29	1.38
1	B	221	VAL	CB-CG1	-5.23	1.41	1.52
1	B	1298	GLY	N-CA	-5.23	1.38	1.46
1	B	1317	SER	CB-OG	-5.23	1.35	1.42
1	B	523	SER	CB-OG	-5.23	1.35	1.42
1	A	409	LYS	CE-NZ	-5.23	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	TRP	CD1-NE1	-5.22	1.29	1.38
1	A	123	VAL	CB-CG1	-5.22	1.41	1.52
1	B	30	VAL	CB-CG2	-5.22	1.41	1.52
1	B	202	TRP	CD1-NE1	-5.22	1.29	1.38
1	B	710	SER	CB-OG	-5.22	1.35	1.42
1	B	1313	TRP	CD1-NE1	-5.22	1.29	1.38
1	B	971	SER	CB-OG	-5.22	1.35	1.42
1	B	110	VAL	CB-CG1	-5.22	1.41	1.52
1	B	115	TRP	CD1-NE1	-5.21	1.29	1.38
1	A	75	GLY	N-CA	-5.21	1.38	1.46
1	B	494	TRP	CD1-NE1	-5.21	1.29	1.38
1	B	621	VAL	CB-CG1	-5.21	1.42	1.52
1	B	969	VAL	CB-CG1	-5.21	1.42	1.52
1	A	889	VAL	CB-CG2	-5.21	1.42	1.52
1	A	108	SER	CB-OG	-5.21	1.35	1.42
1	B	652	VAL	CB-CG1	-5.21	1.42	1.52
1	A	196	TRP	CD1-NE1	-5.20	1.29	1.38
1	A	396	CYS	CB-SG	-5.20	1.73	1.81
1	A	987	VAL	CB-CG2	-5.20	1.42	1.52
1	A	710	SER	CB-OG	-5.19	1.35	1.42
1	A	523	SER	CB-OG	-5.19	1.35	1.42
1	A	652	VAL	CB-CG1	-5.18	1.42	1.52
1	B	196	TRP	CD1-NE1	-5.18	1.29	1.38
1	B	694	VAL	CB-CG1	-5.18	1.42	1.52
1	A	694	VAL	CB-CG1	-5.18	1.42	1.52
1	B	498	VAL	CB-CG2	-5.18	1.42	1.52
1	A	30	VAL	CB-CG2	-5.18	1.42	1.52
1	B	893	TRP	CD1-NE1	-5.17	1.29	1.38
1	A	1326	VAL	CB-CG2	-5.17	1.42	1.52
1	A	88	SER	CB-OG	-5.16	1.35	1.42
1	B	215	VAL	CB-CG1	-5.16	1.42	1.52
1	B	396	CYS	CB-SG	-5.16	1.73	1.81
1	B	772	TRP	CD1-NE1	-5.16	1.29	1.38
1	A	215	VAL	CB-CG1	-5.15	1.42	1.52
1	A	601	VAL	CB-CG2	-5.15	1.42	1.52
1	B	456	VAL	CB-CG1	-5.15	1.42	1.52
1	B	610	SER	CB-OG	-5.15	1.35	1.42
1	A	1326	VAL	CB-CG1	-5.15	1.42	1.52
1	B	88	SER	CB-OG	-5.15	1.35	1.42
1	B	980	GLY	N-CA	-5.14	1.38	1.46
1	B	75	GLY	N-CA	-5.14	1.38	1.46
1	A	498	VAL	CB-CG2	-5.14	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	671	VAL	CB-CG1	-5.14	1.42	1.52
1	B	210	VAL	CB-CG2	-5.14	1.42	1.52
1	A	210	VAL	CB-CG2	-5.13	1.42	1.52
1	A	456	VAL	CB-CG1	-5.13	1.42	1.52
1	B	987	VAL	CB-CG2	-5.13	1.42	1.52
1	B	7	SER	CB-OG	-5.12	1.35	1.42
1	A	7	SER	CB-OG	-5.10	1.35	1.42
1	A	1325	LYS	CE-NZ	-5.10	1.36	1.49
1	B	1325	LYS	CE-NZ	-5.09	1.36	1.49
1	A	384	VAL	CB-CG2	-5.09	1.42	1.52
1	B	93	VAL	CB-CG2	-5.09	1.42	1.52
1	B	1326	VAL	CB-CG2	-5.07	1.42	1.52
1	A	93	VAL	CB-CG2	-5.07	1.42	1.52
1	B	384	VAL	CB-CG2	-5.07	1.42	1.52
1	A	684	VAL	CB-CG2	-5.06	1.42	1.52
1	A	705	LYS	CE-NZ	-5.04	1.36	1.49
1	B	215	VAL	CB-CG2	-5.04	1.42	1.52
1	A	521	CYS	CB-SG	-5.04	1.73	1.81
1	B	1326	VAL	CB-CG1	-5.02	1.42	1.52
1	B	705	LYS	CE-NZ	-5.02	1.36	1.49
1	B	757	SER	CB-OG	-5.02	1.35	1.42
1	A	109	SER	CB-OG	-5.02	1.35	1.42
1	B	981	VAL	CB-CG1	-5.02	1.42	1.52
1	A	981	VAL	CB-CG1	-5.02	1.42	1.52
1	A	215	VAL	CB-CG2	-5.01	1.42	1.52

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	804	TYR	CB-CG-CD2	8.08	125.85	121.00
1	B	804	TYR	CB-CG-CD2	8.08	125.85	121.00
1	A	575	TYR	CB-CG-CD2	7.39	125.44	121.00
1	B	942	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	942	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	513	TYR	CB-CG-CD2	7.04	125.23	121.00
1	A	513	TYR	CB-CG-CD2	7.03	125.22	121.00
1	A	31	ARG	CD-NE-CZ	6.83	133.16	123.60
1	B	31	ARG	CD-NE-CZ	6.81	133.14	123.60
1	B	1329	ARG	CD-NE-CZ	6.81	133.13	123.60
1	A	904	ARG	CD-NE-CZ	6.78	133.09	123.60
1	A	12	ARG	CD-NE-CZ	6.78	133.09	123.60
1	B	12	ARG	CD-NE-CZ	6.78	133.09	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1329	ARG	CD-NE-CZ	6.77	133.08	123.60
1	B	380	ARG	CD-NE-CZ	6.77	133.08	123.60
1	A	805	ARG	CD-NE-CZ	6.77	133.07	123.60
1	B	904	ARG	CD-NE-CZ	6.76	133.07	123.60
1	B	485	ARG	CD-NE-CZ	6.76	133.06	123.60
1	B	71	ARG	CD-NE-CZ	6.73	133.03	123.60
1	A	380	ARG	CD-NE-CZ	6.73	133.02	123.60
1	A	485	ARG	CD-NE-CZ	6.73	133.02	123.60
1	B	805	ARG	CD-NE-CZ	6.72	133.01	123.60
1	A	668	ARG	CD-NE-CZ	6.71	133.00	123.60
1	A	71	ARG	CD-NE-CZ	6.71	132.99	123.60
1	A	558	ARG	CD-NE-CZ	6.68	132.95	123.60
1	A	808	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	882	ARG	CD-NE-CZ	6.67	132.94	123.60
1	A	317	ARG	CD-NE-CZ	6.65	132.91	123.60
1	B	613	ARG	CD-NE-CZ	6.65	132.91	123.60
1	B	558	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	319	ARG	CD-NE-CZ	6.64	132.89	123.60
1	A	875	ARG	CD-NE-CZ	6.64	132.89	123.60
1	B	319	ARG	CD-NE-CZ	6.63	132.89	123.60
1	B	317	ARG	CD-NE-CZ	6.62	132.87	123.60
1	A	930	ARG	CD-NE-CZ	6.62	132.87	123.60
1	B	991	ARG	CD-NE-CZ	6.62	132.86	123.60
1	A	826	ARG	CD-NE-CZ	6.61	132.85	123.60
1	B	875	ARG	CD-NE-CZ	6.61	132.85	123.60
1	B	203	ARG	CD-NE-CZ	6.61	132.85	123.60
1	A	203	ARG	CD-NE-CZ	6.59	132.83	123.60
1	B	229	ARG	CD-NE-CZ	6.58	132.82	123.60
1	A	229	ARG	CD-NE-CZ	6.56	132.79	123.60
1	B	1330	ARG	CD-NE-CZ	6.55	132.78	123.60
1	A	778	ARG	CD-NE-CZ	6.55	132.77	123.60
1	A	1330	ARG	CD-NE-CZ	6.54	132.76	123.60
1	A	991	ARG	CD-NE-CZ	6.54	132.76	123.60
1	B	374	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	778	ARG	CD-NE-CZ	6.49	132.69	123.60
1	B	865	TYR	CB-CG-CD2	-6.49	117.11	121.00
1	A	579	ARG	CD-NE-CZ	6.47	132.65	123.60
1	B	921	ARG	CD-NE-CZ	6.46	132.64	123.60
1	A	588	ARG	CD-NE-CZ	6.44	132.62	123.60
1	A	921	ARG	CD-NE-CZ	6.43	132.61	123.60
1	A	431	ARG	CD-NE-CZ	6.43	132.60	123.60
1	B	924	ARG	CD-NE-CZ	6.41	132.57	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	924	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	541	ARG	CD-NE-CZ	6.36	132.50	123.60
1	B	582	ARG	CD-NE-CZ	6.33	132.47	123.60
1	A	582	ARG	CD-NE-CZ	6.32	132.45	123.60
1	A	269	PHE	CB-CG-CD2	6.32	125.22	120.80
1	B	541	ARG	CD-NE-CZ	6.31	132.44	123.60
1	B	269	PHE	CB-CG-CD2	6.31	125.22	120.80
1	A	793	MET	CA-CB-CG	6.30	124.01	113.30
1	B	793	MET	CA-CB-CG	6.27	123.96	113.30
1	B	48	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	1302	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	576	ARG	CD-NE-CZ	6.11	132.16	123.60
1	A	931	TYR	CB-CG-CD2	6.07	124.64	121.00
1	B	808	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	865	TYR	CB-CG-CD2	-5.96	117.43	121.00
1	A	48	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	352	PHE	CB-CG-CD2	5.94	124.96	120.80
1	A	901	ARG	CD-NE-CZ	5.94	131.91	123.60
1	B	560	PHE	CB-CG-CD2	5.88	124.92	120.80
1	B	352	PHE	CB-CG-CD2	5.88	124.92	120.80
1	B	1302	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	901	ARG	CD-NE-CZ	5.83	131.77	123.60
1	B	1335	MET	CA-CB-CG	5.81	123.17	113.30
1	B	767	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	1335	MET	CA-CB-CG	5.77	123.11	113.30
1	B	521	CYS	CA-CB-SG	5.73	124.32	114.00
1	B	928	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	455	PHE	CB-CG-CD2	5.70	124.79	120.80
1	A	778	ARG	CG-CD-NE	5.67	123.71	111.80
1	B	455	PHE	CB-CG-CD2	5.64	124.75	120.80
1	A	767	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	431	ARG	CG-CD-NE	5.62	123.61	111.80
1	A	374	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	778	ARG	CG-CD-NE	5.60	123.57	111.80
1	B	930	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	348	PHE	CB-CG-CD2	5.53	124.67	120.80
1	A	521	CYS	CA-CB-SG	5.52	123.93	114.00
1	B	348	PHE	CB-CG-CD2	5.48	124.64	120.80
1	B	484	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	B	931	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	320	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	749	PHE	CB-CG-CD2	5.42	124.59	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ARG	CD-NE-CZ	5.41	131.17	123.60
1	A	642	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	924	ARG	CG-CD-NE	5.37	123.08	111.80
1	A	924	ARG	CG-CD-NE	5.36	123.05	111.80
1	A	928	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	930	ARG	CG-CD-NE	5.31	122.95	111.80
1	B	582	ARG	CG-CD-NE	5.30	122.93	111.80
1	B	882	ARG	CG-CD-NE	5.29	122.92	111.80
1	B	57	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	582	ARG	CG-CD-NE	5.28	122.88	111.80
1	A	693	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	B	930	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	114	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	A	276	ARG	CD-NE-CZ	5.25	130.95	123.60
1	B	280	ARG	CD-NE-CZ	5.24	130.94	123.60
1	A	280	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	484	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	A	114	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	875	ARG	CA-CB-CG	5.20	124.83	113.40
1	B	229	ARG	CG-CD-NE	5.19	122.70	111.80
1	B	424	PHE	CB-CG-CD2	5.18	124.43	120.80
1	A	229	ARG	CG-CD-NE	5.18	122.67	111.80
1	A	424	PHE	CB-CG-CD2	5.17	124.42	120.80
1	B	875	ARG	CA-CB-CG	5.16	124.75	113.40
1	B	642	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	686	LEU	CA-CB-CG	5.12	127.08	115.30
1	B	335	ARG	CD-NE-CZ	5.11	130.76	123.60
1	B	31	ARG	CG-CD-NE	5.10	122.51	111.80
1	A	317	ARG	CG-CD-NE	5.10	122.50	111.80
1	A	31	ARG	CG-CD-NE	5.09	122.50	111.80
1	B	317	ARG	CG-CD-NE	5.09	122.50	111.80
1	A	335	ARG	CD-NE-CZ	5.08	130.71	123.60
1	B	921	ARG	CG-CD-NE	5.08	122.47	111.80
1	B	950	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	216	PHE	CB-CG-CD2	5.07	124.34	120.80
1	A	921	ARG	CG-CD-NE	5.06	122.42	111.80
1	A	1328	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	778	ARG	CA-CB-CG	5.05	124.52	113.40
1	A	55	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	686	LEU	CA-CB-CG	5.05	126.92	115.30
1	B	778	ARG	CA-CB-CG	5.03	124.47	113.40
1	B	108	SER	N-CA-CB	5.03	118.04	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	ARG	CG-CD-NE	5.02	122.34	111.80
1	A	431	ARG	CA-CB-CG	5.02	124.44	113.40
1	B	693	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	A	108	SER	N-CA-CB	5.01	118.02	110.50
1	B	631	TYR	CB-CG-CD1	5.01	124.01	121.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	TYR	Sidechain
1	A	696	TYR	Sidechain
1	A	923	TYR	Sidechain
1	B	374	ARG	Sidechain
1	B	696	TYR	Sidechain
1	B	808	ARG	Sidechain
1	B	923	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10199	10245	10243	71	0
1	B	10199	10245	10243	76	0
2	A	21	20	20	0	0
2	B	21	20	20	0	0
3	A	9	5	4	0	0
3	B	9	5	4	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	23	12	12	0	0
5	B	23	12	12	1	0
6	A	6	6	4	0	0
6	B	6	6	4	0	0
All	All	20518	20576	20566	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (144) 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:B:1242:ALA:O	1:B:1246:ASP:N	2.19	0.76
1:A:602:ARG:NH1	1:A:605:ASP:OD2	2.18	0.76
1:A:1242:ALA:O	1:A:1246:ASP:N	2.19	0.75
1:B:602:ARG:NH1	1:B:605:ASP:OD2	2.18	0.75
1:A:358:ARG:NH1	1:A:531:LEU:O	2.20	0.74
1:B:358:ARG:NH1	1:B:531:LEU:O	2.23	0.71
1:A:395:GLU:O	1:A:414:ASN:ND2	2.28	0.67
1:A:901:ARG:NH1	1:B:329:GLU:OE2	2.28	0.66
1:B:395:GLU:O	1:B:414:ASN:ND2	2.28	0.66
1:A:139:ASP:OD1	1:A:222:ARG:NH2	2.30	0.65
1:A:329:GLU:OE2	1:B:901:ARG:NH1	2.30	0.64
1:B:139:ASP:OD1	1:B:222:ARG:NH2	2.30	0.64
1:A:1033:LEU:O	1:A:1038:ARG:NH1	2.33	0.62
1:B:12:ARG:NH1	1:B:35:ASP:OD1	2.33	0.62
1:A:12:ARG:NH1	1:A:35:ASP:OD1	2.33	0.61
1:B:1033:LEU:O	1:B:1038:ARG:NH1	2.33	0.60
1:B:552:THR:OG1	1:B:554:ARG:NH1	2.36	0.58
1:B:385:ILE:HG22	1:B:385:ILE:O	2.03	0.58
1:A:385:ILE:HG22	1:A:385:ILE:O	2.03	0.58
1:A:552:THR:OG1	1:A:554:ARG:NH1	2.36	0.58
1:A:917:ASP:OD1	1:A:918:ALA:N	2.35	0.58
1:B:180:ASP:OD2	1:B:203:ARG:NH1	2.37	0.58
1:A:144:ARG:NH1	1:A:255:TYR:O	2.37	0.58
1:A:180:ASP:OD2	1:A:203:ARG:NH1	2.37	0.58
1:A:210:VAL:HG12	1:A:215:VAL:HG12	1.87	0.57
1:B:144:ARG:NH1	1:B:255:TYR:O	2.37	0.57
1:B:917:ASP:OD1	1:B:918:ALA:N	2.35	0.57
1:A:1058:GLU:OE1	1:A:1061:ARG:NE	2.34	0.57
1:B:210:VAL:HG12	1:B:215:VAL:HG12	1.87	0.56
1:B:1058:GLU:OE1	1:B:1061:ARG:NE	2.34	0.56
1:A:530:ASP:OD1	1:A:882:ARG:NH1	2.39	0.55
1:B:162:ARG:N	1:B:169:GLN:O	2.37	0.54
1:A:1104:ARG:O	1:A:1104:ARG:NE	2.38	0.54
1:B:1104:ARG:O	1:B:1104:ARG:NE	2.37	0.54
1:A:538:GLN:NE2	1:B:919:GLN:O	2.33	0.53
1:B:657:THR:HG22	1:B:658:GLU:H	1.74	0.53
1:A:1023:LEU:HD23	1:A:1041:TRP:CE3	2.43	0.52
1:B:1023:LEU:HD23	1:B:1041:TRP:CE3	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:ASP:OD1	1:A:1231:LEU:N	2.43	0.52
1:B:1230:ASP:OD1	1:B:1231:LEU:N	2.43	0.52
1:B:443:PRO:O	1:B:478:TRP:N	2.43	0.52
1:B:954:ILE:C	1:B:954:ILE:HD12	2.31	0.51
1:B:356:LEU:O	1:B:360:SER:N	2.44	0.51
1:A:443:PRO:O	1:A:478:TRP:N	2.43	0.50
1:A:162:ARG:N	1:A:169:GLN:O	2.37	0.50
1:A:356:LEU:O	1:A:360:SER:N	2.44	0.50
1:B:657:THR:HG22	1:B:658:GLU:N	2.27	0.50
1:A:919:GLN:O	1:B:538:GLN:NE2	2.41	0.49
1:A:1077:LEU:HD13	1:A:1244:LEU:HD11	1.95	0.49
1:A:1247:ASP:OD1	1:A:1248:ARG:N	2.45	0.49
1:B:1181:LEU:O	1:B:1184:GLY:N	2.45	0.49
1:B:620:ALA:O	1:B:624:VAL:HG23	2.12	0.49
1:B:1247:ASP:OD1	1:B:1248:ARG:N	2.45	0.49
1:B:1275:SER:OG	1:B:1276:GLU:N	2.46	0.49
1:A:551:ALA:HB2	1:A:716:ASN:HA	1.95	0.49
1:B:551:ALA:HB2	1:B:716:ASN:HA	1.95	0.48
1:B:1077:LEU:HD13	1:B:1244:LEU:HD11	1.95	0.48
1:A:118:ARG:NH1	1:A:235:ASP:OD2	2.44	0.48
1:B:150:GLU:O	1:B:154:GLN:NE2	2.45	0.48
1:A:620:ALA:O	1:A:624:VAL:HG23	2.12	0.48
1:A:1181:LEU:O	1:A:1184:GLY:N	2.45	0.48
1:A:1275:SER:OG	1:A:1276:GLU:N	2.46	0.48
1:B:118:ARG:NH1	1:B:235:ASP:OD2	2.44	0.48
1:A:150:GLU:O	1:A:154:GLN:NE2	2.45	0.48
1:B:291:TRP:O	1:B:295:LEU:N	2.47	0.48
1:A:291:TRP:O	1:A:295:LEU:N	2.47	0.47
1:A:381:ILE:HD11	1:A:388:PHE:CE1	2.49	0.47
1:A:541:ARG:NH1	1:A:884:VAL:O	2.41	0.47
1:A:1254:GLU:OE1	1:A:1254:GLU:N	2.43	0.47
1:B:530:ASP:OD1	1:B:882:ARG:NH1	2.46	0.47
1:B:875:ARG:NH2	1:B:883:ASP:OD1	2.44	0.47
1:B:1090:LEU:HD13	1:B:1244:LEU:HD13	1.97	0.47
1:B:1117:GLU:O	1:B:1118:ALA:HB3	2.16	0.46
1:A:433:ALA:O	1:A:438:GLN:N	2.45	0.46
1:B:734:LEU:HG	1:B:736:VAL:HG13	1.97	0.46
1:A:1090:LEU:HD13	1:A:1244:LEU:HD13	1.97	0.46
1:A:1117:GLU:O	1:A:1118:ALA:HB3	2.16	0.46
1:B:433:ALA:O	1:B:438:GLN:N	2.45	0.45
1:B:1254:GLU:OE1	1:B:1254:GLU:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ASP:OD1	1:B:467:LEU:N	2.48	0.45
1:A:657:THR:HG22	1:A:658:GLU:N	2.31	0.45
1:A:392:LEU:HD11	1:A:418:ALA:HB1	1.98	0.45
1:B:392:LEU:HD11	1:B:418:ALA:HB1	1.98	0.45
1:B:1093:ASP:OD1	1:B:1095:TRP:N	2.45	0.44
1:A:657:THR:HG22	1:A:658:GLU:H	1.82	0.44
1:A:554:ARG:NH2	1:A:559:ASP:OD2	2.49	0.44
1:B:554:ARG:NH2	1:B:559:ASP:OD2	2.49	0.44
1:B:1291:ASP:OD1	1:B:1292:ALA:N	2.50	0.44
1:A:47:ILE:H	1:A:47:ILE:HD12	1.83	0.44
1:A:1291:ASP:OD1	1:A:1292:ALA:N	2.50	0.44
1:A:849:ASN:ND2	1:A:874:TYR:CE1	2.86	0.44
1:A:364:GLU:OE1	1:A:397:ARG:NH1	2.50	0.44
1:A:693:TYR:CZ	1:A:745:VAL:HG21	2.53	0.43
1:B:1255:LEU:N	1:B:1256:PRO:CD	2.81	0.43
1:B:541:ARG:NH1	1:B:884:VAL:O	2.41	0.43
1:B:923:TYR:O	1:B:923:TYR:CD1	2.71	0.43
1:A:1255:LEU:N	1:A:1256:PRO:CD	2.81	0.43
1:B:364:GLU:OE1	1:B:397:ARG:NH1	2.50	0.43
1:A:923:TYR:CD1	1:A:923:TYR:O	2.71	0.43
1:B:1262:LEU:HD22	1:B:1269:PRO:HB3	2.01	0.42
1:B:721:LEU:HD23	1:B:847:TRP:CZ3	2.55	0.42
1:B:1023:LEU:HD21	1:B:1240:LEU:HD21	2.01	0.42
1:A:1023:LEU:HD21	1:A:1240:LEU:HD21	2.01	0.42
1:B:632:VAL:HG22	1:B:694:VAL:HB	2.01	0.42
1:A:466:ASP:OD1	1:A:467:LEU:N	2.48	0.42
1:A:632:VAL:HG22	1:A:694:VAL:HB	2.01	0.42
1:A:1023:LEU:HD21	1:A:1240:LEU:CD2	2.50	0.42
1:B:849:ASN:ND2	1:B:874:TYR:CE1	2.88	0.42
1:B:1002:LEU:HD22	1:B:1255:LEU:HD21	2.02	0.42
1:B:1026:LEU:HD23	1:B:1041:TRP:CZ3	2.55	0.42
1:A:887:LEU:N	1:A:931:TYR:O	2.43	0.42
1:B:47:ILE:HD12	1:B:47:ILE:H	1.85	0.42
1:A:1221:ARG:NH1	1:A:1222:PRO:O	2.53	0.41
1:B:751:GLY:O	1:B:756:ALA:N	2.53	0.41
1:B:1221:ARG:NH1	1:B:1222:PRO:O	2.53	0.41
1:A:1004:ALA:HB2	1:A:1275:SER:HB2	2.02	0.41
1:B:513:TYR:CZ	1:B:517:LEU:HD11	2.55	0.41
1:A:1262:LEU:HD22	1:A:1269:PRO:HB3	2.02	0.41
1:B:381:ILE:HD11	1:B:388:PHE:CE1	2.55	0.41
1:B:1023:LEU:HD21	1:B:1240:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:LEU:HB3	1:B:666:PRO:CD	2.51	0.41
1:B:817:VAL:HG21	1:B:837:VAL:HG13	2.03	0.41
1:B:1110:GLU:OE1	1:B:1110:GLU:N	2.46	0.41
1:A:502:PRO:HD2	1:A:505:LEU:HD23	2.01	0.41
1:A:875:ARG:NH2	1:A:883:ASP:OD1	2.44	0.41
1:A:513:TYR:CZ	1:A:517:LEU:HD11	2.55	0.41
1:A:1026:LEU:HD23	1:A:1041:TRP:CZ3	2.55	0.41
1:B:368:ASN:HB3	1:B:391:LEU:HD11	2.03	0.41
5:B:1504:AMP:H5'1	5:B:1504:AMP:N9	2.36	0.41
1:A:404:PHE:O	1:A:408:VAL:HG12	2.21	0.41
1:A:1117:GLU:OE1	1:A:1150:ARG:NH2	2.49	0.41
1:B:69:ALA:HB1	1:B:416:HIS:ND1	2.36	0.41
1:B:1004:ALA:HB2	1:B:1275:SER:HB2	2.02	0.41
1:A:893:TRP:CH2	1:A:915:VAL:HG21	2.56	0.40
1:B:877:VAL:HG21	1:B:893:TRP:CE2	2.56	0.40
1:A:1002:LEU:HD22	1:A:1255:LEU:HD21	2.02	0.40
1:B:404:PHE:O	1:B:408:VAL:HG12	2.21	0.40
1:B:613:ARG:NH1	1:B:736:VAL:O	2.52	0.40
1:A:234:LEU:HD21	1:A:239:ALA:HB3	2.04	0.40
1:B:641:ALA:HB3	1:B:1301:GLN:O	2.21	0.40
1:A:325:LEU:N	1:A:490:ILE:O	2.55	0.40
1:A:641:ALA:HB3	1:A:1301:GLN:O	2.21	0.40
1:A:877:VAL:HG21	1:A:893:TRP:CE2	2.56	0.40
1:B:633:PRO:O	1:B:634:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1332/1455 (92%)	1273 (96%)	59 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1332/1455 (92%)	1270 (95%)	61 (5%)	1 (0%)	51	83
All	All	2664/2910 (92%)	2543 (96%)	120 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	748	LEU

### 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	1019/1122 (91%)	1009 (99%)	10 (1%)	76	91
1	B	1019/1122 (91%)	1009 (99%)	10 (1%)	76	91
All	All	2038/2244 (91%)	2018 (99%)	20 (1%)	77	91

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	154	GLN
1	A	230	LEU
1	A	280	ARG
1	A	295	LEU
1	A	345	SER
1	A	676	ARG
1	A	954	ILE
1	A	1109	ARG
1	A	1273	TRP
1	B	31	ARG
1	B	154	GLN
1	B	230	LEU
1	B	280	ARG
1	B	295	LEU

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Mol	Chain	Res	Type
1	B	345	SER
1	B	676	ARG
1	B	954	ILE
1	B	1109	ARG
1	B	1273	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z  > 2$
5	AMP	B	1504	6,4	22,25,25	1.24	2 (9%)	25,38,38	1.73	6 (24%)
6	CYS	B	1505	5	4,5,6	0.77	0	1,5,7	1.58	0
3	SAL	B	1502	2	9,9,10	0.61	0	11,11,13	0.68	0
3	SAL	A	1502	2	9,9,10	0.59	0	11,11,13	0.74	0
2	PNS	B	1501	3,1	13,20,21	0.98	0	18,26,29	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PNS	A	1501	3,1	13,20,21	0.95	0	18,26,29	0.85	1 (5%)
5	AMP	A	1504	6,4	22,25,25	1.27	2 (9%)	25,38,38	1.71	6 (24%)
6	CYS	A	1505	5	4,5,6	0.80	0	1,5,7	0.92	0

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
5	AMP	B	1504	6,4	-	6/6/26/26	0/3/3/3
6	CYS	B	1505	5	-	0/1/4/6	-
3	SAL	B	1502	2	-	2/2/2/4	0/1/1/1
3	SAL	A	1502	2	-	2/2/2/4	0/1/1/1
2	PNS	B	1501	3,1	-	5/24/26/27	-
2	PNS	A	1501	3,1	-	6/24/26/27	-
5	AMP	A	1504	6,4	-	6/6/26/26	0/3/3/3
6	CYS	A	1505	5	-	0/1/4/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1504	AMP	C5-C4	-2.46	1.34	1.40
5	A	1504	AMP	C5-C4	-2.42	1.34	1.40
5	A	1504	AMP	C4-N3	-2.11	1.32	1.35
5	B	1504	AMP	C4-N3	-2.04	1.32	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1504	AMP	C4-C5-N7	4.09	113.66	109.40
5	B	1504	AMP	C4-C5-N7	4.01	113.57	109.40
5	B	1504	AMP	O5'-P-O1P	3.22	115.50	106.47
5	A	1504	AMP	O5'-P-O1P	3.15	115.32	106.47
2	A	1501	PNS	C42-N41-C39	2.34	127.18	122.84
5	A	1504	AMP	C2-N1-C6	-2.26	114.89	118.75
5	B	1504	AMP	C2-N1-C6	-2.25	114.90	118.75
5	B	1504	AMP	O2P-P-O5'	2.23	112.66	106.73
5	A	1504	AMP	N6-C6-N1	-2.20	114.00	118.57
5	B	1504	AMP	C3'-C2'-C1'	2.18	104.26	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1504	AMP	N6-C6-N1	-2.16	114.10	118.57
5	A	1504	AMP	C3'-C2'-C1'	2.13	104.19	100.98
5	A	1504	AMP	O2P-P-O5'	2.09	112.29	106.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

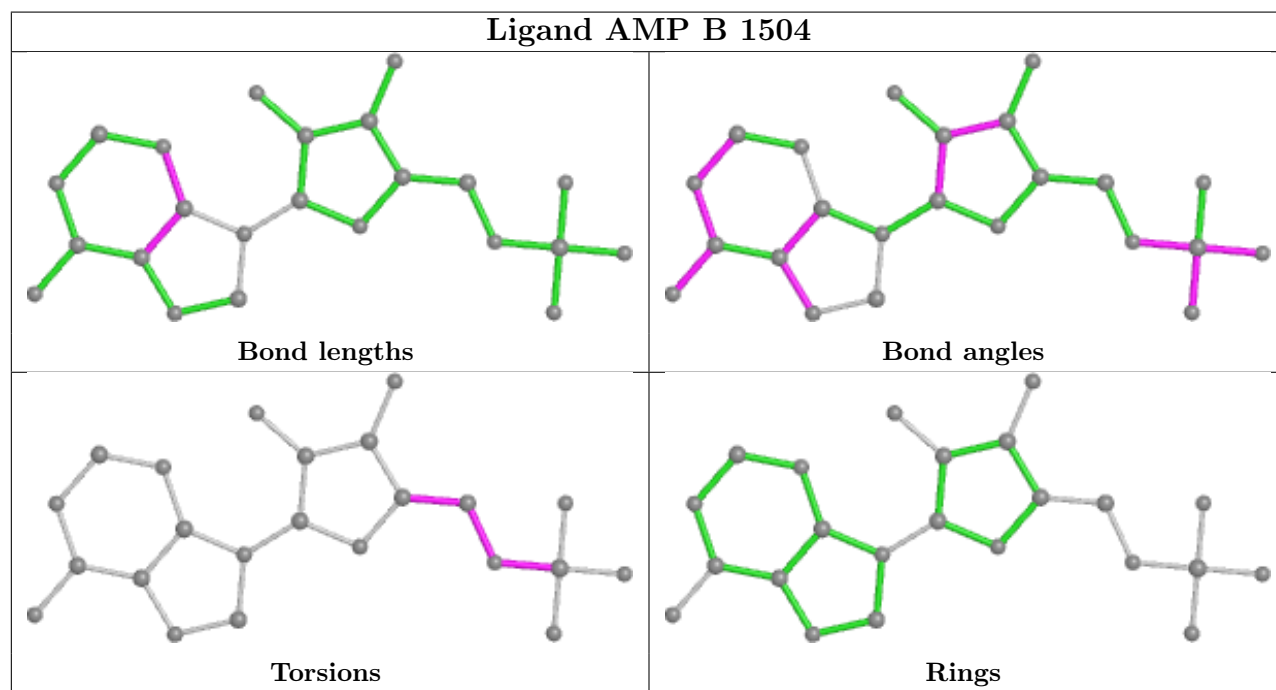
Mol	Chain	Res	Type	Atoms
2	A	1501	PNS	C29-C32-C34-O35
2	A	1501	PNS	C29-C32-C34-N36
2	A	1501	PNS	O33-C32-C34-O35
2	A	1501	PNS	O33-C32-C34-N36
2	A	1501	PNS	C43-C42-N41-C39
2	B	1501	PNS	C29-C32-C34-O35
2	B	1501	PNS	O33-C32-C34-O35
2	B	1501	PNS	O33-C32-C34-N36
2	B	1501	PNS	C43-C42-N41-C39
3	A	1502	SAL	C2-C1-C1'-O1'
5	A	1504	AMP	C5'-O5'-P-O2P
5	A	1504	AMP	C5'-O5'-P-O3P
5	A	1504	AMP	O4'-C4'-C5'-O5'
5	B	1504	AMP	C5'-O5'-P-O2P
5	B	1504	AMP	C5'-O5'-P-O3P
5	B	1504	AMP	O4'-C4'-C5'-O5'
3	B	1502	SAL	C2-C1-C1'-O1'
5	B	1504	AMP	C3'-C4'-C5'-O5'
5	B	1504	AMP	C4'-C5'-O5'-P
5	A	1504	AMP	C3'-C4'-C5'-O5'
5	A	1504	AMP	C4'-C5'-O5'-P
5	A	1504	AMP	C5'-O5'-P-O1P
5	B	1504	AMP	C5'-O5'-P-O1P
2	B	1501	PNS	C29-C32-C34-N36
3	B	1502	SAL	C6-C1-C1'-O1'
3	A	1502	SAL	C6-C1-C1'-O1'
2	A	1501	PNS	O35-C34-N36-C37

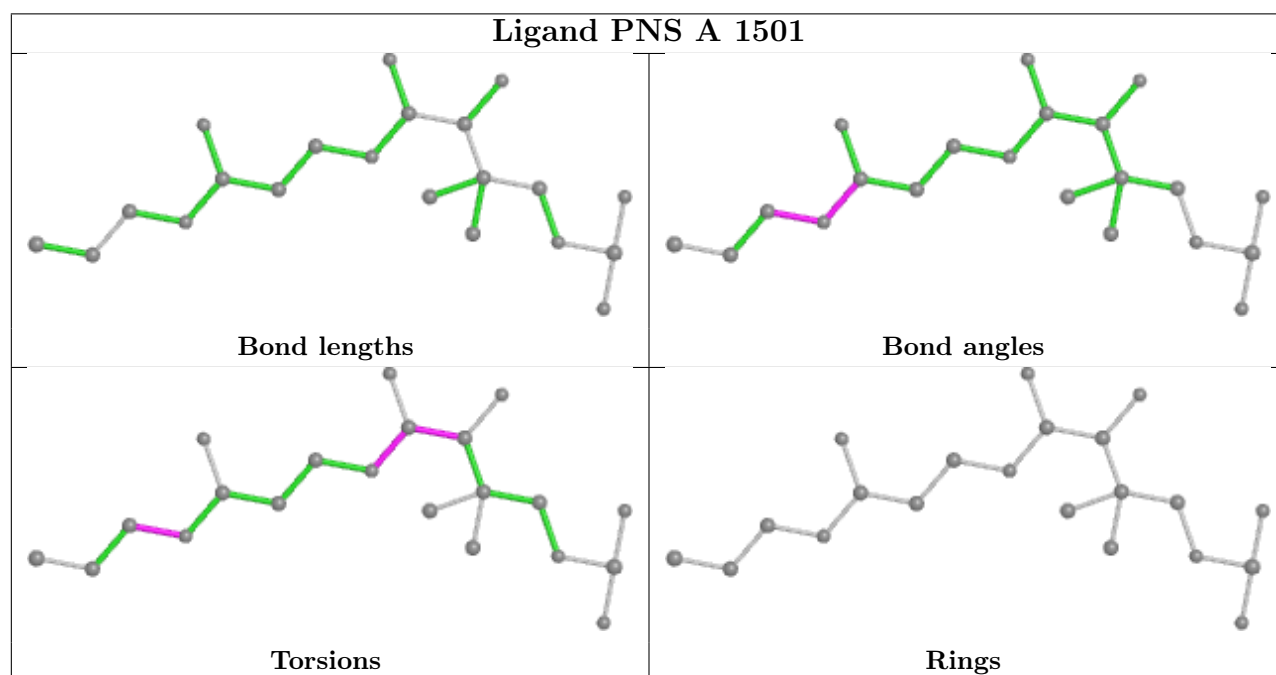
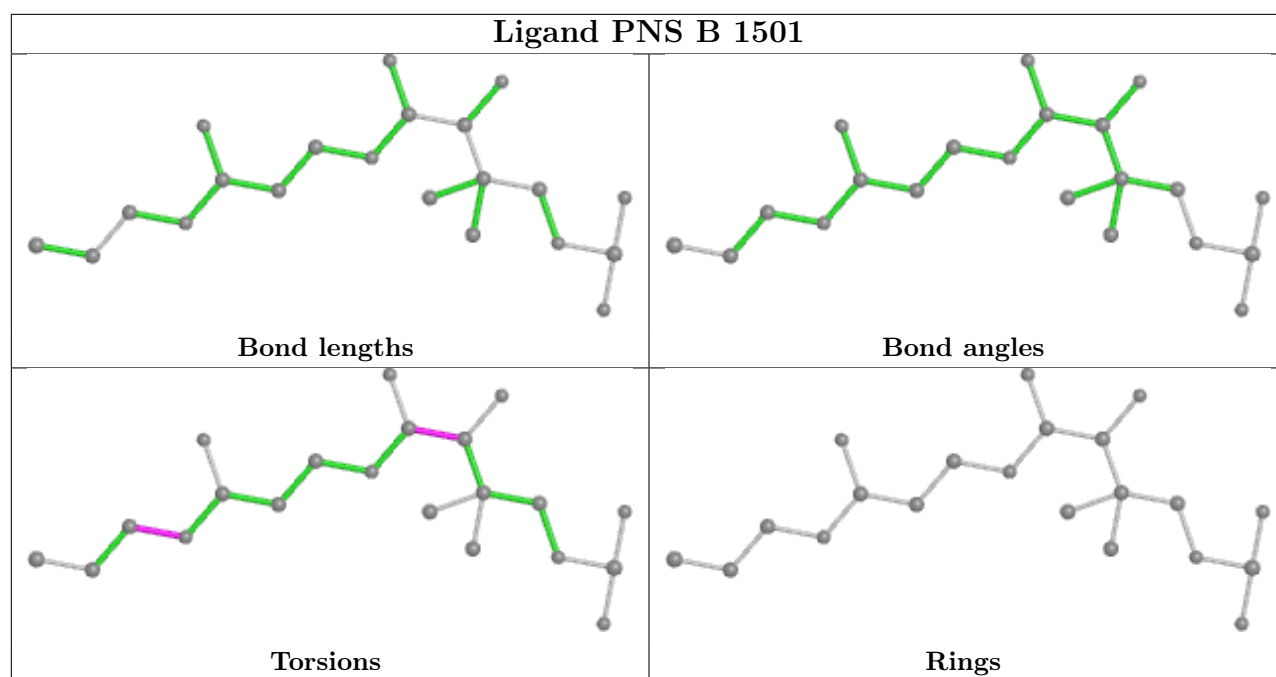
There are no ring outliers.

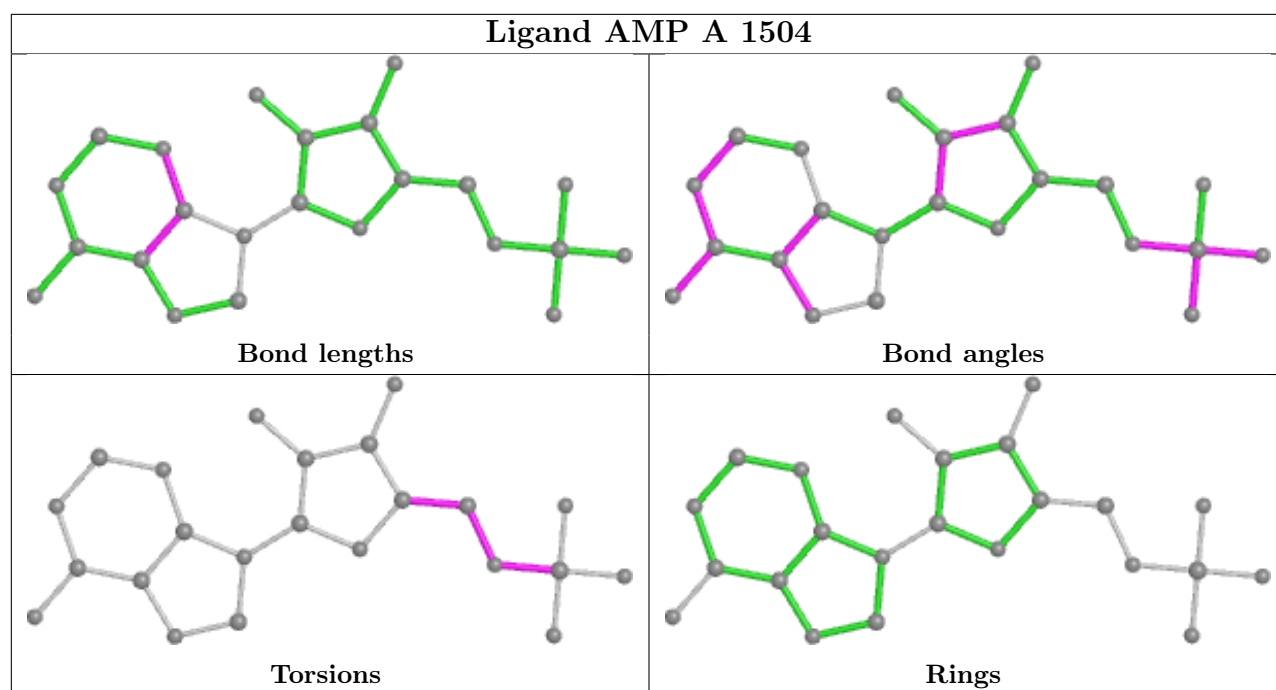
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1504	AMP	1	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

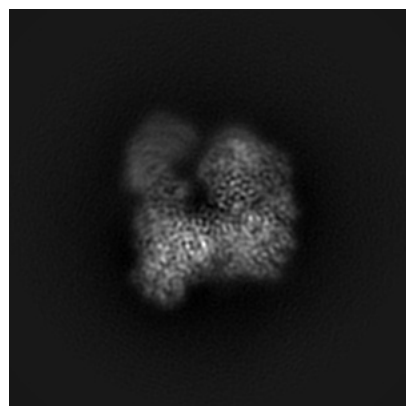
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31198. These allow visual inspection of the internal detail of the map and identification of artifacts.

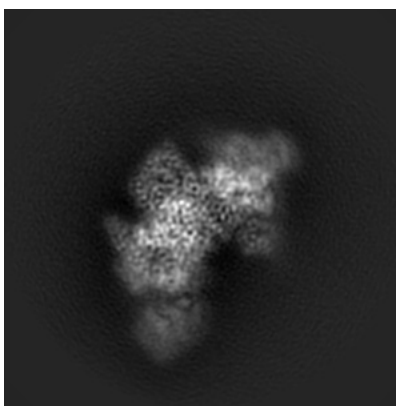
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

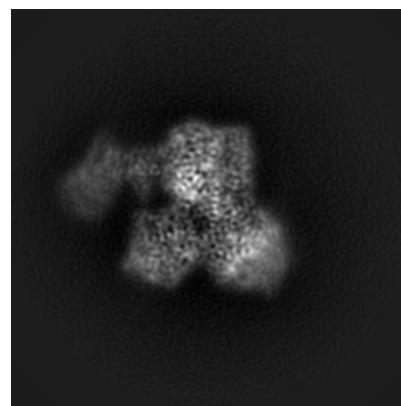
#### 6.1.1 Primary map



X

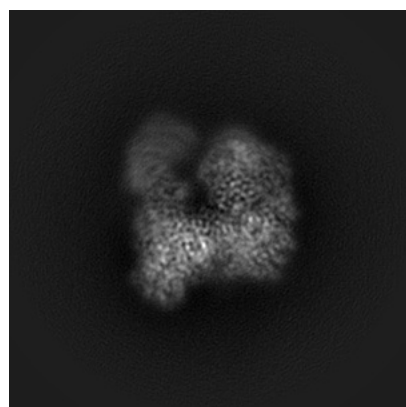


Y

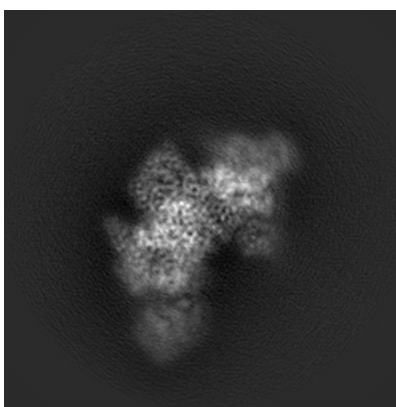


Z

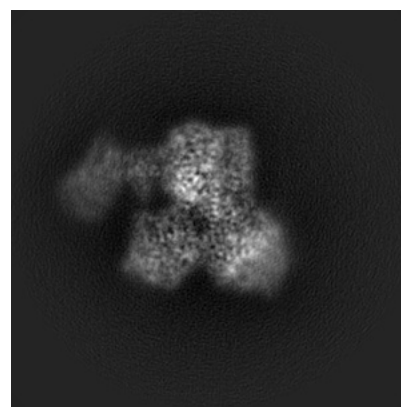
#### 6.1.2 Raw map



X



Y

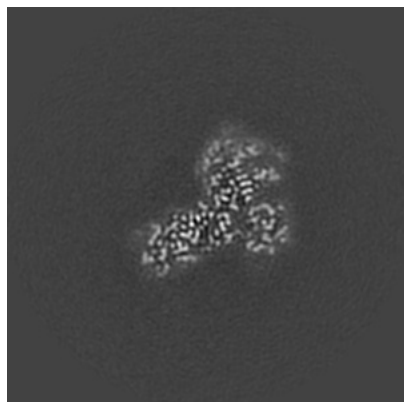


Z

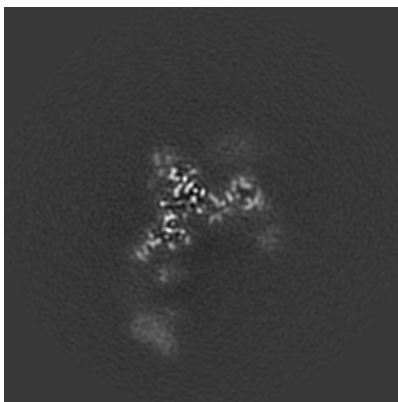
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

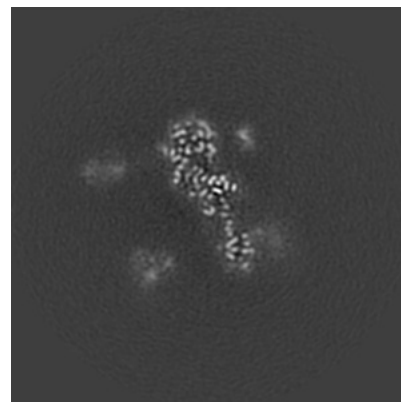
### 6.2.1 Primary map



X Index: 125

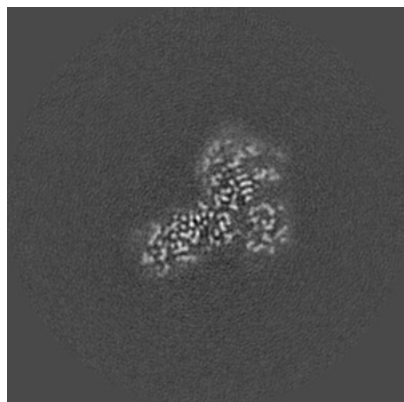


Y Index: 125

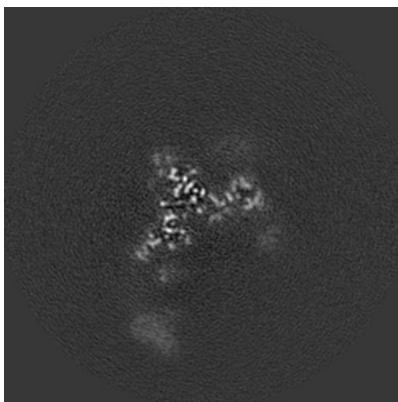


Z Index: 125

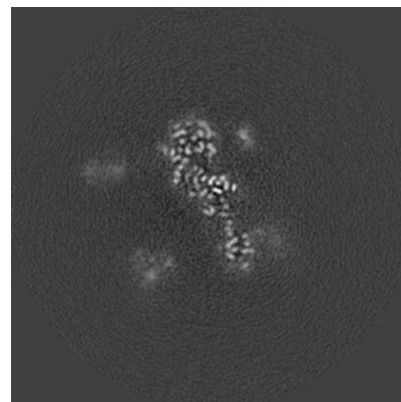
### 6.2.2 Raw map



X Index: 125



Y Index: 125



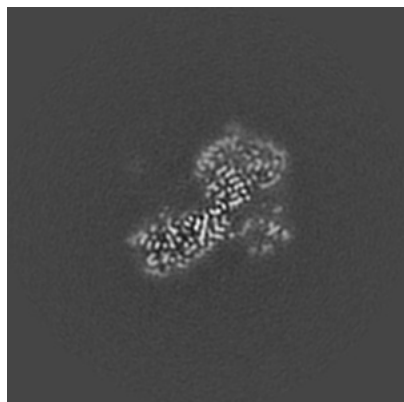
Z Index: 125

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

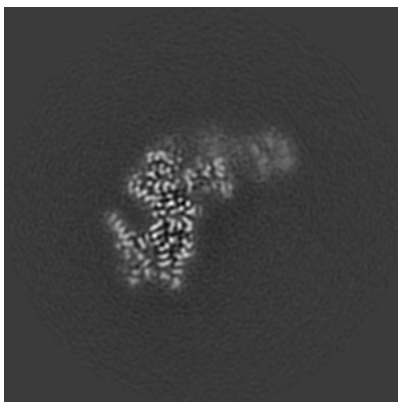


## 6.3 Largest variance slices [i](#)

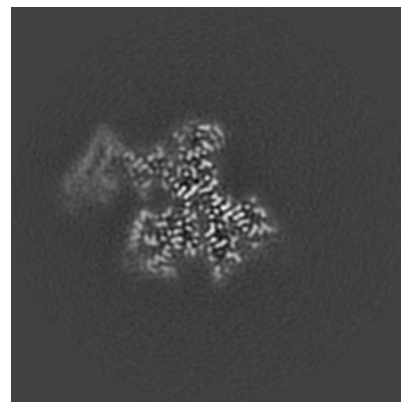
### 6.3.1 Primary map



X Index: 128

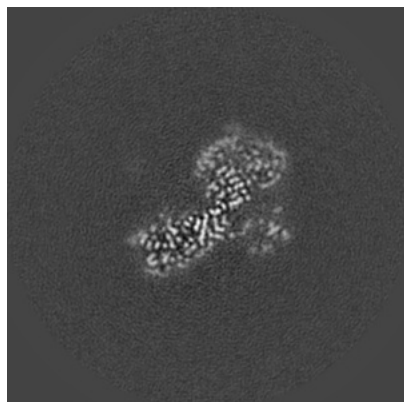


Y Index: 106

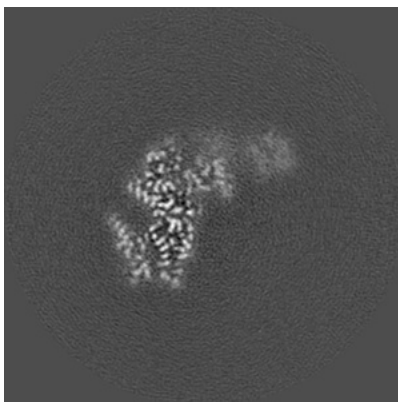


Z Index: 107

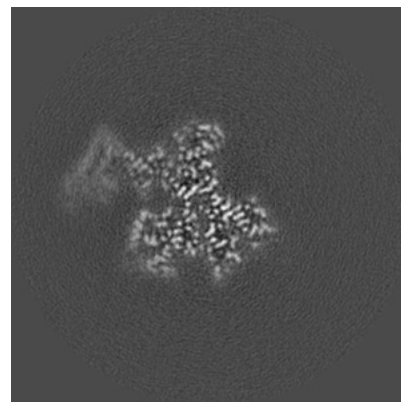
### 6.3.2 Raw map



X Index: 128



Y Index: 107

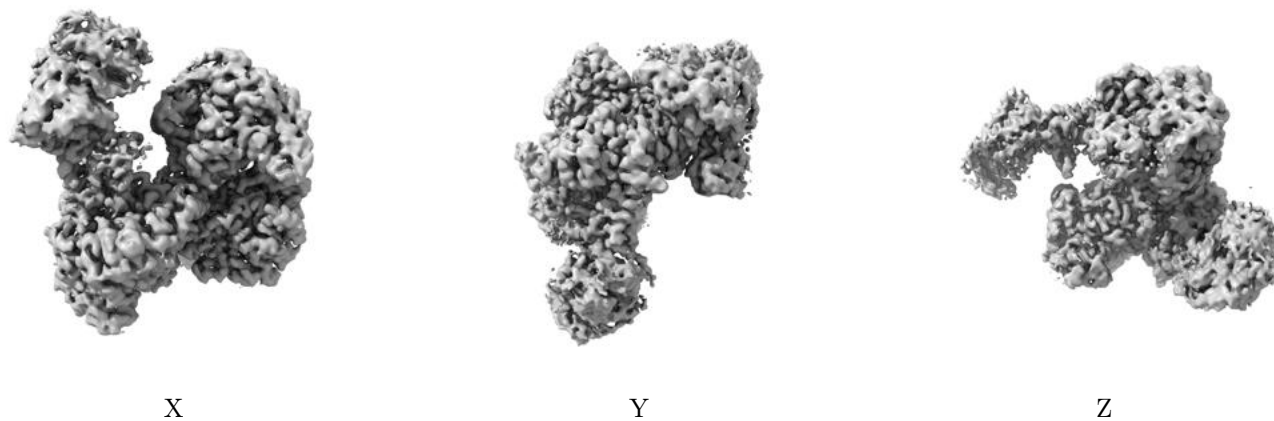


Z Index: 107

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

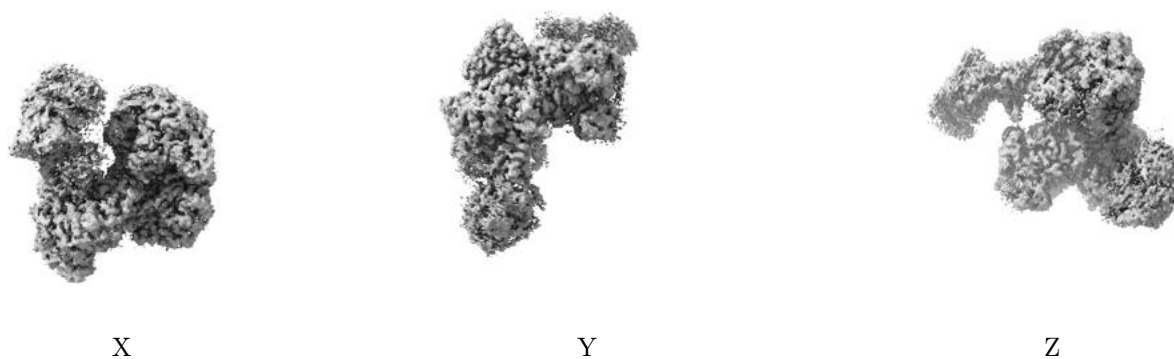
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

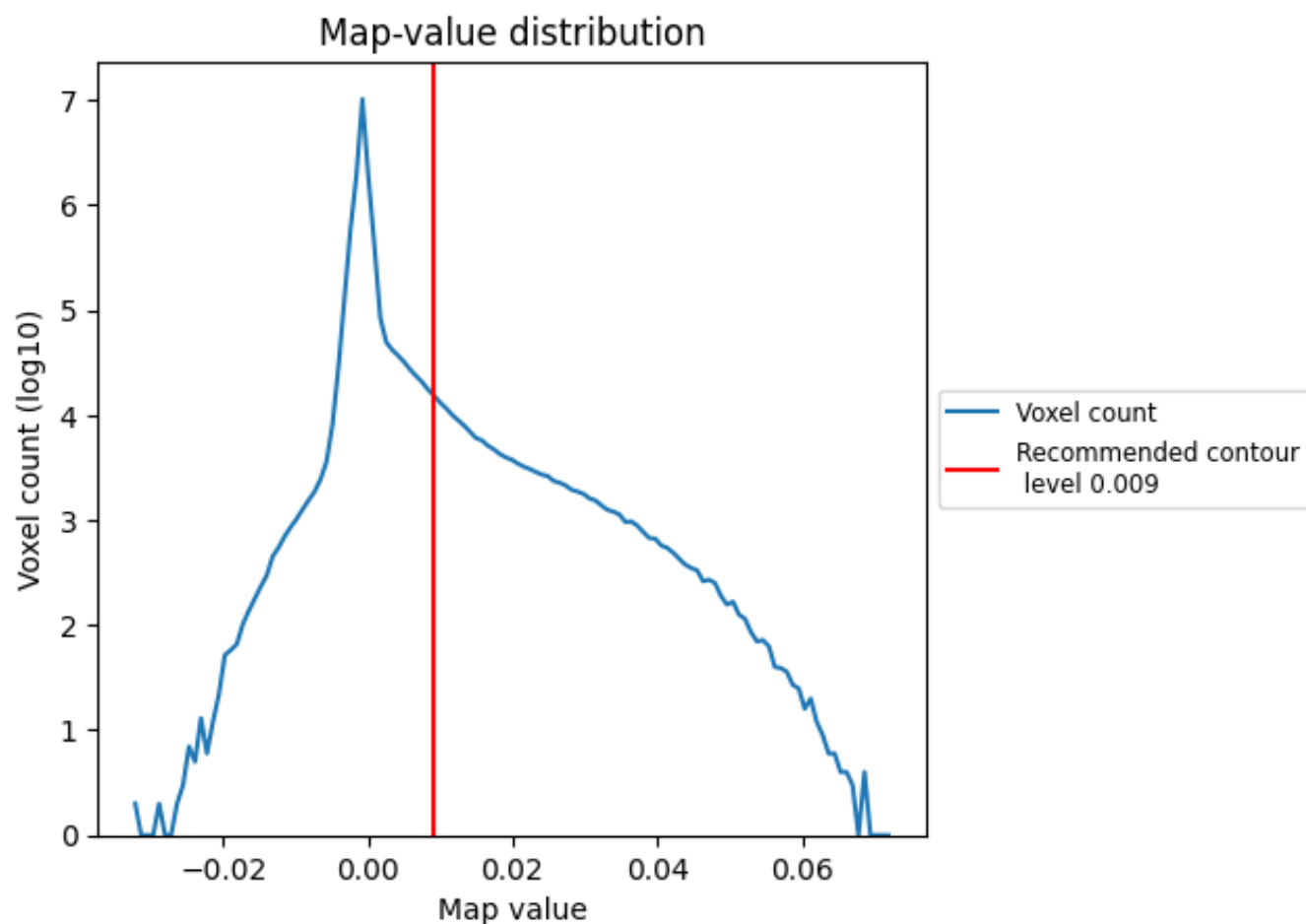
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

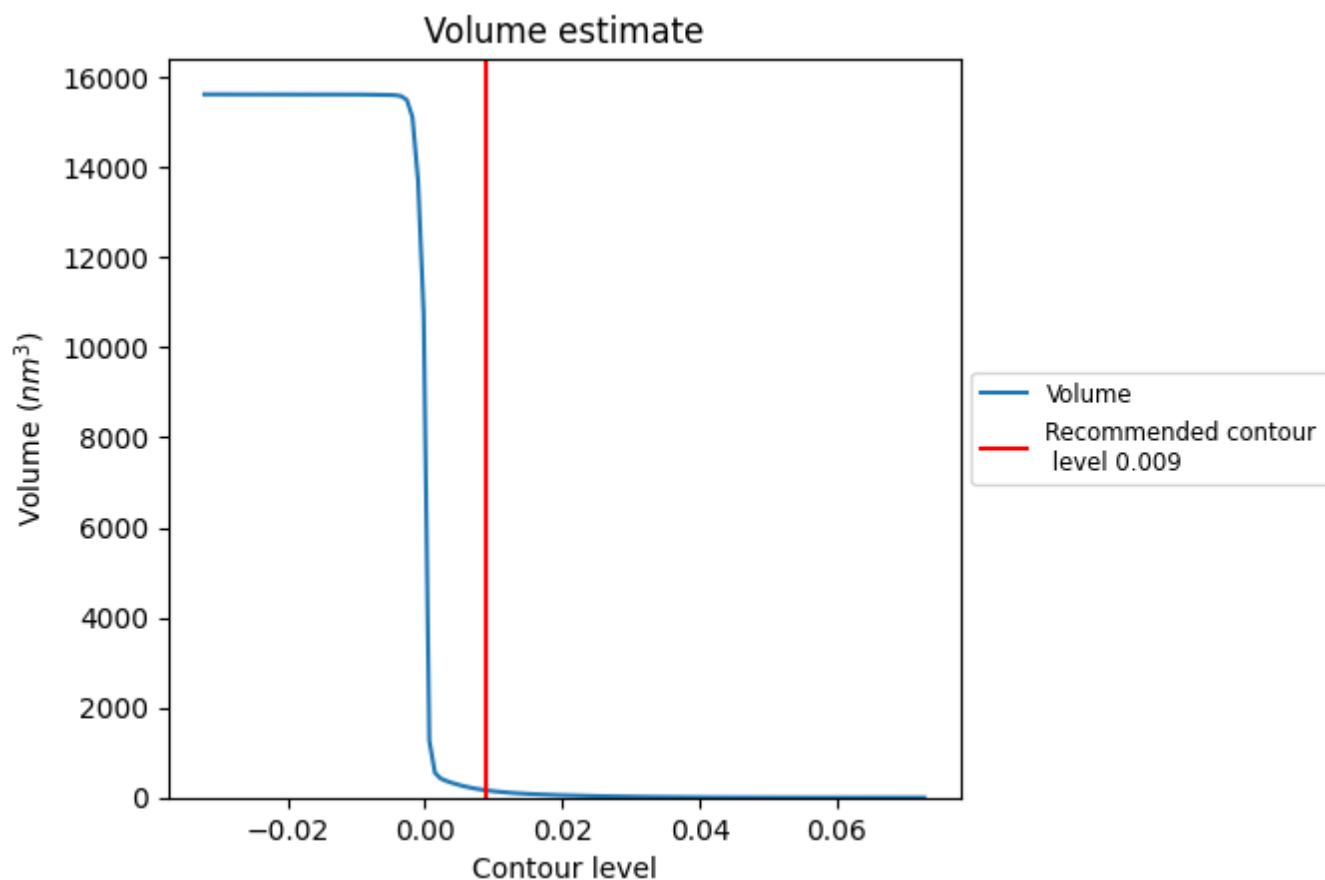
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

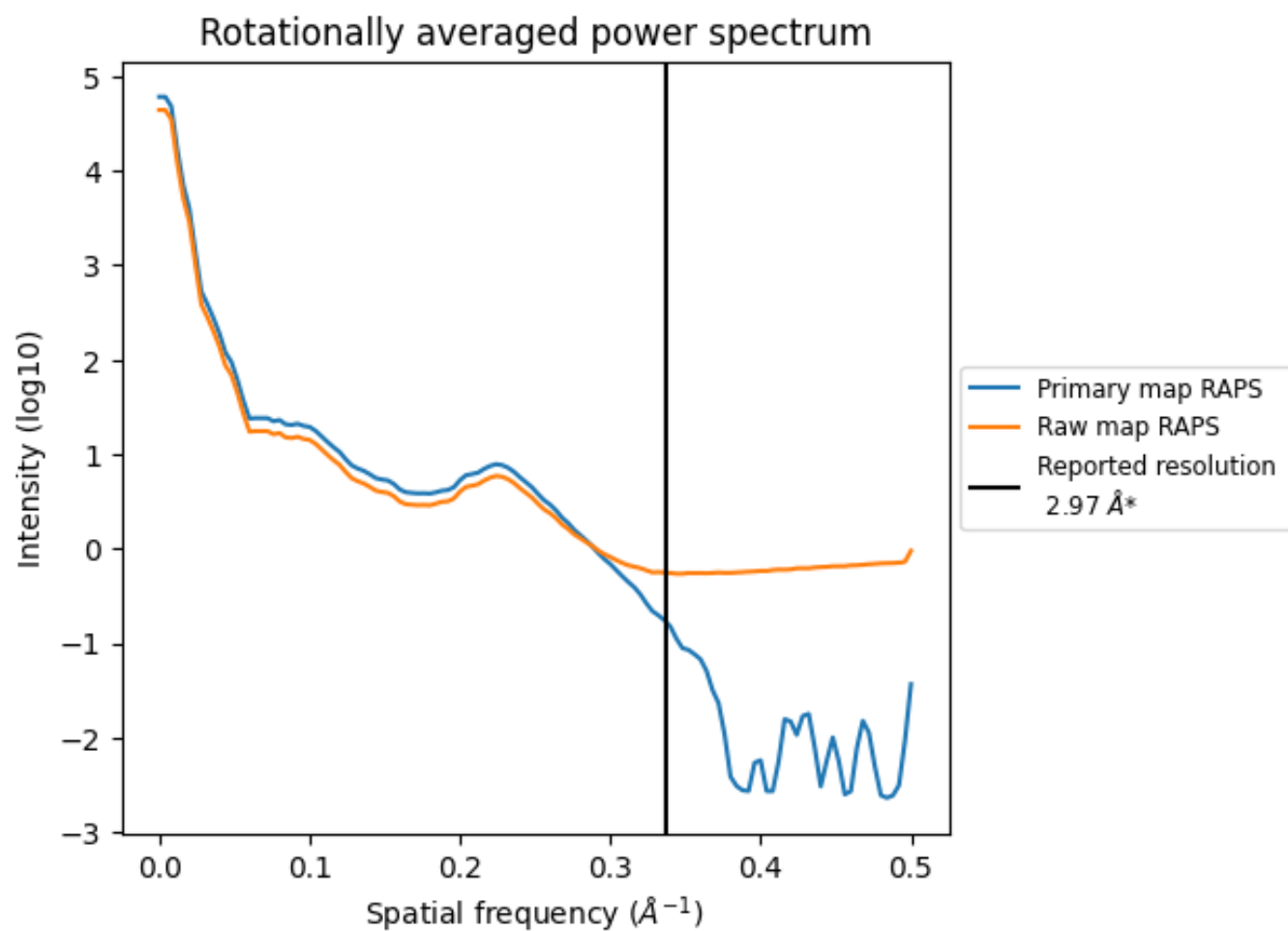
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm<sup>3</sup>; this corresponds to an approximate mass of 144 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 ⓘ

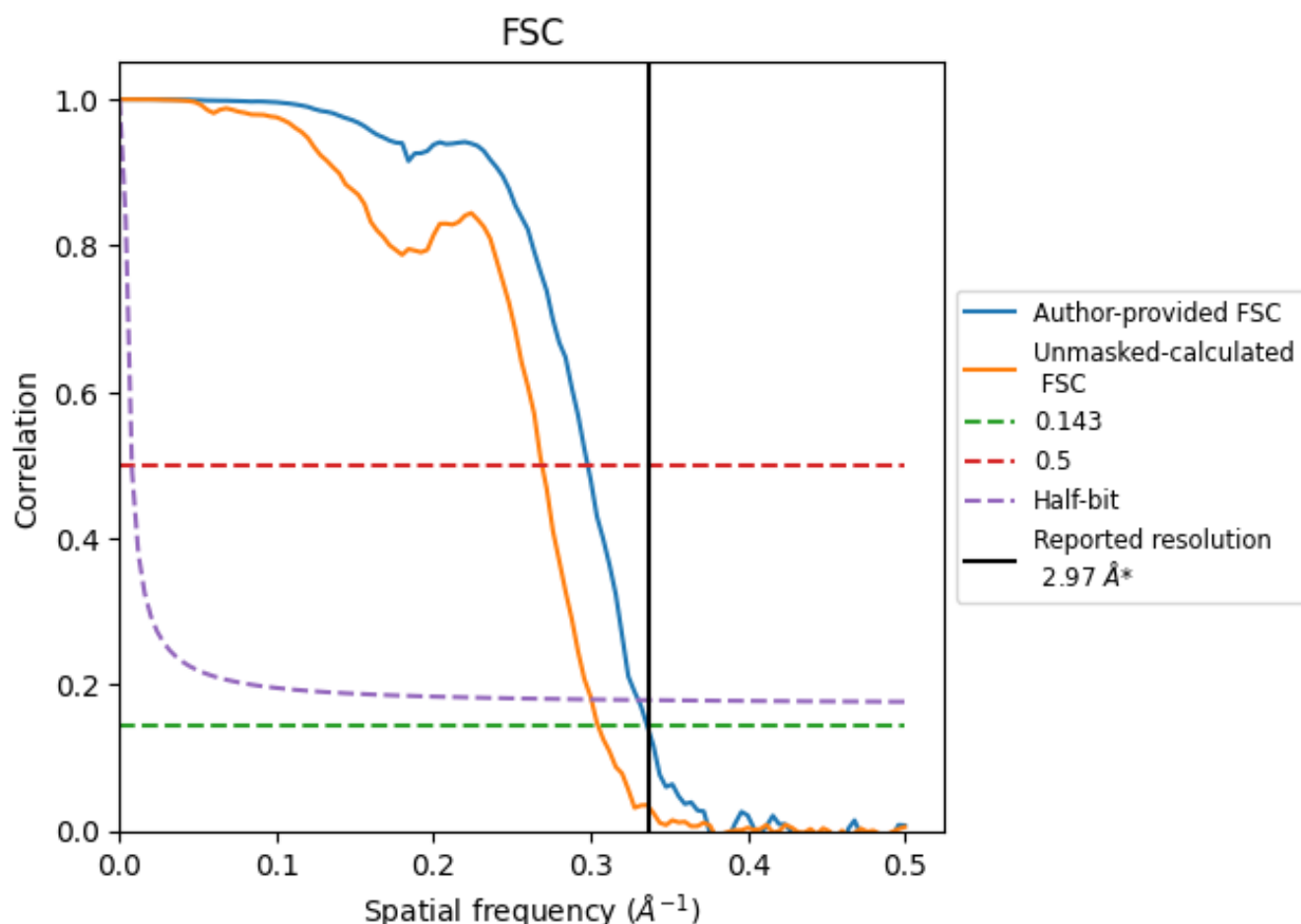


\*Reported resolution corresponds to spatial frequency of  $0.337 \text{ \AA}^{-1}$

## 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 0.337  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

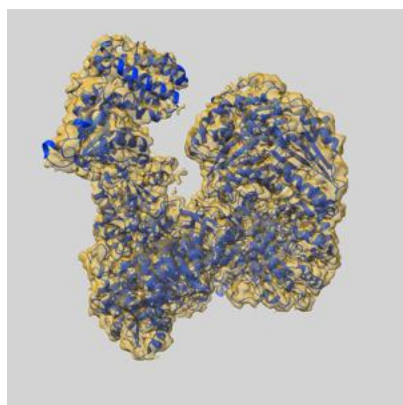
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.98	3.35	3.03
Unmasked-calculated*	3.28	3.72	3.33

\*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 3.28 differs from the reported value 2.97 by more than 10 %

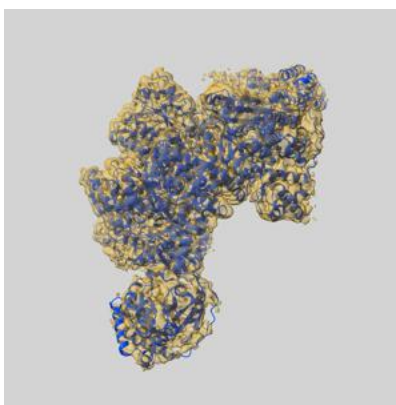
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31198 and PDB model 7EMY. Per-residue inclusion information can be found in section [3](#) on page [7](#).

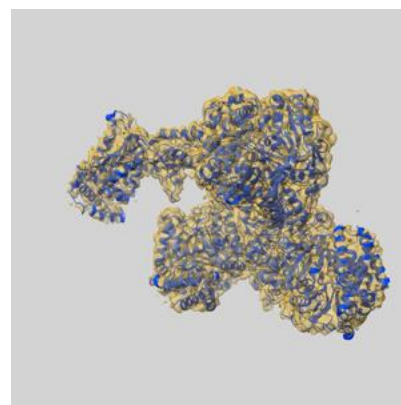
### 9.1 Map-model overlay [i](#)



X



Y

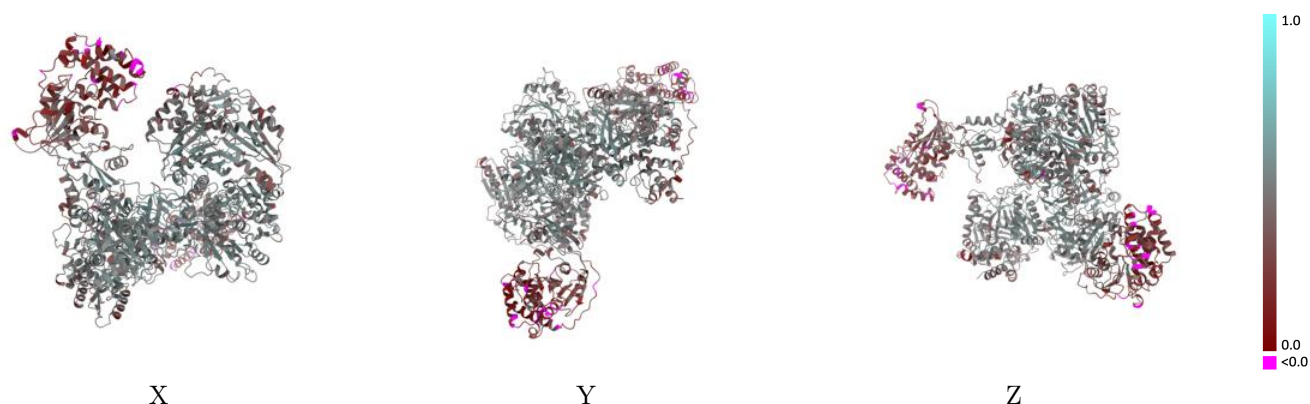


Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

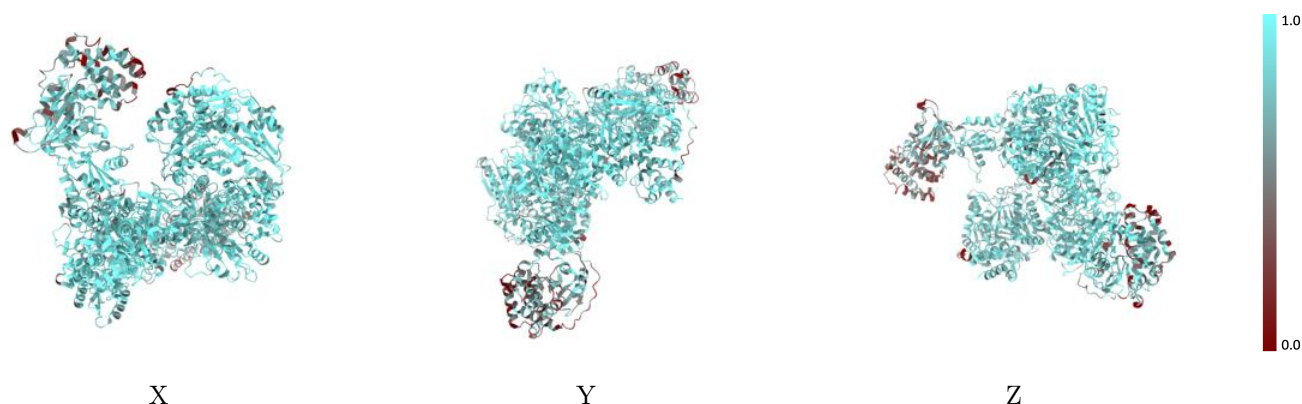


## 9.2 Q-score mapped to coordinate model [i](#)



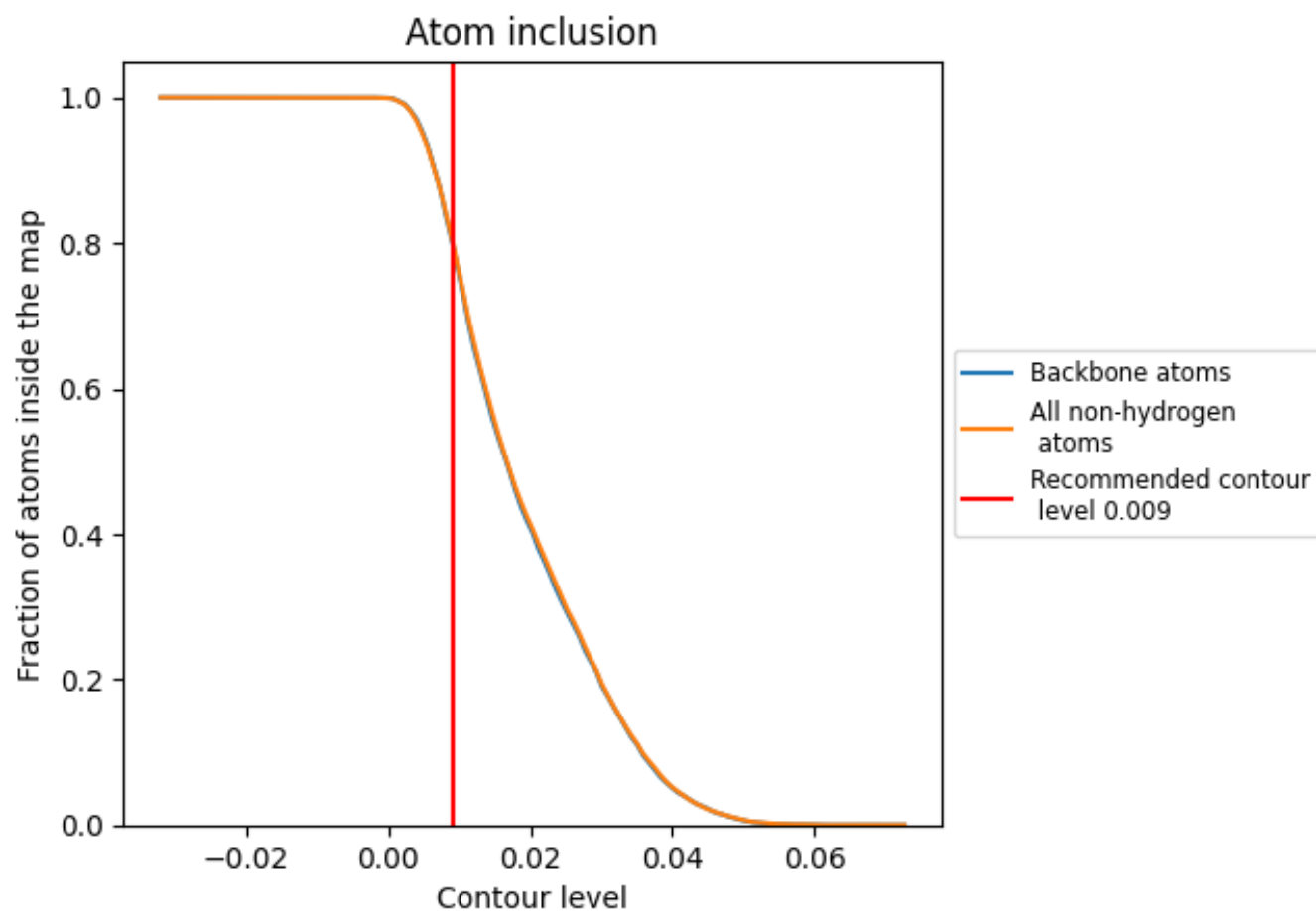
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8034	<div></div> 0.4300
A	<div></div> 0.7897	<div></div> 0.4220
B	<div></div> 0.8520	<div></div> 0.4380

