



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:08 AM UTC

PDB ID : 6OLA / pdb_00006ola
EMDB ID : EMD-20113
Title : Structure of the PCV2d virus-like particle
Authors : Khayat, R.; Wen, K.; Alimova, A.; Galarza, J.; Gottlieb, P.
Deposited on : 2019-04-16
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

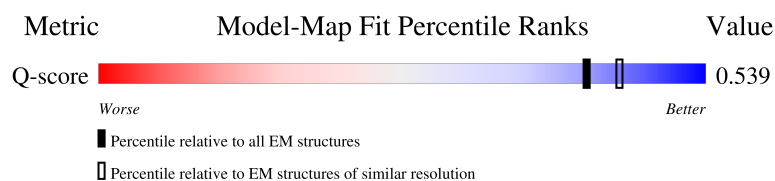
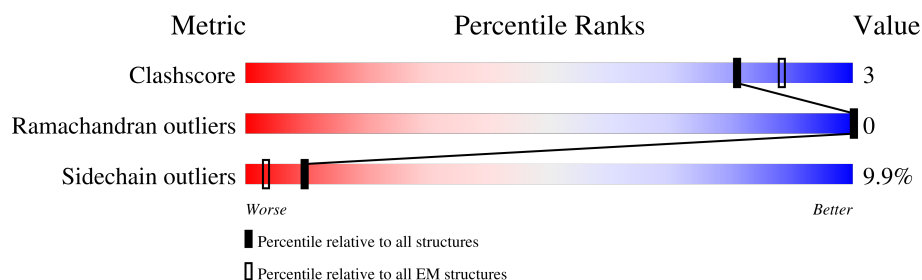
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	196	
1	A1	196	
1	A2	196	
1	A3	196	

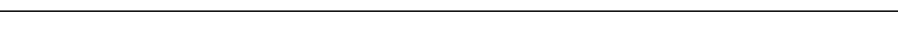
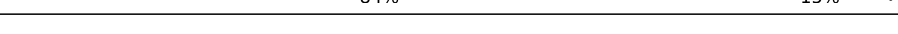
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Mol	Chain	Length	Quality of chain
1	A4	196	 83% 16% .
1	A5	196	 84% 15% .
1	A6	196	 85% 14% .
1	A7	196	 84% 15% .
1	A8	196	 83% 16% .
1	A9	196	 84% 15% .
1	AA	196	 84% 15% .
1	AB	196	 85% 14% .
1	AC	196	 84% 15% .
1	AD	196	 84% 15% .
1	AE	196	 84% 15% .
1	AF	196	 84% 15% .
1	AG	196	 84% 15% .
1	AH	196	 84% 15% .
1	AI	196	 84% 15% .
1	AJ	196	 85% 14% .
1	AK	196	 84% 15% .
1	AL	196	 85% 14% .
1	AM	196	 83% 16% .
1	AN	196	 84% 15% .
1	AO	196	 83% 16% .
1	AP	196	 83% 16% .
1	AQ	196	 83% 16% .
1	AR	196	 85% 14% .
1	AS	196	 84% 15% .

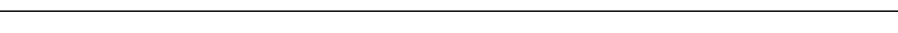
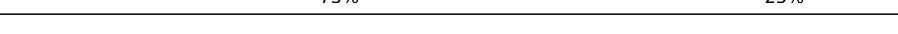
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Mol	Chain	Length	Quality of chain	
1	AT	196		.
1	AU	196		.
1	AV	196		.
1	AW	196		.
1	AX	196		.
1	AY	196		.
1	AZ	196		.
1	Aa	196		.
1	Ab	196		.
1	Ac	196		.
1	Ad	196		.
1	Ae	196		.
1	Af	196		.
1	Ag	196		.
1	Ah	196		.
1	Ai	196		.
1	Aj	196		.
1	Ak	196		.
1	Al	196		.
1	Am	196		.
1	An	196		.
1	Ao	196		.
1	Ap	196		.
1	Aq	196		.
1	Ar	196		.

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Mol	Chain	Length	Quality of chain
1	As	196	 84% 15% .
1	At	196	 84% 15% .
1	Au	196	 85% 14% .
1	Av	196	 84% 15% .
1	Aw	196	 85% 14% .
1	Ax	196	 84% 15% .
2	B0	4	 50% 50%
2	B1	4	 75% 25%
2	B2	4	 50% 50%
2	B3	4	 50% 50%
2	B4	4	 75% 25%
2	B5	4	 50% 50%
2	B6	4	 75% 25%
2	B7	4	 75% 25%
2	B8	4	 75% 25%
2	B9	4	 50% 50%
2	BA	4	 50% 50%
2	BB	4	 50% 50%
2	BC	4	 75% 25%
2	BD	4	 50% 50%
2	BE	4	 50% 50%
2	BF	4	 75% 25%
2	BG	4	 50% 50%
2	BH	4	 50% 50%
2	BI	4	 50% 50%

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Mol	Chain	Length	Quality of chain	
2	BJ	4		50%
2	BK	4		50%
2	BL	4		50%
2	BM	4		50%
2	BN	4		50%
2	BO	4		50%
2	BP	4		50%
2	BQ	4		50%
2	BR	4		50%
2	BS	4		75%
2	BT	4		50%
2	BU	4		50%
2	BV	4		50%
2	BW	4		50%
2	BX	4		50%
2	BY	4		50%
2	BZ	4		75%
2	Ba	4		50%
2	Bb	4		50%
2	Bc	4		50%
2	Bd	4		50%
2	Be	4		50%
2	Bf	4		50%
2	Bg	4		50%
2	Bh	4		50%

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Mol	Chain	Length	Quality of chain
2	Bi	4	50% 50%
2	Bj	4	50% 50%
2	Bk	4	50% 50%
2	Bl	4	75% 25%
2	Bm	4	50% 50%
2	Bn	4	50% 50%
2	Bo	4	50% 50%
2	Bp	4	50% 50%
2	Bq	4	50% 50%
2	Br	4	75% 25%
2	Bs	4	50% 50%
2	Bt	4	50% 50%
2	Bu	4	50% 50%
2	Bv	4	50% 50%
2	Bw	4	75% 25%
2	Bx	4	75% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 200820 atoms, of which 97920 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A0	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A1	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A2	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A3	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A4	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A5	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A6	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A7	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A8	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	A9	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	AA	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	AB	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	AC	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	AD	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	AE	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	AF	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		
1	AG	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	AH	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AI	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AJ	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AK	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AL	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AM	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AN	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AO	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AP	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AQ	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AR	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AS	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AT	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AU	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AV	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AW	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AX	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AY	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	AZ	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Aa	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ab	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ac	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ad	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ae	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Af	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ag	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ah	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ai	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Aj	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ak	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Al	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Am	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	An	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ao	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ap	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Aq	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Ar	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	As	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	At	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Au	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Av	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0
1	Aw	196	Total 3220	C 1046	H 1587	N 289	O 294	S 4	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ax	196	Total	C	H	N	O	S	0	0
			3220	1046	1587	289	294	4		

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B0	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B1	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B2	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B3	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B4	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B5	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B6	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B7	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B8	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	B9	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BA	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BB	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BC	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BD	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BE	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BF	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BG	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		
2	BH	4	Total	C	H	N	O	P	0	0
			127	38	45	16	24	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	BI	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BJ	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BK	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BL	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BM	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BN	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BO	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BP	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BQ	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BR	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BS	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BT	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BU	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BV	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BW	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BX	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BY	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	BZ	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Ba	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bb	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bc	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0

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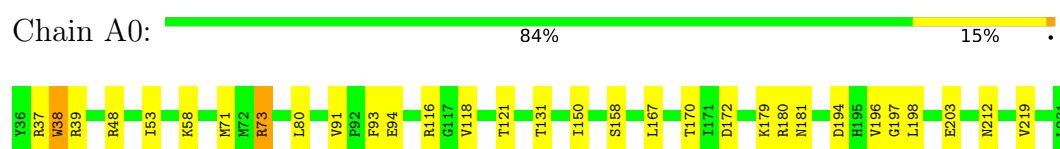
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Mol	Chain	Residues	Atoms						AltConf	Trace
2	Bd	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Be	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bf	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bg	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bh	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bi	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bj	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bk	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bl	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bm	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bn	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bo	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bp	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bq	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Br	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bs	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bt	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bu	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bv	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bw	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0
2	Bx	4	Total 127	C 38	H 45	N 16	O 24	P 4	0	0

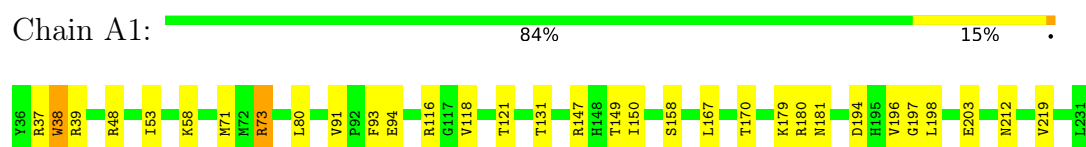
3 Residue-property plots

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

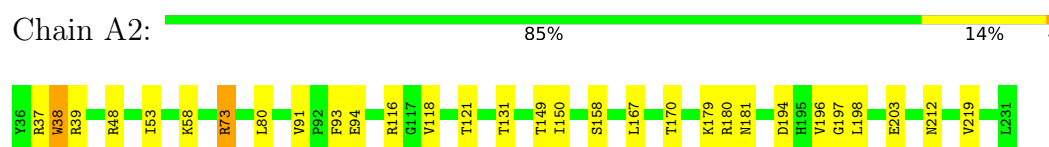
- Molecule 1: Capsid protein



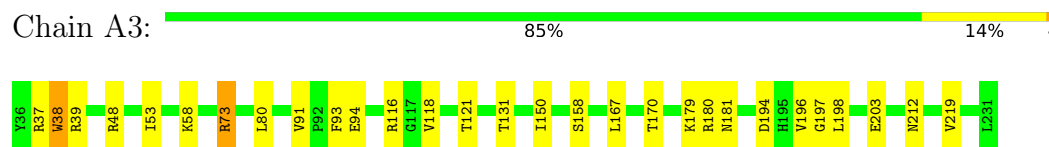
- Molecule 1: Capsid protein



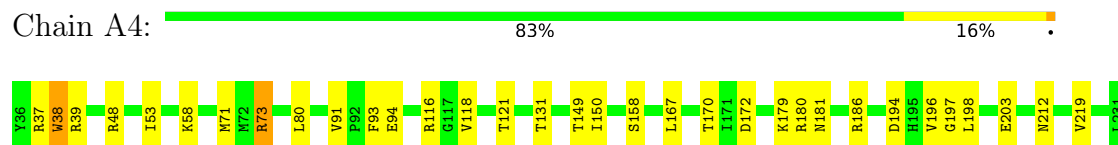
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

Chain A5:  84% 15% .



• Molecule 1: Capsid protein

Chain A6:  85% 14% .



• Molecule 1: Capsid protein

Chain A7:  84% 15% .



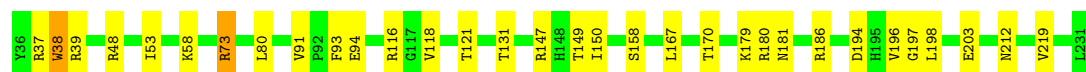
• Molecule 1: Capsid protein

Chain A8:  83% 16% .



• Molecule 1: Capsid protein

Chain A9:  84% 15% .



• Molecule 1: Capsid protein

Chain AA:  84% 15% .

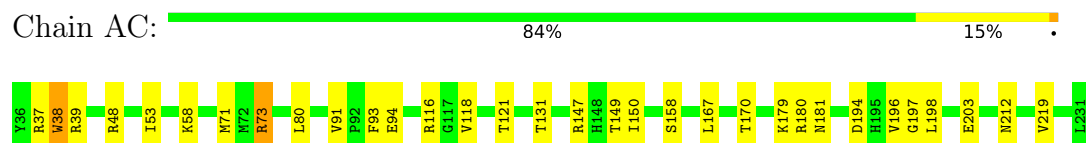


• Molecule 1: Capsid protein

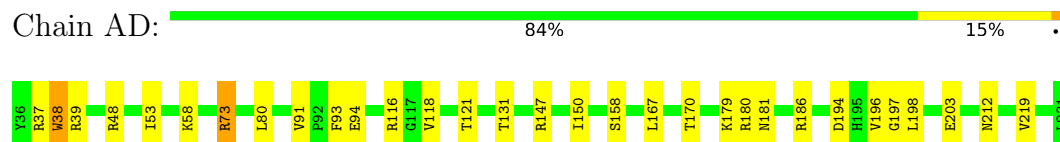
Chain AB:  85% 14% .



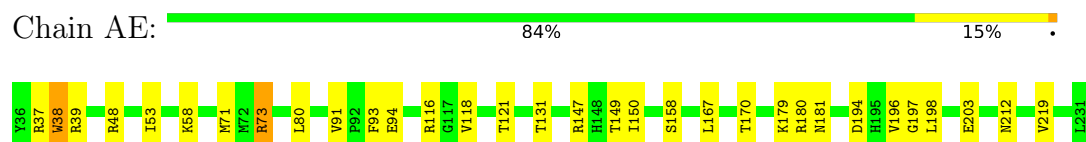
• Molecule 1: Capsid protein



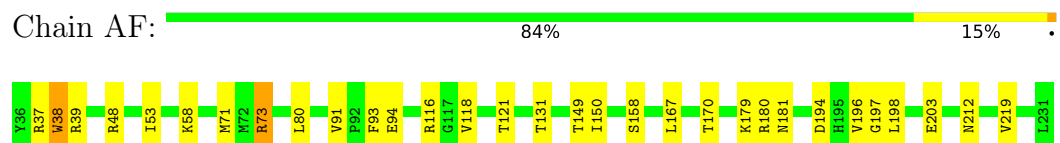
- Molecule 1: Capsid protein



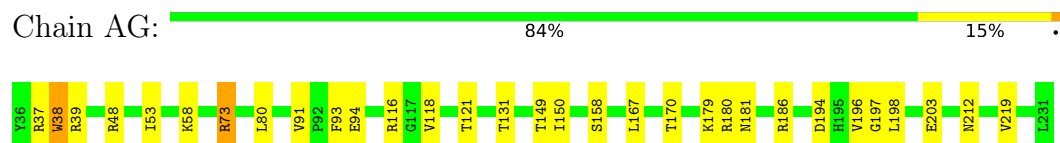
- Molecule 1: Capsid protein



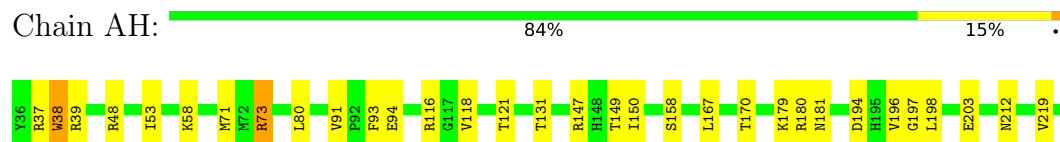
- Molecule 1: Capsid protein



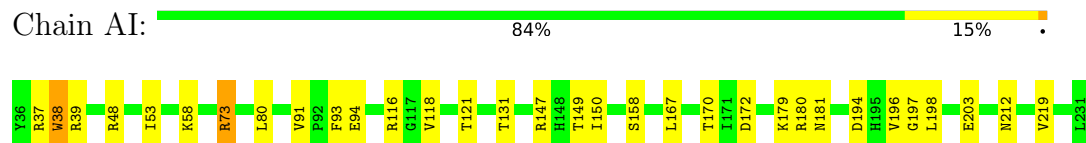
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



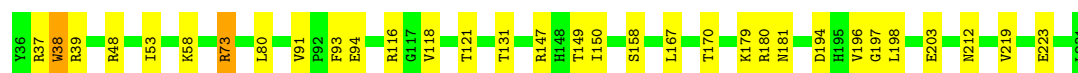
- Molecule 1: Capsid protein

Chain AJ:  85% 14%



- Molecule 1: Capsid protein

Chain AK:  84% 15%



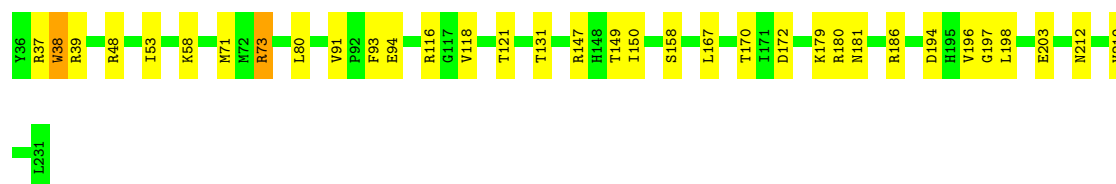
- Molecule 1: Capsid protein

Chain AL:  85% 14%



- Molecule 1: Capsid protein

Chain AM:  83% 16%



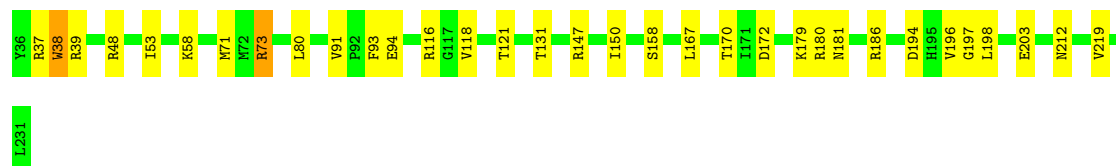
- Molecule 1: Capsid protein

Chain AN:  84% 15%



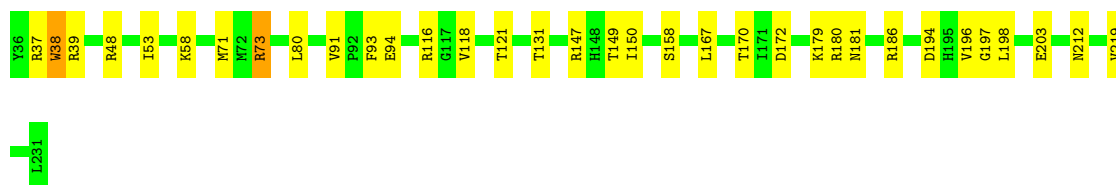
- Molecule 1: Capsid protein

Chain AO:  83% 16%



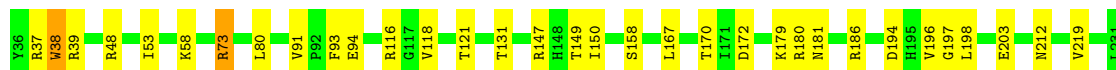
- Molecule 1: Capsid protein

Chain AP:  83% 16%



- Molecule 1: Capsid protein

Chain AQ: 83% 16%



- Molecule 1: Capsid protein

Chain AR: 85% 14%



- Molecule 1: Capsid protein

Chain AS: 84% 15%



- Molecule 1: Capsid protein

Chain AT: 84% 15%



- Molecule 1: Capsid protein

Chain AU: 84% 15%



- Molecule 1: Capsid protein

Chain AV: 84% 15%



- Molecule 1: Capsid protein

Chain AW:  83% 16% .



- Molecule 1: Capsid protein

Chain AX:  83% 16% .



- Molecule 1: Capsid protein

Chain AY:  83% 16% .



- Molecule 1: Capsid protein

Chain AZ:  83% 16% .



- Molecule 1: Capsid protein

Chain Aa:  83% 16% .



- Molecule 1: Capsid protein

Chain Ab:  85% 14% .



- Molecule 1: Capsid protein

Chain Ac:  84% 15% .



- Molecule 1: Capsid protein

Chain Ad:  84% 15%



- Molecule 1: Capsid protein

Chain Ae:  85% 14%



- Molecule 1: Capsid protein

Chain Af:  84% 15%



- Molecule 1: Capsid protein

Chain Ag:  84% 15%



- Molecule 1: Capsid protein

Chain Ah:  84% 15%



- Molecule 1: Capsid protein

Chain Ai:  85% 14%



- Molecule 1: Capsid protein

Chain Aj:  85% 14%



- Molecule 1: Capsid protein

Chain Ak:  84% 15% .



• Molecule 1: Capsid protein

Chain Al:  84% 15% .



• Molecule 1: Capsid protein

Chain Am:  84% 15% .



• Molecule 1: Capsid protein

Chain An:  84% 15% .



• Molecule 1: Capsid protein

Chain Ao:  85% 14% .



• Molecule 1: Capsid protein

Chain Ap:  83% 16% .



• Molecule 1: Capsid protein

Chain Aq:  84% 15% .



• Molecule 1: Capsid protein

Chain Ar:  84% 15% .



• Molecule 1: Capsid protein

Chain As:  84% 15% .



• Molecule 1: Capsid protein

Chain At:  84% 15% .



• Molecule 1: Capsid protein

Chain Au:  85% 14% .



• Molecule 1: Capsid protein

Chain Av:  84% 15% .



• Molecule 1: Capsid protein

Chain Aw:  85% 14% .



• Molecule 1: Capsid protein

Chain Ax:  84% 15% .



• Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B0:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B1:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B2:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B3:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B4:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B5:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B6:  75% 25%

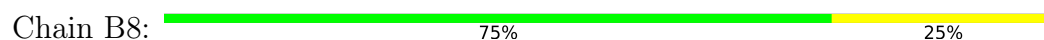


- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain B7:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



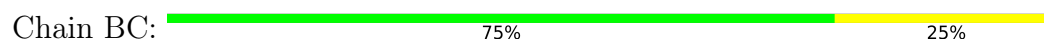
- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BF:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BG:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BH:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BI:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BJ:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BK:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BL:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BM:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BU:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BV:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BW:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BX:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BY:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain BZ:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Ba:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bb:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bj:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bk:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bl:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bm:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bn:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bo:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bp:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bq:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Br:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bs:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bt:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bu:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bv:  50% 50%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bw:  75% 25%



- Molecule 2: DNA (5'-D(P*CP*CP*GP*G)-3')

Chain Bx:  75% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4442	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A0	0.52	0/1682	0.67	4/2289 (0.2%)
1	A1	0.53	0/1682	0.67	4/2289 (0.2%)
1	A2	0.53	0/1682	0.67	4/2289 (0.2%)
1	A3	0.53	0/1682	0.67	4/2289 (0.2%)
1	A4	0.53	0/1682	0.67	4/2289 (0.2%)
1	A5	0.53	0/1682	0.67	4/2289 (0.2%)
1	A6	0.53	0/1682	0.67	4/2289 (0.2%)
1	A7	0.53	0/1682	0.67	4/2289 (0.2%)
1	A8	0.53	0/1682	0.67	4/2289 (0.2%)
1	A9	0.53	0/1682	0.67	4/2289 (0.2%)
1	AA	0.52	0/1682	0.67	4/2289 (0.2%)
1	AB	0.53	0/1682	0.67	4/2289 (0.2%)
1	AC	0.53	0/1682	0.67	4/2289 (0.2%)
1	AD	0.52	0/1682	0.67	4/2289 (0.2%)
1	AE	0.53	0/1682	0.67	4/2289 (0.2%)
1	AF	0.53	0/1682	0.67	4/2289 (0.2%)
1	AG	0.53	0/1682	0.67	4/2289 (0.2%)
1	AH	0.53	0/1682	0.67	4/2289 (0.2%)
1	AI	0.53	0/1682	0.67	4/2289 (0.2%)
1	AJ	0.53	0/1682	0.67	4/2289 (0.2%)
1	AK	0.53	0/1682	0.67	4/2289 (0.2%)
1	AL	0.53	0/1682	0.67	4/2289 (0.2%)
1	AM	0.53	0/1682	0.67	4/2289 (0.2%)
1	AN	0.53	0/1682	0.67	4/2289 (0.2%)
1	AO	0.53	0/1682	0.67	4/2289 (0.2%)
1	AP	0.53	0/1682	0.67	4/2289 (0.2%)
1	AQ	0.53	0/1682	0.67	4/2289 (0.2%)
1	AR	0.53	0/1682	0.67	4/2289 (0.2%)
1	AS	0.53	0/1682	0.67	4/2289 (0.2%)
1	AT	0.53	0/1682	0.67	4/2289 (0.2%)
1	AU	0.53	0/1682	0.67	4/2289 (0.2%)
1	AV	0.53	0/1682	0.67	4/2289 (0.2%)
1	AW	0.53	0/1682	0.67	4/2289 (0.2%)
1	AX	0.53	0/1682	0.67	4/2289 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AY	0.53	0/1682	0.67	4/2289 (0.2%)
1	AZ	0.53	0/1682	0.67	4/2289 (0.2%)
1	Aa	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ab	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ac	0.52	0/1682	0.67	4/2289 (0.2%)
1	Ad	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ae	0.53	0/1682	0.67	4/2289 (0.2%)
1	Af	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ag	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ah	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ai	0.53	0/1682	0.67	4/2289 (0.2%)
1	Aj	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ak	0.53	0/1682	0.67	4/2289 (0.2%)
1	Al	0.53	0/1682	0.67	4/2289 (0.2%)
1	Am	0.53	0/1682	0.67	4/2289 (0.2%)
1	An	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ao	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ap	0.53	0/1682	0.67	4/2289 (0.2%)
1	Aq	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ar	0.53	0/1682	0.67	4/2289 (0.2%)
1	As	0.53	0/1682	0.67	4/2289 (0.2%)
1	At	0.53	0/1682	0.67	4/2289 (0.2%)
1	Au	0.53	0/1682	0.67	4/2289 (0.2%)
1	Av	0.53	0/1682	0.67	4/2289 (0.2%)
1	Aw	0.53	0/1682	0.67	4/2289 (0.2%)
1	Ax	0.52	0/1682	0.67	4/2289 (0.2%)
2	B0	0.42	0/91	0.68	0/138
2	B1	0.42	0/91	0.68	0/138
2	B2	0.42	0/91	0.68	0/138
2	B3	0.42	0/91	0.68	0/138
2	B4	0.42	0/91	0.68	0/138
2	B5	0.42	0/91	0.68	0/138
2	B6	0.42	0/91	0.68	0/138
2	B7	0.42	0/91	0.68	0/138
2	B8	0.42	0/91	0.68	0/138
2	B9	0.42	0/91	0.68	0/138
2	BA	0.42	0/91	0.68	0/138
2	BB	0.42	0/91	0.68	0/138
2	BC	0.42	0/91	0.68	0/138
2	BD	0.42	0/91	0.68	0/138
2	BE	0.42	0/91	0.68	0/138
2	BF	0.42	0/91	0.68	0/138
2	BG	0.42	0/91	0.68	0/138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BH	0.42	0/91	0.68	0/138
2	BI	0.42	0/91	0.68	0/138
2	BJ	0.42	0/91	0.68	0/138
2	BK	0.42	0/91	0.68	0/138
2	BL	0.42	0/91	0.68	0/138
2	BM	0.42	0/91	0.68	0/138
2	BN	0.42	0/91	0.68	0/138
2	BO	0.42	0/91	0.68	0/138
2	BP	0.42	0/91	0.68	0/138
2	BQ	0.42	0/91	0.68	0/138
2	BR	0.42	0/91	0.68	0/138
2	BS	0.42	0/91	0.68	0/138
2	BT	0.42	0/91	0.68	0/138
2	BU	0.42	0/91	0.68	0/138
2	BV	0.42	0/91	0.68	0/138
2	BW	0.42	0/91	0.68	0/138
2	BX	0.42	0/91	0.68	0/138
2	BY	0.42	0/91	0.68	0/138
2	BZ	0.42	0/91	0.68	0/138
2	Ba	0.42	0/91	0.68	0/138
2	Bb	0.42	0/91	0.68	0/138
2	Bc	0.42	0/91	0.68	0/138
2	Bd	0.42	0/91	0.68	0/138
2	Be	0.42	0/91	0.68	0/138
2	Bf	0.42	0/91	0.68	0/138
2	Bg	0.42	0/91	0.68	0/138
2	Bh	0.42	0/91	0.68	0/138
2	Bi	0.42	0/91	0.68	0/138
2	Bj	0.42	0/91	0.68	0/138
2	Bk	0.42	0/91	0.68	0/138
2	Bl	0.42	0/91	0.68	0/138
2	Bm	0.42	0/91	0.68	0/138
2	Bn	0.42	0/91	0.68	0/138
2	Bo	0.42	0/91	0.68	0/138
2	Bp	0.42	0/91	0.68	0/138
2	Bq	0.42	0/91	0.68	0/138
2	Br	0.42	0/91	0.68	0/138
2	Bs	0.42	0/91	0.68	0/138
2	Bt	0.42	0/91	0.68	0/138
2	Bu	0.42	0/91	0.68	0/138
2	Bv	0.42	0/91	0.68	0/138
2	Bw	0.42	0/91	0.68	0/138
2	Bx	0.42	0/91	0.68	0/138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.52	0/106380	0.67	240/145620 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A0	0	1
1	A1	0	1
1	A2	0	1
1	A3	0	1
1	A4	0	1
1	A5	0	1
1	A6	0	1
1	A7	0	1
1	A8	0	1
1	A9	0	1
1	AA	0	1
1	AB	0	1
1	AC	0	1
1	AD	0	1
1	AE	0	1
1	AF	0	1
1	AG	0	1
1	AH	0	1
1	AI	0	1
1	AJ	0	1
1	AK	0	1
1	AL	0	1
1	AM	0	1
1	AN	0	1
1	AO	0	1
1	AP	0	1
1	AQ	0	1
1	AR	0	1
1	AS	0	1
1	AT	0	1
1	AU	0	1
1	AV	0	1
1	AW	0	1
1	AX	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	AY	0	1
1	AZ	0	1
1	Aa	0	1
1	Ab	0	1
1	Ac	0	1
1	Ad	0	1
1	Ae	0	1
1	Af	0	1
1	Ag	0	1
1	Ah	0	1
1	Ai	0	1
1	Aj	0	1
1	Ak	0	1
1	Al	0	1
1	Am	0	1
1	An	0	1
1	Ao	0	1
1	Ap	0	1
1	Aq	0	1
1	Ar	0	1
1	As	0	1
1	At	0	1
1	Au	0	1
1	Av	0	1
1	Aw	0	1
1	Ax	0	1
All	All	0	60

There are no bond length outliers.

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A9	38	TRP	CA-C-N	14.07	148.41	121.54
1	A9	38	TRP	C-N-CA	14.07	148.41	121.54
1	Ao	38	TRP	CA-C-N	14.07	148.41	121.54
1	Ao	38	TRP	C-N-CA	14.07	148.41	121.54
1	A4	38	TRP	CA-C-N	14.06	148.40	121.54
1	A4	38	TRP	C-N-CA	14.06	148.40	121.54
1	A7	38	TRP	CA-C-N	14.06	148.40	121.54
1	A7	38	TRP	C-N-CA	14.06	148.40	121.54
1	Aa	38	TRP	CA-C-N	14.06	148.40	121.54
1	Aa	38	TRP	C-N-CA	14.06	148.40	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AO	38	TRP	CA-C-N	14.06	148.39	121.54
1	AO	38	TRP	C-N-CA	14.06	148.39	121.54
1	AY	38	TRP	CA-C-N	14.06	148.39	121.54
1	AY	38	TRP	C-N-CA	14.06	148.39	121.54
1	AH	38	TRP	CA-C-N	14.05	148.37	121.54
1	AH	38	TRP	C-N-CA	14.05	148.37	121.54
1	AV	38	TRP	CA-C-N	14.05	148.37	121.54
1	AV	38	TRP	C-N-CA	14.05	148.37	121.54
1	AF	38	TRP	CA-C-N	14.04	148.36	121.54
1	AF	38	TRP	C-N-CA	14.04	148.36	121.54
1	AI	38	TRP	CA-C-N	14.04	148.37	121.54
1	AI	38	TRP	C-N-CA	14.04	148.37	121.54
1	Aw	38	TRP	CA-C-N	14.04	148.37	121.54
1	Aw	38	TRP	C-N-CA	14.04	148.37	121.54
1	An	38	TRP	CA-C-N	14.04	148.36	121.54
1	An	38	TRP	C-N-CA	14.04	148.36	121.54
1	As	38	TRP	CA-C-N	14.04	148.36	121.54
1	As	38	TRP	C-N-CA	14.04	148.36	121.54
1	AP	38	TRP	CA-C-N	14.04	148.35	121.54
1	AP	38	TRP	C-N-CA	14.04	148.35	121.54
1	AT	38	TRP	CA-C-N	14.04	148.36	121.54
1	AT	38	TRP	C-N-CA	14.04	148.36	121.54
1	Al	38	TRP	CA-C-N	14.04	148.36	121.54
1	Al	38	TRP	C-N-CA	14.04	148.36	121.54
1	Ad	38	TRP	CA-C-N	14.04	148.35	121.54
1	Ad	38	TRP	C-N-CA	14.04	148.35	121.54
1	Ae	38	TRP	CA-C-N	14.04	148.35	121.54
1	Ae	38	TRP	C-N-CA	14.04	148.35	121.54
1	A3	38	TRP	CA-C-N	14.04	148.35	121.54
1	A3	38	TRP	C-N-CA	14.04	148.35	121.54
1	AC	38	TRP	CA-C-N	14.04	148.35	121.54
1	Av	38	TRP	CA-C-N	14.04	148.35	121.54
1	A2	38	TRP	CA-C-N	14.03	148.34	121.54
1	A2	38	TRP	C-N-CA	14.03	148.34	121.54
1	A8	38	TRP	CA-C-N	14.04	148.35	121.54
1	A8	38	TRP	C-N-CA	14.04	148.35	121.54
1	AC	38	TRP	C-N-CA	14.04	148.35	121.54
1	Av	38	TRP	C-N-CA	14.04	148.35	121.54
1	AR	38	TRP	CA-C-N	14.03	148.35	121.54
1	AR	38	TRP	C-N-CA	14.03	148.35	121.54
1	AG	38	TRP	CA-C-N	14.03	148.34	121.54
1	AG	38	TRP	C-N-CA	14.03	148.34	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AJ	38	TRP	CA-C-N	14.03	148.34	121.54
1	AJ	38	TRP	C-N-CA	14.03	148.34	121.54
1	Aj	38	TRP	CA-C-N	14.03	148.34	121.54
1	Aj	38	TRP	C-N-CA	14.03	148.34	121.54
1	AN	38	TRP	CA-C-N	14.03	148.34	121.54
1	AN	38	TRP	C-N-CA	14.03	148.34	121.54
1	At	38	TRP	CA-C-N	14.03	148.34	121.54
1	At	38	TRP	C-N-CA	14.03	148.34	121.54
1	A6	38	TRP	CA-C-N	14.03	148.33	121.54
1	A6	38	TRP	C-N-CA	14.03	148.33	121.54
1	Af	38	TRP	CA-C-N	14.03	148.34	121.54
1	Af	38	TRP	C-N-CA	14.03	148.34	121.54
1	A0	38	TRP	CA-C-N	14.03	148.33	121.54
1	A0	38	TRP	C-N-CA	14.03	148.33	121.54
1	Ap	38	TRP	CA-C-N	14.03	148.33	121.54
1	Ap	38	TRP	C-N-CA	14.03	148.33	121.54
1	Am	38	TRP	CA-C-N	14.02	148.33	121.54
1	Am	38	TRP	C-N-CA	14.02	148.33	121.54
1	A1	38	TRP	CA-C-N	14.02	148.32	121.54
1	A1	38	TRP	C-N-CA	14.02	148.32	121.54
1	Ac	38	TRP	CA-C-N	14.02	148.32	121.54
1	Ac	38	TRP	C-N-CA	14.02	148.32	121.54
1	Ai	38	TRP	CA-C-N	14.02	148.32	121.54
1	Ai	38	TRP	C-N-CA	14.02	148.32	121.54
1	AK	38	TRP	CA-C-N	14.02	148.32	121.54
1	AK	38	TRP	C-N-CA	14.02	148.32	121.54
1	AW	38	TRP	CA-C-N	14.02	148.32	121.54
1	AW	38	TRP	C-N-CA	14.02	148.32	121.54
1	AB	38	TRP	CA-C-N	14.02	148.32	121.54
1	AB	38	TRP	C-N-CA	14.02	148.32	121.54
1	AS	38	TRP	CA-C-N	14.02	148.31	121.54
1	AS	38	TRP	C-N-CA	14.02	148.31	121.54
1	Ab	38	TRP	CA-C-N	14.02	148.31	121.54
1	Ab	38	TRP	C-N-CA	14.02	148.31	121.54
1	Ah	38	TRP	CA-C-N	14.01	148.31	121.54
1	Ah	38	TRP	C-N-CA	14.01	148.31	121.54
1	AE	38	TRP	CA-C-N	14.01	148.30	121.54
1	AE	38	TRP	C-N-CA	14.01	148.30	121.54
1	Ax	38	TRP	CA-C-N	14.01	148.30	121.54
1	Ax	38	TRP	C-N-CA	14.01	148.30	121.54
1	AZ	38	TRP	CA-C-N	14.01	148.30	121.54
1	AZ	38	TRP	C-N-CA	14.01	148.30	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ak	38	TRP	CA-C-N	14.01	148.30	121.54
1	Ak	38	TRP	C-N-CA	14.01	148.30	121.54
1	AM	38	TRP	CA-C-N	14.01	148.29	121.54
1	AM	38	TRP	C-N-CA	14.01	148.29	121.54
1	AD	38	TRP	CA-C-N	14.01	148.29	121.54
1	AD	38	TRP	C-N-CA	14.01	148.29	121.54
1	AU	38	TRP	CA-C-N	14.01	148.29	121.54
1	AU	38	TRP	C-N-CA	14.01	148.29	121.54
1	Au	38	TRP	CA-C-N	14.01	148.29	121.54
1	Au	38	TRP	C-N-CA	14.01	148.29	121.54
1	AA	38	TRP	CA-C-N	14.00	148.29	121.54
1	AA	38	TRP	C-N-CA	14.00	148.29	121.54
1	AL	38	TRP	CA-C-N	14.00	148.29	121.54
1	AL	38	TRP	C-N-CA	14.00	148.29	121.54
1	AX	38	TRP	CA-C-N	14.00	148.28	121.54
1	AX	38	TRP	C-N-CA	14.00	148.28	121.54
1	Ag	38	TRP	CA-C-N	14.00	148.28	121.54
1	Ag	38	TRP	C-N-CA	14.00	148.28	121.54
1	AQ	38	TRP	CA-C-N	14.00	148.28	121.54
1	AQ	38	TRP	C-N-CA	14.00	148.28	121.54
1	Ar	38	TRP	CA-C-N	14.00	148.28	121.54
1	Ar	38	TRP	C-N-CA	14.00	148.28	121.54
1	A5	38	TRP	CA-C-N	14.00	148.27	121.54
1	A5	38	TRP	C-N-CA	14.00	148.27	121.54
1	Aq	38	TRP	CA-C-N	13.99	148.26	121.54
1	Aq	38	TRP	C-N-CA	13.99	148.26	121.54
1	A8	39	ARG	CA-C-N	5.23	131.11	121.70
1	A8	39	ARG	C-N-CA	5.23	131.11	121.70
1	AQ	39	ARG	CA-C-N	5.23	131.11	121.70
1	AQ	39	ARG	C-N-CA	5.23	131.11	121.70
1	Ar	39	ARG	CA-C-N	5.23	131.11	121.70
1	Ar	39	ARG	C-N-CA	5.23	131.11	121.70
1	Ax	39	ARG	CA-C-N	5.23	131.11	121.70
1	Ax	39	ARG	C-N-CA	5.23	131.11	121.70
1	AW	39	ARG	CA-C-N	5.22	131.10	121.70
1	AW	39	ARG	C-N-CA	5.22	131.10	121.70
1	Af	39	ARG	CA-C-N	5.22	131.10	121.70
1	Af	39	ARG	C-N-CA	5.22	131.10	121.70
1	AI	39	ARG	CA-C-N	5.22	131.10	121.70
1	AI	39	ARG	C-N-CA	5.22	131.10	121.70
1	AO	39	ARG	CA-C-N	5.22	131.10	121.70
1	AO	39	ARG	C-N-CA	5.22	131.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	An	39	ARG	CA-C-N	5.22	131.10	121.70
1	An	39	ARG	C-N-CA	5.22	131.10	121.70
1	Ao	39	ARG	CA-C-N	5.22	131.10	121.70
1	Ao	39	ARG	C-N-CA	5.22	131.10	121.70
1	A9	39	ARG	CA-C-N	5.22	131.10	121.70
1	A9	39	ARG	C-N-CA	5.22	131.10	121.70
1	Ac	39	ARG	CA-C-N	5.22	131.09	121.70
1	Ac	39	ARG	C-N-CA	5.22	131.09	121.70
1	Aj	39	ARG	CA-C-N	5.22	131.10	121.70
1	Aj	39	ARG	C-N-CA	5.22	131.10	121.70
1	AA	39	ARG	CA-C-N	5.22	131.09	121.70
1	AA	39	ARG	C-N-CA	5.22	131.09	121.70
1	AP	39	ARG	CA-C-N	5.22	131.09	121.70
1	AP	39	ARG	C-N-CA	5.22	131.09	121.70
1	Ab	39	ARG	CA-C-N	5.22	131.09	121.70
1	Ab	39	ARG	C-N-CA	5.22	131.09	121.70
1	Ak	39	ARG	CA-C-N	5.22	131.09	121.70
1	Ak	39	ARG	C-N-CA	5.22	131.09	121.70
1	Aw	39	ARG	CA-C-N	5.22	131.09	121.70
1	Aw	39	ARG	C-N-CA	5.22	131.09	121.70
1	AB	39	ARG	CA-C-N	5.21	131.09	121.70
1	AB	39	ARG	C-N-CA	5.21	131.09	121.70
1	AV	39	ARG	CA-C-N	5.21	131.09	121.70
1	AV	39	ARG	C-N-CA	5.21	131.09	121.70
1	AZ	39	ARG	CA-C-N	5.21	131.09	121.70
1	AZ	39	ARG	C-N-CA	5.21	131.09	121.70
1	Au	39	ARG	CA-C-N	5.21	131.09	121.70
1	Au	39	ARG	C-N-CA	5.21	131.09	121.70
1	AX	39	ARG	CA-C-N	5.21	131.08	121.70
1	AX	39	ARG	C-N-CA	5.21	131.08	121.70
1	Ae	39	ARG	CA-C-N	5.21	131.08	121.70
1	Ae	39	ARG	C-N-CA	5.21	131.08	121.70
1	A4	39	ARG	CA-C-N	5.21	131.08	121.70
1	A4	39	ARG	C-N-CA	5.21	131.08	121.70
1	AJ	39	ARG	CA-C-N	5.21	131.08	121.70
1	AJ	39	ARG	C-N-CA	5.21	131.08	121.70
1	AL	39	ARG	CA-C-N	5.21	131.08	121.70
1	AL	39	ARG	C-N-CA	5.21	131.08	121.70
1	AC	39	ARG	CA-C-N	5.21	131.08	121.70
1	AC	39	ARG	C-N-CA	5.21	131.08	121.70
1	Al	39	ARG	CA-C-N	5.21	131.08	121.70
1	Al	39	ARG	C-N-CA	5.21	131.08	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Am	39	ARG	CA-C-N	5.21	131.08	121.70
1	Am	39	ARG	C-N-CA	5.21	131.08	121.70
1	AK	39	ARG	CA-C-N	5.21	131.07	121.70
1	AK	39	ARG	C-N-CA	5.21	131.07	121.70
1	Ad	39	ARG	CA-C-N	5.21	131.07	121.70
1	Ad	39	ARG	C-N-CA	5.21	131.07	121.70
1	AS	39	ARG	CA-C-N	5.21	131.07	121.70
1	AS	39	ARG	C-N-CA	5.21	131.07	121.70
1	AU	39	ARG	CA-C-N	5.21	131.07	121.70
1	AU	39	ARG	C-N-CA	5.21	131.07	121.70
1	Ag	39	ARG	CA-C-N	5.21	131.07	121.70
1	Ag	39	ARG	C-N-CA	5.21	131.07	121.70
1	A3	39	ARG	CA-C-N	5.21	131.07	121.70
1	A3	39	ARG	C-N-CA	5.21	131.07	121.70
1	AE	39	ARG	CA-C-N	5.21	131.07	121.70
1	AE	39	ARG	C-N-CA	5.21	131.07	121.70
1	A0	39	ARG	CA-C-N	5.20	131.07	121.70
1	A0	39	ARG	C-N-CA	5.20	131.07	121.70
1	AN	39	ARG	CA-C-N	5.20	131.07	121.70
1	AN	39	ARG	C-N-CA	5.20	131.07	121.70
1	AT	39	ARG	CA-C-N	5.20	131.07	121.70
1	AT	39	ARG	C-N-CA	5.20	131.07	121.70
1	Ai	39	ARG	CA-C-N	5.20	131.07	121.70
1	Ai	39	ARG	C-N-CA	5.20	131.07	121.70
1	A1	39	ARG	CA-C-N	5.20	131.06	121.70
1	A1	39	ARG	C-N-CA	5.20	131.06	121.70
1	A2	39	ARG	CA-C-N	5.20	131.06	121.70
1	A2	39	ARG	C-N-CA	5.20	131.06	121.70
1	AF	39	ARG	CA-C-N	5.20	131.06	121.70
1	AF	39	ARG	C-N-CA	5.20	131.06	121.70
1	Ah	39	ARG	CA-C-N	5.20	131.06	121.70
1	Ah	39	ARG	C-N-CA	5.20	131.06	121.70
1	As	39	ARG	CA-C-N	5.20	131.06	121.70
1	As	39	ARG	C-N-CA	5.20	131.06	121.70
1	AM	39	ARG	CA-C-N	5.20	131.06	121.70
1	AM	39	ARG	C-N-CA	5.20	131.06	121.70
1	AR	39	ARG	CA-C-N	5.20	131.05	121.70
1	AR	39	ARG	C-N-CA	5.20	131.05	121.70
1	AY	39	ARG	CA-C-N	5.20	131.05	121.70
1	AY	39	ARG	C-N-CA	5.20	131.05	121.70
1	A5	39	ARG	CA-C-N	5.19	131.04	121.70
1	A5	39	ARG	C-N-CA	5.19	131.04	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A6	39	ARG	CA-C-N	5.19	131.04	121.70
1	A6	39	ARG	C-N-CA	5.19	131.04	121.70
1	AD	39	ARG	CA-C-N	5.19	131.05	121.70
1	AD	39	ARG	C-N-CA	5.19	131.05	121.70
1	AG	39	ARG	CA-C-N	5.19	131.04	121.70
1	AG	39	ARG	C-N-CA	5.19	131.04	121.70
1	AH	39	ARG	CA-C-N	5.19	131.04	121.70
1	AH	39	ARG	C-N-CA	5.19	131.04	121.70
1	Ap	39	ARG	CA-C-N	5.19	131.03	121.70
1	Ap	39	ARG	C-N-CA	5.19	131.03	121.70
1	Aa	39	ARG	CA-C-N	5.18	131.03	121.70
1	Aa	39	ARG	C-N-CA	5.18	131.03	121.70
1	At	39	ARG	CA-C-N	5.18	131.03	121.70
1	At	39	ARG	C-N-CA	5.18	131.03	121.70
1	Aq	39	ARG	CA-C-N	5.18	131.02	121.70
1	Aq	39	ARG	C-N-CA	5.18	131.02	121.70
1	A7	39	ARG	CA-C-N	5.17	131.00	121.70
1	A7	39	ARG	C-N-CA	5.17	131.00	121.70
1	Av	39	ARG	CA-C-N	5.16	131.00	121.70
1	Av	39	ARG	C-N-CA	5.16	131.00	121.70

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A0	38	TRP	Peptide
1	A1	38	TRP	Peptide
1	A2	38	TRP	Peptide
1	A3	38	TRP	Peptide
1	A4	38	TRP	Peptide
1	A5	38	TRP	Peptide
1	A6	38	TRP	Peptide
1	A7	38	TRP	Peptide
1	A8	38	TRP	Peptide
1	A9	38	TRP	Peptide
1	AA	38	TRP	Peptide
1	AB	38	TRP	Peptide
1	AC	38	TRP	Peptide
1	AD	38	TRP	Peptide
1	AE	38	TRP	Peptide
1	AF	38	TRP	Peptide
1	AG	38	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	AH	38	TRP	Peptide
1	AI	38	TRP	Peptide
1	AJ	38	TRP	Peptide
1	AK	38	TRP	Peptide
1	AL	38	TRP	Peptide
1	AM	38	TRP	Peptide
1	AN	38	TRP	Peptide
1	AO	38	TRP	Peptide
1	AP	38	TRP	Peptide
1	AQ	38	TRP	Peptide
1	AR	38	TRP	Peptide
1	AS	38	TRP	Peptide
1	AT	38	TRP	Peptide
1	AU	38	TRP	Peptide
1	AV	38	TRP	Peptide
1	AW	38	TRP	Peptide
1	AX	38	TRP	Peptide
1	AY	38	TRP	Peptide
1	AZ	38	TRP	Peptide
1	Aa	38	TRP	Peptide
1	Ab	38	TRP	Peptide
1	Ac	38	TRP	Peptide
1	Ad	38	TRP	Peptide
1	Ae	38	TRP	Peptide
1	Af	38	TRP	Peptide
1	Ag	38	TRP	Peptide
1	Ah	38	TRP	Peptide
1	Ai	38	TRP	Peptide
1	Aj	38	TRP	Peptide
1	Ak	38	TRP	Peptide
1	Al	38	TRP	Peptide
1	Am	38	TRP	Peptide
1	An	38	TRP	Peptide
1	Ao	38	TRP	Peptide
1	Ap	38	TRP	Peptide
1	Aq	38	TRP	Peptide
1	Ar	38	TRP	Peptide
1	As	38	TRP	Peptide
1	At	38	TRP	Peptide
1	Au	38	TRP	Peptide
1	Av	38	TRP	Peptide
1	Aw	38	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	Ax	38	TRP	Peptide

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	A0	1633	1587	1591	8	0
1	A1	1633	1587	1591	9	0
1	A2	1633	1587	1591	7	0
1	A3	1633	1587	1591	7	0
1	A4	1633	1587	1591	11	0
1	A5	1633	1587	1591	9	0
1	A6	1633	1587	1591	8	0
1	A7	1633	1587	1591	9	0
1	A8	1633	1587	1591	11	0
1	A9	1633	1587	1591	10	0
1	AA	1633	1587	1591	9	0
1	AB	1633	1587	1591	6	0
1	AC	1633	1587	1591	11	0
1	AD	1633	1587	1591	9	0
1	AE	1633	1587	1591	9	0
1	AF	1633	1587	1591	9	0
1	AG	1633	1587	1591	8	0
1	AH	1633	1587	1591	9	0
1	AI	1633	1587	1591	10	0
1	AJ	1633	1587	1591	7	0
1	AK	1633	1587	1591	9	0
1	AL	1633	1587	1591	7	0
1	AM	1633	1587	1591	11	0
1	AN	1633	1587	1591	8	0
1	AO	1633	1587	1591	11	0
1	AP	1633	1587	1591	11	0
1	AQ	1633	1587	1591	11	0
1	AR	1633	1587	1591	8	0
1	AS	1633	1587	1591	9	0
1	AT	1633	1587	1591	10	0
1	AU	1633	1587	1591	9	0
1	AV	1633	1587	1591	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AW	1633	1587	1591	10	0
1	AX	1633	1587	1591	10	0
1	AY	1633	1587	1591	10	0
1	AZ	1633	1587	1591	10	0
1	Aa	1633	1587	1591	11	0
1	Ab	1633	1587	1591	7	0
1	Ac	1633	1587	1591	9	0
1	Ad	1633	1587	1591	9	0
1	Ae	1633	1587	1591	7	0
1	Af	1633	1587	1591	10	0
1	Ag	1633	1587	1591	9	0
1	Ah	1633	1587	1591	10	0
1	Ai	1633	1587	1591	7	0
1	Aj	1633	1587	1591	9	0
1	Ak	1633	1587	1591	8	0
1	Al	1633	1587	1591	10	0
1	Am	1633	1587	1591	9	0
1	An	1633	1587	1591	8	0
1	Ao	1633	1587	1591	7	0
1	Ap	1633	1587	1591	10	0
1	Aq	1633	1587	1591	8	0
1	Ar	1633	1587	1591	9	0
1	As	1633	1587	1591	9	0
1	At	1633	1587	1591	10	0
1	Au	1633	1587	1591	8	0
1	Av	1633	1587	1591	8	0
1	Aw	1633	1587	1591	6	0
1	Ax	1633	1587	1591	10	0
2	B0	82	45	45	2	0
2	B1	82	45	45	1	0
2	B2	82	45	45	3	0
2	B3	82	45	45	2	0
2	B4	82	45	45	1	0
2	B5	82	45	45	3	0
2	B6	82	45	45	1	0
2	B7	82	45	45	1	0
2	B8	82	45	45	1	0
2	B9	82	45	45	4	0
2	BA	82	45	45	3	0
2	BB	82	45	45	3	0
2	BC	82	45	45	1	0
2	BD	82	45	45	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BE	82	45	45	2	0
2	BF	82	45	45	1	0
2	BG	82	45	45	2	0
2	BH	82	45	45	2	0
2	BI	82	45	45	3	0
2	BJ	82	45	45	3	0
2	BK	82	45	45	2	0
2	BL	82	45	45	3	0
2	BM	82	45	45	2	0
2	BN	82	45	45	3	0
2	BO	82	45	45	2	0
2	BP	82	45	45	2	0
2	BQ	82	45	45	3	0
2	BR	82	45	45	3	0
2	BS	82	45	45	1	0
2	BT	82	45	45	2	0
2	BU	82	45	45	2	0
2	BV	82	45	45	2	0
2	BW	82	45	45	2	0
2	BX	82	45	45	3	0
2	BY	82	45	45	3	0
2	BZ	82	45	45	1	0
2	Ba	82	45	45	3	0
2	Bb	82	45	45	3	0
2	Bc	82	45	45	2	0
2	Bd	82	45	45	2	0
2	Be	82	45	45	2	0
2	Bf	82	45	45	2	0
2	Bg	82	45	45	3	0
2	Bh	82	45	45	2	0
2	Bi	82	45	45	2	0
2	Bj	82	45	45	2	0
2	Bk	82	45	45	3	0
2	Bl	82	45	45	1	0
2	Bm	82	45	45	2	0
2	Bn	82	45	45	3	0
2	Bo	82	45	45	2	0
2	Bp	82	45	45	2	0
2	Bq	82	45	45	3	0
2	Br	82	45	45	1	0
2	Bs	82	45	45	2	0
2	Bt	82	45	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bu	82	45	45	2	0
2	Bv	82	45	45	2	0
2	Bw	82	45	45	1	0
2	Bx	82	45	45	1	0
All	All	102900	97920	98160	515	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 (515) 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:Af:121:THR:HG23	1:Af:150:ILE:HD11	1.54	0.90
1:Ax:121:THR:HG23	1:Ax:150:ILE:HD11	1.54	0.90
1:Aa:121:THR:HG23	1:Aa:150:ILE:HD11	1.54	0.90
1:Al:121:THR:HG23	1:Al:150:ILE:HD11	1.54	0.90
1:Aw:121:THR:HG23	1:Aw:150:ILE:HD11	1.54	0.89
1:Ae:121:THR:HG23	1:Ae:150:ILE:HD11	1.54	0.89
1:AB:121:THR:HG23	1:AB:150:ILE:HD11	1.54	0.89
1:AY:121:THR:HG23	1:AY:150:ILE:HD11	1.54	0.89
1:A1:121:THR:HG23	1:A1:150:ILE:HD11	1.54	0.89
1:AN:121:THR:HG23	1:AN:150:ILE:HD11	1.54	0.89
1:AH:121:THR:HG23	1:AH:150:ILE:HD11	1.54	0.88
1:Ab:121:THR:HG23	1:Ab:150:ILE:HD11	1.54	0.88
1:Ad:121:THR:HG23	1:Ad:150:ILE:HD11	1.54	0.88
1:Aq:121:THR:HG23	1:Aq:150:ILE:HD11	1.54	0.88
1:AI:121:THR:HG23	1:AI:150:ILE:HD11	1.54	0.88
1:Aj:121:THR:HG23	1:Aj:150:ILE:HD11	1.54	0.88
1:AS:121:THR:HG23	1:AS:150:ILE:HD11	1.54	0.88
1:A6:121:THR:HG23	1:A6:150:ILE:HD11	1.54	0.88
1:AT:121:THR:HG23	1:AT:150:ILE:HD11	1.54	0.88
1:A2:121:THR:HG23	1:A2:150:ILE:HD11	1.54	0.88
1:AC:121:THR:HG23	1:AC:150:ILE:HD11	1.54	0.88
1:AR:121:THR:HG23	1:AR:150:ILE:HD11	1.54	0.88
1:Ac:121:THR:HG23	1:Ac:150:ILE:HD11	1.54	0.88
1:Ah:121:THR:HG23	1:Ah:150:ILE:HD11	1.54	0.88
1:Am:121:THR:HG23	1:Am:150:ILE:HD11	1.54	0.88
1:A5:121:THR:HG23	1:A5:150:ILE:HD11	1.54	0.88
1:A7:121:THR:HG23	1:A7:150:ILE:HD11	1.54	0.88
1:A8:121:THR:HG23	1:A8:150:ILE:HD11	1.54	0.88
1:Av:121:THR:HG23	1:Av:150:ILE:HD11	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:121:THR:HG23	1:A0:150:ILE:HD11	1.54	0.88
1:AP:121:THR:HG23	1:AP:150:ILE:HD11	1.54	0.88
1:AU:121:THR:HG23	1:AU:150:ILE:HD11	1.54	0.88
1:An:121:THR:HG23	1:An:150:ILE:HD11	1.54	0.88
1:Ai:121:THR:HG23	1:Ai:150:ILE:HD11	1.54	0.88
1:A4:121:THR:HG23	1:A4:150:ILE:HD11	1.54	0.87
1:AG:121:THR:HG23	1:AG:150:ILE:HD11	1.54	0.87
1:AL:121:THR:HG23	1:AL:150:ILE:HD11	1.54	0.87
1:Ao:121:THR:HG23	1:Ao:150:ILE:HD11	1.54	0.87
1:Au:121:THR:HG23	1:Au:150:ILE:HD11	1.54	0.87
1:AK:121:THR:HG23	1:AK:150:ILE:HD11	1.54	0.87
1:AM:121:THR:HG23	1:AM:150:ILE:HD11	1.54	0.87
1:Ap:121:THR:HG23	1:Ap:150:ILE:HD11	1.54	0.87
1:As:121:THR:HG23	1:As:150:ILE:HD11	1.54	0.87
1:A3:121:THR:HG23	1:A3:150:ILE:HD11	1.54	0.87
1:AF:121:THR:HG23	1:AF:150:ILE:HD11	1.54	0.87
1:Ar:121:THR:HG23	1:Ar:150:ILE:HD11	1.54	0.87
1:AO:121:THR:HG23	1:AO:150:ILE:HD11	1.54	0.87
1:AW:121:THR:HG23	1:AW:150:ILE:HD11	1.54	0.87
1:AE:121:THR:HG23	1:AE:150:ILE:HD11	1.54	0.87
1:Ag:121:THR:HG23	1:Ag:150:ILE:HD11	1.54	0.87
1:At:121:THR:HG23	1:At:150:ILE:HD11	1.54	0.87
1:AJ:121:THR:HG23	1:AJ:150:ILE:HD11	1.54	0.86
1:AX:121:THR:HG23	1:AX:150:ILE:HD11	1.54	0.86
1:A9:121:THR:HG23	1:A9:150:ILE:HD11	1.54	0.86
1:AA:121:THR:HG23	1:AA:150:ILE:HD11	1.54	0.86
1:AD:121:THR:HG23	1:AD:150:ILE:HD11	1.54	0.86
1:AQ:121:THR:HG23	1:AQ:150:ILE:HD11	1.54	0.86
1:AV:121:THR:HG23	1:AV:150:ILE:HD11	1.54	0.86
1:Ak:121:THR:HG23	1:Ak:150:ILE:HD11	1.54	0.85
1:AZ:121:THR:HG23	1:AZ:150:ILE:HD11	1.54	0.85
1:AU:48:ARG:NH1	2:BU:358:DG:OP2	2.17	0.78
1:AW:48:ARG:NH1	2:BW:358:DG:OP2	2.17	0.78
1:A2:48:ARG:NH1	2:B2:358:DG:OP2	2.17	0.78
1:AC:48:ARG:NH1	2:BC:358:DG:OP2	2.17	0.78
1:AE:48:ARG:NH1	2:BE:358:DG:OP2	2.17	0.78
1:AQ:48:ARG:NH1	2:BQ:358:DG:OP2	2.17	0.78
1:Ad:48:ARG:NH1	2:Bd:358:DG:OP2	2.17	0.78
1:Ae:48:ARG:NH1	2:Be:358:DG:OP2	2.17	0.78
1:Au:48:ARG:NH1	2:Bu:358:DG:OP2	2.17	0.78
1:Aw:48:ARG:NH1	2:Bw:358:DG:OP2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:48:ARG:NH1	2:B5:358:DG:OP2	2.17	0.78
1:A6:48:ARG:NH1	2:B6:358:DG:OP2	2.17	0.78
1:A8:48:ARG:NH1	2:B8:358:DG:OP2	2.17	0.78
1:A9:48:ARG:NH1	2:B9:358:DG:OP2	2.17	0.78
1:AI:48:ARG:NH1	2:BI:358:DG:OP2	2.17	0.78
1:AL:48:ARG:NH1	2:BL:358:DG:OP2	2.17	0.78
1:AP:48:ARG:NH1	2:BP:358:DG:OP2	2.17	0.78
1:AR:48:ARG:NH1	2:BR:358:DG:OP2	2.17	0.78
1:AS:48:ARG:NH1	2:BS:358:DG:OP2	2.17	0.78
1:Ah:48:ARG:NH1	2:Bh:358:DG:OP2	2.17	0.78
1:Aj:48:ARG:NH1	2:Bj:358:DG:OP2	2.17	0.78
1:Ao:48:ARG:NH1	2:Bo:358:DG:OP2	2.17	0.78
1:Ar:48:ARG:NH1	2:Br:358:DG:OP2	2.17	0.78
1:AB:48:ARG:NH1	2:BB:358:DG:OP2	2.17	0.78
1:AO:48:ARG:NH1	2:BO:358:DG:OP2	2.17	0.78
1:AZ:48:ARG:NH1	2:BZ:358:DG:OP2	2.17	0.78
1:Ak:48:ARG:NH1	2:Bk:358:DG:OP2	2.17	0.78
1:AY:48:ARG:NH1	2:BY:358:DG:OP2	2.17	0.78
1:A1:48:ARG:NH1	2:B1:358:DG:OP2	2.17	0.77
1:AA:48:ARG:NH1	2:BA:358:DG:OP2	2.17	0.77
1:AD:48:ARG:NH1	2:BD:358:DG:OP2	2.17	0.77
1:AV:48:ARG:NH1	2:BV:358:DG:OP2	2.17	0.77
1:Ai:48:ARG:NH1	2:Bi:358:DG:OP2	2.17	0.77
1:Av:48:ARG:NH1	2:Bv:358:DG:OP2	2.17	0.77
1:A4:48:ARG:NH1	2:B4:358:DG:OP2	2.17	0.77
1:AF:48:ARG:NH1	2:BF:358:DG:OP2	2.17	0.77
1:AX:48:ARG:NH1	2:BX:358:DG:OP2	2.17	0.77
1:Ac:48:ARG:NH1	2:Bc:358:DG:OP2	2.17	0.77
1:An:48:ARG:NH1	2:Bn:358:DG:OP2	2.17	0.77
1:AH:48:ARG:NH1	2:BH:358:DG:OP2	2.17	0.77
1:AK:48:ARG:NH1	2:BK:358:DG:OP2	2.17	0.77
1:AN:48:ARG:NH1	2:BN:358:DG:OP2	2.17	0.77
1:Aa:48:ARG:NH1	2:Ba:358:DG:OP2	2.17	0.77
1:Al:48:ARG:NH1	2:Bl:358:DG:OP2	2.17	0.77
1:As:48:ARG:NH1	2:Bs:358:DG:OP2	2.17	0.77
1:Aq:48:ARG:NH1	2:Bq:358:DG:OP2	2.17	0.77
1:At:48:ARG:NH1	2:Bt:358:DG:OP2	2.17	0.77
1:AG:48:ARG:NH1	2:BG:358:DG:OP2	2.17	0.77
1:AJ:48:ARG:NH1	2:BJ:358:DG:OP2	2.17	0.77
1:Ag:48:ARG:NH1	2:Bg:358:DG:OP2	2.17	0.77
1:A0:48:ARG:NH1	2:B0:358:DG:OP2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:48:ARG:NH1	2:B3:358:DG:OP2	2.17	0.77
1:A7:48:ARG:NH1	2:B7:358:DG:OP2	2.17	0.77
1:Ab:48:ARG:NH1	2:Bb:358:DG:OP2	2.17	0.77
1:Am:48:ARG:NH1	2:Bm:358:DG:OP2	2.17	0.77
1:AT:48:ARG:NH1	2:BT:358:DG:OP2	2.17	0.77
1:Ax:48:ARG:NH1	2:Bx:358:DG:OP2	2.17	0.77
1:Af:48:ARG:NH1	2:Bf:358:DG:OP2	2.17	0.76
1:AM:48:ARG:NH1	2:BM:358:DG:OP2	2.17	0.76
1:Ap:48:ARG:NH1	2:Bp:358:DG:OP2	2.17	0.76
1:AC:149:THR:OG1	2:BD:357:DC:OP2	2.16	0.63
1:A8:149:THR:OG1	2:B9:357:DC:OP2	2.19	0.61
1:AX:172:ASP:OD2	1:Am:186:ARG:NH2	2.33	0.59
1:Ab:149:THR:OG1	2:Bc:357:DC:OP2	2.20	0.59
1:AD:186:ARG:NH2	1:Ah:172:ASP:OD2	2.35	0.58
1:Ac:149:THR:OG1	2:Bd:357:DC:OP2	2.21	0.58
1:AG:149:THR:OG1	2:BH:357:DC:OP2	2.22	0.57
1:AP:147:ARG:NH2	2:BQ:357:DC:OP2	2.39	0.56
1:AF:149:THR:OG1	2:BG:357:DC:OP2	2.22	0.55
1:An:149:THR:OG1	2:Bj:357:DC:OP2	2.26	0.54
1:AK:149:THR:OG1	2:BL:357:DC:OP2	2.26	0.54
1:Al:149:THR:OG1	2:Bm:357:DC:OP2	2.25	0.53
1:AT:149:THR:OG1	2:BP:357:DC:OP2	2.28	0.52
1:Af:149:THR:OG1	2:Bg:357:DC:OP2	2.27	0.52
1:A7:91:VAL:HG12	1:A7:93:PHE:HD2	1.75	0.52
1:A8:91:VAL:HG12	1:A8:93:PHE:HD2	1.75	0.52
1:AP:91:VAL:HG12	1:AP:93:PHE:HD2	1.75	0.52
1:AV:91:VAL:HG12	1:AV:93:PHE:HD2	1.75	0.52
1:AZ:149:THR:OG1	2:Ba:357:DC:OP2	2.28	0.52
1:AD:91:VAL:HG12	1:AD:93:PHE:HD2	1.75	0.52
1:AS:91:VAL:HG12	1:AS:93:PHE:HD2	1.75	0.52
1:AT:91:VAL:HG12	1:AT:93:PHE:HD2	1.75	0.52
1:Aq:91:VAL:HG12	1:Aq:93:PHE:HD2	1.75	0.52
1:Au:91:VAL:HG12	1:Au:93:PHE:HD2	1.75	0.52
1:A6:91:VAL:HG12	1:A6:93:PHE:HD2	1.75	0.52
1:AE:91:VAL:HG12	1:AE:93:PHE:HD2	1.75	0.52
1:AN:91:VAL:HG12	1:AN:93:PHE:HD2	1.75	0.52
1:AQ:91:VAL:HG12	1:AQ:93:PHE:HD2	1.75	0.52
1:AW:91:VAL:HG12	1:AW:93:PHE:HD2	1.75	0.52
1:Ah:91:VAL:HG12	1:Ah:93:PHE:HD2	1.75	0.52
1:Am:149:THR:OG1	2:Bn:357:DC:OP2	2.28	0.52
1:A3:91:VAL:HG12	1:A3:93:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:91:VAL:HG12	1:AJ:93:PHE:HD2	1.75	0.52
1:A9:91:VAL:HG12	1:A9:93:PHE:HD2	1.75	0.52
1:Ad:91:VAL:HG12	1:Ad:93:PHE:HD2	1.75	0.52
1:Ae:91:VAL:HG12	1:Ae:93:PHE:HD2	1.75	0.52
1:A0:91:VAL:HG12	1:A0:93:PHE:HD2	1.75	0.52
1:Ac:91:VAL:HG12	1:Ac:93:PHE:HD2	1.75	0.52
1:Aj:91:VAL:HG12	1:Aj:93:PHE:HD2	1.75	0.52
1:An:91:VAL:HG12	1:An:93:PHE:HD2	1.75	0.52
1:Ax:149:THR:OG1	2:Bt:357:DC:OP2	2.27	0.52
1:Aw:91:VAL:HG12	1:Aw:93:PHE:HD2	1.75	0.52
1:Ax:91:VAL:HG12	1:Ax:93:PHE:HD2	1.75	0.52
1:AG:91:VAL:HG12	1:AG:93:PHE:HD2	1.75	0.51
1:AI:91:VAL:HG12	1:AI:93:PHE:HD2	1.75	0.51
1:AX:91:VAL:HG12	1:AX:93:PHE:HD2	1.75	0.51
1:AY:91:VAL:HG12	1:AY:93:PHE:HD2	1.75	0.51
1:Aa:91:VAL:HG12	1:Aa:93:PHE:HD2	1.75	0.51
1:Af:91:VAL:HG12	1:Af:93:PHE:HD2	1.75	0.51
1:Al:91:VAL:HG12	1:Al:93:PHE:HD2	1.75	0.51
1:A2:91:VAL:HG12	1:A2:93:PHE:HD2	1.75	0.51
1:AB:91:VAL:HG12	1:AB:93:PHE:HD2	1.75	0.51
1:AZ:91:VAL:HG12	1:AZ:93:PHE:HD2	1.75	0.51
1:Ak:91:VAL:HG12	1:Ak:93:PHE:HD2	1.75	0.51
1:Ao:91:VAL:HG12	1:Ao:93:PHE:HD2	1.75	0.51
1:AL:91:VAL:HG12	1:AL:93:PHE:HD2	1.75	0.51
1:AA:91:VAL:HG12	1:AA:93:PHE:HD2	1.75	0.51
1:AH:91:VAL:HG12	1:AH:93:PHE:HD2	1.75	0.51
1:Ao:149:THR:OG1	2:Bp:357:DC:OP2	2.27	0.51
1:A1:91:VAL:HG12	1:A1:93:PHE:HD2	1.75	0.51
1:A5:91:VAL:HG12	1:A5:93:PHE:HD2	1.75	0.51
1:AK:91:VAL:HG12	1:AK:93:PHE:HD2	1.75	0.51
1:A4:91:VAL:HG12	1:A4:93:PHE:HD2	1.75	0.51
1:AC:91:VAL:HG12	1:AC:93:PHE:HD2	1.75	0.51
1:AF:91:VAL:HG12	1:AF:93:PHE:HD2	1.75	0.51
1:AR:91:VAL:HG12	1:AR:93:PHE:HD2	1.75	0.51
1:AU:91:VAL:HG12	1:AU:93:PHE:HD2	1.75	0.51
1:A1:149:THR:OG1	2:B2:357:DC:OP2	2.29	0.51
1:As:91:VAL:HG12	1:As:93:PHE:HD2	1.75	0.51
1:AO:91:VAL:HG12	1:AO:93:PHE:HD2	1.75	0.51
1:Ai:91:VAL:HG12	1:Ai:93:PHE:HD2	1.75	0.50
1:Aj:149:THR:OG1	2:Bk:357:DC:OP2	2.28	0.50
1:Ar:91:VAL:HG12	1:Ar:93:PHE:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:147:ARG:NH2	2:BE:357:DC:OP2	2.45	0.50
1:AM:91:VAL:HG12	1:AM:93:PHE:HD2	1.75	0.50
1:Ag:91:VAL:HG12	1:Ag:93:PHE:HD2	1.75	0.50
1:At:91:VAL:HG12	1:At:93:PHE:HD2	1.75	0.50
1:Av:91:VAL:HG12	1:Av:93:PHE:HD2	1.75	0.50
1:Am:91:VAL:HG12	1:Am:93:PHE:HD2	1.75	0.50
1:Ap:91:VAL:HG12	1:Ap:93:PHE:HD2	1.75	0.50
1:Ab:91:VAL:HG12	1:Ab:93:PHE:HD2	1.75	0.50
1:A4:149:THR:OG1	2:B0:357:DC:OP2	2.27	0.50
1:Ad:186:ARG:NH2	1:Av:172:ASP:OD2	2.44	0.49
1:AU:149:THR:OG1	2:BV:357:DC:OP2	2.30	0.49
1:As:172:ASP:OD2	1:At:186:ARG:NH2	2.43	0.49
1:AE:149:THR:OG1	2:BA:357:DC:OP2	2.30	0.49
1:AX:149:THR:OG1	2:BY:357:DC:OP2	2.29	0.49
1:AP:149:THR:OG1	2:BQ:357:DC:OP2	2.30	0.49
1:AI:149:THR:OG1	2:BJ:357:DC:OP2	2.31	0.48
1:AN:149:THR:OG1	2:BO:357:DC:OP2	2.31	0.48
1:Af:147:ARG:NH2	2:Bg:357:DC:OP2	2.47	0.48
1:AQ:147:ARG:NH2	2:BR:357:DC:OP2	2.46	0.48
1:AQ:149:THR:OG1	2:BR:357:DC:OP2	2.31	0.48
1:AM:147:ARG:NH2	2:BN:357:DC:OP2	2.47	0.48
1:AH:149:THR:OG1	2:BI:357:DC:OP2	2.29	0.47
1:A0:172:ASP:OD2	1:AM:186:ARG:NH2	2.47	0.47
1:Ah:149:THR:OG1	2:Bi:357:DC:OP2	2.28	0.47
1:A1:147:ARG:NH2	2:B2:357:DC:OP2	2.47	0.47
1:A9:147:ARG:NH2	2:B5:357:DC:OP2	2.47	0.47
1:AA:149:THR:OG1	2:BB:357:DC:OP2	2.31	0.47
1:Aq:118:VAL:N	1:Aq:203:GLU:OE1	2.47	0.47
1:AN:118:VAL:N	1:AN:203:GLU:OE1	2.47	0.46
1:A8:149:THR:HG1	2:B9:357:DC:P	2.36	0.46
1:AX:147:ARG:NH2	2:BY:357:DC:OP2	2.49	0.46
1:Am:118:VAL:N	1:Am:203:GLU:OE1	2.47	0.46
1:Ab:118:VAL:N	1:Ab:203:GLU:OE1	2.47	0.46
1:Am:147:ARG:NH2	2:Bn:357:DC:OP2	2.47	0.46
1:A2:149:THR:OG1	2:B3:357:DC:OP2	2.33	0.46
1:A4:172:ASP:OD2	1:A5:186:ARG:NH2	2.48	0.46
1:AM:149:THR:OG1	2:BN:357:DC:OP2	2.32	0.46
1:AU:186:ARG:NH2	1:Ad:172:ASP:OD2	2.48	0.46
1:AY:172:ASP:OD2	1:AZ:186:ARG:NH2	2.48	0.46
1:AE:147:ARG:NH2	2:BA:357:DC:OP2	2.49	0.46
1:AI:172:ASP:OD2	1:Ac:186:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:172:ASP:OD2	1:As:186:ARG:NH2	2.48	0.45
1:AB:118:VAL:N	1:AB:203:GLU:OE1	2.47	0.45
1:AO:147:ARG:NH2	2:BK:357:DC:OP2	2.49	0.45
1:AY:118:VAL:N	1:AY:203:GLU:OE1	2.47	0.45
1:Ao:196:VAL:HG22	1:Ao:197:GLY:H	1.82	0.45
1:Ap:196:VAL:HG22	1:Ap:197:GLY:H	1.82	0.45
1:AM:196:VAL:HG22	1:AM:197:GLY:H	1.82	0.45
1:AS:196:VAL:HG22	1:AS:197:GLY:H	1.82	0.45
1:AV:149:THR:OG1	2:BW:357:DC:OP2	2.32	0.45
1:At:196:VAL:HG22	1:At:197:GLY:H	1.82	0.45
1:A4:186:ARG:NH2	1:AW:172:ASP:OD2	2.49	0.45
1:A6:196:VAL:HG22	1:A6:197:GLY:H	1.82	0.45
1:AK:196:VAL:HG22	1:AK:197:GLY:H	1.82	0.45
1:AL:196:VAL:HG22	1:AL:197:GLY:H	1.82	0.45
1:AP:196:VAL:HG22	1:AP:197:GLY:H	1.82	0.45
1:Ae:196:VAL:HG22	1:Ae:197:GLY:H	1.82	0.45
1:An:196:VAL:HG22	1:An:197:GLY:H	1.82	0.45
1:As:196:VAL:HG22	1:As:197:GLY:H	1.82	0.45
1:A8:196:VAL:HG22	1:A8:197:GLY:H	1.82	0.45
1:Ac:196:VAL:HG22	1:Ac:197:GLY:H	1.82	0.45
1:Ag:196:VAL:HG22	1:Ag:197:GLY:H	1.82	0.45
1:A9:149:THR:OG1	2:B5:357:DC:OP2	2.34	0.45
1:AZ:196:VAL:HG22	1:AZ:197:GLY:H	1.82	0.45
1:Ab:196:VAL:HG22	1:Ab:197:GLY:H	1.82	0.45
1:Ax:196:VAL:HG22	1:Ax:197:GLY:H	1.82	0.45
1:A9:186:ARG:NH2	1:AM:172:ASP:OD2	2.50	0.45
1:AA:196:VAL:HG22	1:AA:197:GLY:H	1.82	0.45
1:AB:196:VAL:HG22	1:AB:197:GLY:H	1.82	0.45
1:AO:172:ASP:OD2	1:AP:186:ARG:NH2	2.46	0.45
1:Af:196:VAL:HG22	1:Af:197:GLY:H	1.82	0.45
1:Ak:196:VAL:HG22	1:Ak:197:GLY:H	1.82	0.45
1:Am:196:VAL:HG22	1:Am:197:GLY:H	1.82	0.45
1:Aw:196:VAL:HG22	1:Aw:197:GLY:H	1.82	0.45
1:A0:196:VAL:HG22	1:A0:197:GLY:H	1.82	0.45
1:A9:196:VAL:HG22	1:A9:197:GLY:H	1.82	0.45
1:AN:196:VAL:HG22	1:AN:197:GLY:H	1.82	0.45
1:AX:196:VAL:HG22	1:AX:197:GLY:H	1.82	0.45
1:Aq:196:VAL:HG22	1:Aq:197:GLY:H	1.82	0.45
1:A7:196:VAL:HG22	1:A7:197:GLY:H	1.82	0.45
1:AO:118:VAL:N	1:AO:203:GLU:OE1	2.47	0.45
1:AQ:121:THR:CG2	1:AQ:150:ILE:HD11	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:196:VAL:HG22	1:AQ:197:GLY:H	1.82	0.45
1:AT:196:VAL:HG22	1:AT:197:GLY:H	1.82	0.45
1:AV:118:VAL:N	1:AV:203:GLU:OE1	2.47	0.45
1:AY:196:VAL:HG22	1:AY:197:GLY:H	1.82	0.45
1:AI:149:THR:OG1	2:Be:357:DC:OP2	2.31	0.45
1:A2:196:VAL:HG22	1:A2:197:GLY:H	1.82	0.44
1:AE:196:VAL:HG22	1:AE:197:GLY:H	1.82	0.44
1:AG:196:VAL:HG22	1:AG:197:GLY:H	1.82	0.44
1:AI:118:VAL:N	1:AI:203:GLU:OE1	2.47	0.44
1:AO:196:VAL:HG22	1:AO:197:GLY:H	1.82	0.44
1:AA:147:ARG:NH2	2:BB:357:DC:OP2	2.51	0.44
1:AC:118:VAL:N	1:AC:203:GLU:OE1	2.47	0.44
1:AK:147:ARG:NH2	2:BL:357:DC:OP2	2.50	0.44
1:AL:118:VAL:N	1:AL:203:GLU:OE1	2.47	0.44
1:AW:196:VAL:HG22	1:AW:197:GLY:H	1.82	0.44
1:Ar:118:VAL:N	1:Ar:203:GLU:OE1	2.47	0.44
1:Ar:196:VAL:HG22	1:Ar:197:GLY:H	1.82	0.44
1:A2:118:VAL:N	1:A2:203:GLU:OE1	2.47	0.44
1:A4:196:VAL:HG22	1:A4:197:GLY:H	1.82	0.44
1:A9:121:THR:CG2	1:A9:150:ILE:HD11	2.39	0.44
1:AD:118:VAL:N	1:AD:203:GLU:OE1	2.47	0.44
1:AW:147:ARG:NH2	2:BX:357:DC:OP2	2.51	0.44
1:Ao:118:VAL:N	1:Ao:203:GLU:OE1	2.47	0.44
1:A8:147:ARG:NH2	2:B9:357:DC:OP2	2.50	0.44
1:AF:196:VAL:HG22	1:AF:197:GLY:H	1.82	0.44
1:AI:196:VAL:HG22	1:AI:197:GLY:H	1.82	0.44
1:Ae:149:THR:OG1	2:Bf:357:DC:OP2	2.35	0.44
1:Ag:149:THR:OG1	2:Bh:357:DC:OP2	2.31	0.44
1:Ah:196:VAL:HG22	1:Ah:197:GLY:H	1.82	0.44
1:Ap:118:VAL:N	1:Ap:203:GLU:OE1	2.47	0.44
1:AU:118:VAL:N	1:AU:203:GLU:OE1	2.47	0.44
1:Ag:121:THR:CG2	1:Ag:150:ILE:HD11	2.39	0.44
1:Aj:196:VAL:HG22	1:Aj:197:GLY:H	1.82	0.44
1:Ar:71:MET:SD	1:Ar:71:MET:N	2.89	0.44
1:Ar:147:ARG:NH2	2:Bs:357:DC:OP2	2.50	0.44
1:Au:196:VAL:HG22	1:Au:197:GLY:H	1.82	0.44
1:A3:118:VAL:N	1:A3:203:GLU:OE1	2.47	0.44
1:AJ:118:VAL:N	1:AJ:203:GLU:OE1	2.47	0.44
1:AM:118:VAL:N	1:AM:203:GLU:OE1	2.47	0.44
1:AR:118:VAL:N	1:AR:203:GLU:OE1	2.47	0.44
1:AS:172:ASP:OD2	1:Ah:186:ARG:NH2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:196:VAL:HG22	1:Ai:197:GLY:H	1.82	0.44
1:At:121:THR:CG2	1:At:150:ILE:HD11	2.39	0.44
1:Ad:196:VAL:HG22	1:Ad:197:GLY:H	1.82	0.44
1:Av:196:VAL:HG22	1:Av:197:GLY:H	1.82	0.44
1:A5:196:VAL:HG22	1:A5:197:GLY:H	1.82	0.44
1:A5:118:VAL:N	1:A5:203:GLU:OE1	2.47	0.44
1:AD:196:VAL:HG22	1:AD:197:GLY:H	1.82	0.44
1:AK:73:ARG:HD2	1:AK:196:VAL:HG23	2.00	0.44
1:AO:71:MET:SD	1:AO:71:MET:N	2.89	0.44
1:AO:121:THR:CG2	1:AO:150:ILE:HD11	2.39	0.44
1:AR:196:VAL:HG22	1:AR:197:GLY:H	1.82	0.44
1:AV:196:VAL:HG22	1:AV:197:GLY:H	1.82	0.44
1:A1:71:MET:SD	1:A1:71:MET:N	2.89	0.43
1:AG:73:ARG:HD2	1:AG:196:VAL:HG23	2.00	0.43
1:AU:196:VAL:HG22	1:AU:197:GLY:H	1.82	0.43
1:Ar:73:ARG:HD2	1:Ar:196:VAL:HG23	2.00	0.43
1:A0:73:ARG:HD2	1:A0:196:VAL:HG23	2.00	0.43
1:A7:121:THR:CG2	1:A7:150:ILE:HD11	2.39	0.43
1:AV:121:THR:CG2	1:AV:150:ILE:HD11	2.39	0.43
1:Aa:71:MET:SD	1:Aa:71:MET:N	2.89	0.43
1:Ab:73:ARG:HD2	1:Ab:196:VAL:HG23	2.00	0.43
1:Ar:121:THR:CG2	1:Ar:150:ILE:HD11	2.39	0.43
1:As:73:ARG:HD2	1:As:196:VAL:HG23	2.01	0.43
1:At:118:VAL:N	1:At:203:GLU:OE1	2.47	0.43
1:A3:196:VAL:HG22	1:A3:197:GLY:H	1.82	0.43
1:AC:147:ARG:NH2	2:BD:357:DC:OP2	2.50	0.43
1:AD:121:THR:CG2	1:AD:150:ILE:HD11	2.39	0.43
1:AM:73:ARG:HD2	1:AM:196:VAL:HG23	2.00	0.43
1:AO:73:ARG:HD2	1:AO:196:VAL:HG23	2.01	0.43
1:Am:73:ARG:HD2	1:Am:196:VAL:HG23	2.00	0.43
1:Ap:73:ARG:HD2	1:Ap:196:VAL:HG23	2.00	0.43
1:A1:73:ARG:HD2	1:A1:196:VAL:HG23	2.01	0.43
1:AF:118:VAL:N	1:AF:203:GLU:OE1	2.47	0.43
1:AH:73:ARG:HD2	1:AH:196:VAL:HG23	2.00	0.43
1:AJ:196:VAL:HG22	1:AJ:197:GLY:H	1.82	0.43
1:AZ:73:ARG:HD2	1:AZ:196:VAL:HG23	2.00	0.43
1:Aa:73:ARG:HD2	1:Aa:196:VAL:HG23	2.01	0.43
1:Ae:73:ARG:HD2	1:Ae:196:VAL:HG23	2.00	0.43
1:Ag:118:VAL:N	1:Ag:203:GLU:OE1	2.47	0.43
1:Ah:73:ARG:HD2	1:Ah:196:VAL:HG23	2.00	0.43
1:Ak:73:ARG:HD2	1:Ak:196:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:71:MET:SD	1:Al:71:MET:N	2.89	0.43
1:Al:73:ARG:HD2	1:Al:196:VAL:HG23	2.00	0.43
1:Au:73:ARG:HD2	1:Au:196:VAL:HG23	2.00	0.43
1:Aw:73:ARG:HD2	1:Aw:196:VAL:HG23	2.00	0.43
1:A4:73:ARG:HD2	1:A4:196:VAL:HG23	2.01	0.43
1:AD:73:ARG:HD2	1:AD:196:VAL:HG23	2.00	0.43
1:AG:118:VAL:N	1:AG:203:GLU:OE1	2.47	0.43
1:AK:118:VAL:N	1:AK:203:GLU:OE1	2.47	0.43
1:AO:186:ARG:NH2	1:Aq:172:ASP:OD2	2.47	0.43
1:AX:73:ARG:HD2	1:AX:196:VAL:HG23	2.00	0.43
1:Ag:73:ARG:HD2	1:Ag:196:VAL:HG23	2.01	0.43
1:A1:196:VAL:HG22	1:A1:197:GLY:H	1.82	0.43
1:A2:73:ARG:HD2	1:A2:196:VAL:HG23	2.01	0.43
1:AA:73:ARG:HD2	1:AA:196:VAL:HG23	2.01	0.43
1:AC:196:VAL:HG22	1:AC:197:GLY:H	1.82	0.43
1:AF:73:ARG:HD2	1:AF:196:VAL:HG23	2.01	0.43
1:AH:71:MET:SD	1:AH:71:MET:N	2.89	0.43
1:AQ:186:ARG:NH2	1:Ap:172:ASP:OD2	2.48	0.43
1:AV:73:ARG:HD2	1:AV:196:VAL:HG23	2.00	0.43
1:Aa:147:ARG:NH2	2:Bb:357:DC:OP2	2.52	0.43
1:Ad:118:VAL:N	1:Ad:203:GLU:OE1	2.47	0.43
1:At:73:ARG:HD2	1:At:196:VAL:HG23	2.01	0.43
1:A4:118:VAL:N	1:A4:203:GLU:OE1	2.47	0.43
1:A8:118:VAL:N	1:A8:203:GLU:OE1	2.47	0.43
1:AA:118:VAL:N	1:AA:203:GLU:OE1	2.47	0.43
1:AI:73:ARG:HD2	1:AI:196:VAL:HG23	2.01	0.43
1:AT:118:VAL:N	1:AT:203:GLU:OE1	2.47	0.43
1:AX:118:VAL:N	1:AX:203:GLU:OE1	2.47	0.43
1:Al:196:VAL:HG22	1:Al:197:GLY:H	1.82	0.43
1:As:118:VAL:N	1:As:203:GLU:OE1	2.47	0.43
1:A0:118:VAL:N	1:A0:203:GLU:OE1	2.47	0.43
1:A7:118:VAL:N	1:A7:203:GLU:OE1	2.47	0.43
1:A9:73:ARG:HD2	1:A9:196:VAL:HG23	2.00	0.43
1:AB:73:ARG:HD2	1:AB:196:VAL:HG23	2.01	0.43
1:AH:196:VAL:HG22	1:AH:197:GLY:H	1.82	0.43
1:AL:73:ARG:HD2	1:AL:196:VAL:HG23	2.00	0.43
1:AT:121:THR:CG2	1:AT:150:ILE:HD11	2.39	0.43
1:Aa:149:THR:OG1	2:Bb:357:DC:OP2	2.34	0.43
1:Aa:196:VAL:HG22	1:Aa:197:GLY:H	1.82	0.43
1:Ag:71:MET:SD	1:Ag:71:MET:N	2.89	0.43
1:Aj:118:VAL:N	1:Aj:203:GLU:OE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:73:ARG:HD2	1:Ao:196:VAL:HG23	2.00	0.43
1:At:71:MET:SD	1:At:71:MET:N	2.89	0.43
1:Ax:73:ARG:HD2	1:Ax:196:VAL:HG23	2.00	0.43
1:AT:71:MET:SD	1:AT:71:MET:N	2.89	0.43
1:Aj:73:ARG:HD2	1:Aj:196:VAL:HG23	2.01	0.43
1:Au:149:THR:OG1	2:Bv:357:DC:OP2	2.34	0.43
1:AQ:73:ARG:HD2	1:AQ:196:VAL:HG23	2.00	0.43
1:AY:73:ARG:HD2	1:AY:196:VAL:HG23	2.01	0.43
1:AY:186:ARG:NH2	1:Al:172:ASP:OD2	2.49	0.43
1:Ad:73:ARG:HD2	1:Ad:196:VAL:HG23	2.00	0.43
1:Ax:147:ARG:NH2	2:Bt:357:DC:OP2	2.51	0.43
1:AC:121:THR:CG2	1:AC:150:ILE:HD11	2.39	0.42
1:AP:118:VAL:N	1:AP:203:GLU:OE1	2.47	0.42
1:Af:73:ARG:HD2	1:Af:196:VAL:HG23	2.01	0.42
1:An:71:MET:SD	1:An:71:MET:N	2.89	0.42
1:A7:71:MET:SD	1:A7:71:MET:N	2.89	0.42
1:AH:118:VAL:N	1:AH:203:GLU:OE1	2.47	0.42
1:AN:73:ARG:HD2	1:AN:196:VAL:HG23	2.00	0.42
1:Ac:73:ARG:HD2	1:Ac:196:VAL:HG23	2.00	0.42
1:At:149:THR:OG1	2:Bu:357:DC:OP2	2.35	0.42
1:Ax:71:MET:SD	1:Ax:71:MET:N	2.89	0.42
1:AX:71:MET:SD	1:AX:71:MET:N	2.89	0.42
1:Ac:71:MET:SD	1:Ac:71:MET:N	2.89	0.42
1:An:73:ARG:HD2	1:An:196:VAL:HG23	2.00	0.42
1:A6:73:ARG:HD2	1:A6:196:VAL:HG23	2.00	0.42
1:AJ:73:ARG:HD2	1:AJ:196:VAL:HG23	2.00	0.42
1:AY:149:THR:OG1	2:BU:357:DC:OP2	2.31	0.42
1:Aa:118:VAL:N	1:Aa:203:GLU:OE1	2.47	0.42
1:Af:71:MET:SD	1:Af:71:MET:N	2.89	0.42
1:Af:118:VAL:N	1:Af:203:GLU:OE1	2.47	0.42
1:Aj:149:THR:HG1	2:Bk:357:DC:P	2.42	0.42
1:Al:118:VAL:N	1:Al:203:GLU:OE1	2.47	0.42
1:Aq:73:ARG:HD2	1:Aq:196:VAL:HG23	2.01	0.42
1:AA:71:MET:SD	1:AA:71:MET:N	2.89	0.42
1:AF:121:THR:CG2	1:AF:150:ILE:HD11	2.39	0.42
1:AP:172:ASP:OD2	1:Aq:186:ARG:NH2	2.48	0.42
1:AS:73:ARG:HD2	1:AS:196:VAL:HG23	2.00	0.42
1:Ax:118:VAL:N	1:Ax:203:GLU:OE1	2.47	0.42
1:AC:73:ARG:HD2	1:AC:196:VAL:HG23	2.00	0.42
1:AH:147:ARG:NH2	2:BI:357:DC:OP2	2.53	0.42
1:AR:73:ARG:HD2	1:AR:196:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:73:ARG:HD2	1:AU:196:VAL:HG23	2.01	0.42
1:AW:73:ARG:HD2	1:AW:196:VAL:HG23	2.00	0.42
1:AW:118:VAL:N	1:AW:203:GLU:OE1	2.47	0.42
1:Aa:186:ARG:NH2	1:Ak:172:ASP:OD2	2.51	0.42
1:Ai:73:ARG:HD2	1:Ai:196:VAL:HG23	2.00	0.42
1:A1:118:VAL:N	1:A1:203:GLU:OE1	2.47	0.42
1:A3:73:ARG:HD2	1:A3:196:VAL:HG23	2.01	0.42
1:A5:73:ARG:HD2	1:A5:196:VAL:HG23	2.01	0.42
1:A8:73:ARG:HD2	1:A8:196:VAL:HG23	2.00	0.42
1:AJ:121:THR:CG2	1:AJ:150:ILE:HD11	2.39	0.42
1:Aa:121:THR:CG2	1:Aa:150:ILE:HD11	2.39	0.42
1:Ai:118:VAL:N	1:Ai:203:GLU:OE1	2.47	0.42
1:A9:118:VAL:N	1:A9:203:GLU:OE1	2.47	0.42
1:AE:71:MET:SD	1:AE:71:MET:N	2.89	0.42
1:AE:73:ARG:HD2	1:AE:196:VAL:HG23	2.01	0.42
1:AW:149:THR:OG1	2:BX:357:DC:OP2	2.35	0.42
1:Ah:121:THR:CG2	1:Ah:150:ILE:HD11	2.39	0.42
1:Av:73:ARG:HD2	1:Av:196:VAL:HG23	2.00	0.42
1:Av:118:VAL:N	1:Av:203:GLU:OE1	2.47	0.42
1:A3:121:THR:CG2	1:A3:150:ILE:HD11	2.39	0.42
1:AP:73:ARG:HD2	1:AP:196:VAL:HG23	2.00	0.42
1:AW:71:MET:SD	1:AW:71:MET:N	2.89	0.42
1:Au:121:THR:CG2	1:Au:150:ILE:HD11	2.39	0.42
1:A4:121:THR:CG2	1:A4:150:ILE:HD11	2.39	0.42
1:AE:118:VAL:N	1:AE:203:GLU:OE1	2.47	0.42
1:As:149:THR:OG1	2:Bo:357:DC:OP2	2.35	0.42
1:A4:71:MET:SD	1:A4:71:MET:N	2.89	0.41
1:AL:149:THR:OG1	2:BM:357:DC:OP2	2.36	0.41
1:Ac:118:VAL:N	1:Ac:203:GLU:OE1	2.47	0.41
1:Al:121:THR:CG2	1:Al:150:ILE:HD11	2.39	0.41
1:An:118:VAL:N	1:An:203:GLU:OE1	2.47	0.41
1:Au:118:VAL:N	1:Au:203:GLU:OE1	2.47	0.41
1:AZ:118:VAL:N	1:AZ:203:GLU:OE1	2.47	0.41
1:A7:73:ARG:HD2	1:A7:196:VAL:HG23	2.00	0.41
1:AF:71:MET:SD	1:AF:71:MET:N	2.89	0.41
1:AQ:118:VAL:N	1:AQ:203:GLU:OE1	2.47	0.41
1:AC:71:MET:SD	1:AC:71:MET:N	2.89	0.41
1:AZ:71:MET:SD	1:AZ:71:MET:N	2.89	0.41
1:Ak:71:MET:SD	1:Ak:71:MET:N	2.89	0.41
1:Ak:118:VAL:N	1:Ak:203:GLU:OE1	2.47	0.41
1:Aw:118:VAL:N	1:Aw:203:GLU:OE1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:73:ARG:HD2	1:AT:196:VAL:HG23	2.00	0.41
1:Ax:121:THR:CG2	1:Ax:150:ILE:HD11	2.39	0.41
1:AK:223:GLU:OE2	1:AT:146:SER:OG	2.33	0.41
1:AU:71:MET:SD	1:AU:71:MET:N	2.89	0.41
1:Aj:121:THR:CG2	1:Aj:150:ILE:HD11	2.39	0.41
1:AR:71:MET:SD	1:AR:71:MET:N	2.89	0.41
1:A5:71:MET:SD	1:A5:71:MET:N	2.89	0.41
1:A6:121:THR:CG2	1:A6:150:ILE:HD11	2.39	0.41
1:AS:118:VAL:N	1:AS:203:GLU:OE1	2.47	0.41
1:Ad:121:THR:CG2	1:Ad:150:ILE:HD11	2.39	0.41
1:Ae:118:VAL:N	1:Ae:203:GLU:OE1	2.47	0.41
1:Af:121:THR:CG2	1:Af:150:ILE:HD11	2.39	0.41
1:Ah:118:VAL:N	1:Ah:203:GLU:OE1	2.47	0.41
1:A6:118:VAL:N	1:A6:203:GLU:OE1	2.47	0.41
1:A6:186:ARG:NH2	1:AV:172:ASP:OD2	2.52	0.41
1:A8:71:MET:SD	1:A8:71:MET:N	2.89	0.41
1:AI:121:THR:CG2	1:AI:150:ILE:HD11	2.39	0.41
1:Ap:147:ARG:NH2	2:Bq:357:DC:OP2	2.54	0.41
1:AC:149:THR:HG1	2:BD:357:DC:P	2.41	0.40
1:AM:71:MET:SD	1:AM:71:MET:N	2.89	0.40
1:AP:71:MET:SD	1:AP:71:MET:N	2.89	0.40
1:AR:121:THR:CG2	1:AR:150:ILE:HD11	2.39	0.40
1:AS:121:THR:CG2	1:AS:150:ILE:HD11	2.39	0.40
1:Ap:71:MET:SD	1:Ap:71:MET:N	2.89	0.40
1:AZ:147:ARG:NH2	2:Ba:357:DC:OP2	2.54	0.40
1:Ap:149:THR:OG1	2:Bq:357:DC:OP2	2.39	0.40
1:Av:71:MET:SD	1:Av:71:MET:N	2.89	0.40
1:AV:71:MET:SD	1:AV:71:MET:N	2.89	0.40
1:AY:71:MET:SD	1:AY:71:MET:N	2.89	0.40
1:A5:121:THR:CG2	1:A5:150:ILE:HD11	2.39	0.40
1:AG:186:ARG:NH2	1:AQ:172:ASP:OD2	2.51	0.40
1:AS:149:THR:OG1	2:BT:357:DC:OP2	2.36	0.40
1:A0:71:MET:SD	1:A0:71:MET:N	2.89	0.40
1:A8:172:ASP:OD2	1:AN:186:ARG:NH2	2.52	0.40
1:AI:147:ARG:NH2	2:BJ:357:DC:OP2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A0	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A1	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A2	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A3	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A4	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A5	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A6	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A7	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A8	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	A9	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AA	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AB	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AC	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AD	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AE	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AF	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AG	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AH	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AI	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AJ	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AK	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AL	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AM	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AN	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AO	194/196 (99%)	178 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AP	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AQ	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AR	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AS	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AT	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AU	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AV	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AW	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AX	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AY	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	AZ	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Aa	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ab	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ac	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ad	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ae	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Af	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ag	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ah	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ai	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Aj	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ak	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Al	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Am	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	An	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ao	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ap	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Aq	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ar	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	As	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	At	194/196 (99%)	178 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Au	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Av	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Aw	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
1	Ax	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
All	All	11640/11760 (99%)	10680 (92%)	960 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	A0	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A1	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A2	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A3	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A4	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A5	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A6	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A7	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A8	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	A9	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AA	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AB	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AC	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AD	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AE	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AF	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AG	181/181 (100%)	163 (90%)	18 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AH	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AI	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AJ	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AK	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AL	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AM	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AN	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AO	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AP	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AQ	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AR	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AS	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AT	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AU	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AV	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AW	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AX	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AY	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	AZ	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Aa	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ab	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ac	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ad	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ae	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Af	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ag	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ah	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ai	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Aj	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ak	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Al	181/181 (100%)	163 (90%)	18 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Am	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	An	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ao	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ap	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Aq	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ar	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	As	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	At	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Au	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Av	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Aw	181/181 (100%)	163 (90%)	18 (10%)	7	27
1	Ax	181/181 (100%)	163 (90%)	18 (10%)	7	27
All	All	10860/10860 (100%)	9780 (90%)	1080 (10%)	10	27

All (1080) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	37	ARG
1	A0	53	ILE
1	A0	58	LYS
1	A0	73	ARG
1	A0	80	LEU
1	A0	94	GLU
1	A0	116	ARG
1	A0	131	THR
1	A0	158	SER
1	A0	167	LEU
1	A0	170	THR
1	A0	179	LYS
1	A0	180	ARG
1	A0	181	ASN
1	A0	194	ASP
1	A0	198	LEU
1	A0	212	ASN
1	A0	219	VAL
1	A1	37	ARG
1	A1	53	ILE
1	A1	58	LYS

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Mol	Chain	Res	Type
1	A1	73	ARG
1	A1	80	LEU
1	A1	94	GLU
1	A1	116	ARG
1	A1	131	THR
1	A1	158	SER
1	A1	167	LEU
1	A1	170	THR
1	A1	179	LYS
1	A1	180	ARG
1	A1	181	ASN
1	A1	194	ASP
1	A1	198	LEU
1	A1	212	ASN
1	A1	219	VAL
1	A2	37	ARG
1	A2	53	ILE
1	A2	58	LYS
1	A2	73	ARG
1	A2	80	LEU
1	A2	94	GLU
1	A2	116	ARG
1	A2	131	THR
1	A2	158	SER
1	A2	167	LEU
1	A2	170	THR
1	A2	179	LYS
1	A2	180	ARG
1	A2	181	ASN
1	A2	194	ASP
1	A2	198	LEU
1	A2	212	ASN
1	A2	219	VAL
1	A3	37	ARG
1	A3	53	ILE
1	A3	58	LYS
1	A3	73	ARG
1	A3	80	LEU
1	A3	94	GLU
1	A3	116	ARG
1	A3	131	THR
1	A3	158	SER

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Mol	Chain	Res	Type
1	A3	167	LEU
1	A3	170	THR
1	A3	179	LYS
1	A3	180	ARG
1	A3	181	ASN
1	A3	194	ASP
1	A3	198	LEU
1	A3	212	ASN
1	A3	219	VAL
1	A4	37	ARG
1	A4	53	ILE
1	A4	58	LYS
1	A4	73	ARG
1	A4	80	LEU
1	A4	94	GLU
1	A4	116	ARG
1	A4	131	THR
1	A4	158	SER
1	A4	167	LEU
1	A4	170	THR
1	A4	179	LYS
1	A4	180	ARG
1	A4	181	ASN
1	A4	194	ASP
1	A4	198	LEU
1	A4	212	ASN
1	A4	219	VAL
1	A5	37	ARG
1	A5	53	ILE
1	A5	58	LYS
1	A5	73	ARG
1	A5	80	LEU
1	A5	94	GLU
1	A5	116	ARG
1	A5	131	THR
1	A5	158	SER
1	A5	167	LEU
1	A5	170	THR
1	A5	179	LYS
1	A5	180	ARG
1	A5	181	ASN
1	A5	194	ASP

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Mol	Chain	Res	Type
1	A5	198	LEU
1	A5	212	ASN
1	A5	219	VAL
1	A6	37	ARG
1	A6	53	ILE
1	A6	58	LYS
1	A6	73	ARG
1	A6	80	LEU
1	A6	94	GLU
1	A6	116	ARG
1	A6	131	THR
1	A6	158	SER
1	A6	167	LEU
1	A6	170	THR
1	A6	179	LYS
1	A6	180	ARG
1	A6	181	ASN
1	A6	194	ASP
1	A6	198	LEU
1	A6	212	ASN
1	A6	219	VAL
1	A7	37	ARG
1	A7	53	ILE
1	A7	58	LYS
1	A7	73	ARG
1	A7	80	LEU
1	A7	94	GLU
1	A7	116	ARG
1	A7	131	THR
1	A7	158	SER
1	A7	167	LEU
1	A7	170	THR
1	A7	179	LYS
1	A7	180	ARG
1	A7	181	ASN
1	A7	194	ASP
1	A7	198	LEU
1	A7	212	ASN
1	A7	219	VAL
1	A8	37	ARG
1	A8	53	ILE
1	A8	58	LYS

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Mol	Chain	Res	Type
1	A8	73	ARG
1	A8	80	LEU
1	A8	94	GLU
1	A8	116	ARG
1	A8	131	THR
1	A8	158	SER
1	A8	167	LEU
1	A8	170	THR
1	A8	179	LYS
1	A8	180	ARG
1	A8	181	ASN
1	A8	194	ASP
1	A8	198	LEU
1	A8	212	ASN
1	A8	219	VAL
1	A9	37	ARG
1	A9	53	ILE
1	A9	58	LYS
1	A9	73	ARG
1	A9	80	LEU
1	A9	94	GLU
1	A9	116	ARG
1	A9	131	THR
1	A9	158	SER
1	A9	167	LEU
1	A9	170	THR
1	A9	179	LYS
1	A9	180	ARG
1	A9	181	ASN
1	A9	194	ASP
1	A9	198	LEU
1	A9	212	ASN
1	A9	219	VAL
1	AA	37	ARG
1	AA	53	ILE
1	AA	58	LYS
1	AA	73	ARG
1	AA	80	LEU
1	AA	94	GLU
1	AA	116	ARG
1	AA	131	THR
1	AA	158	SER

Continued on next page...

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Mol	Chain	Res	Type
1	AA	167	LEU
1	AA	170	THR
1	AA	179	LYS
1	AA	180	ARG
1	AA	181	ASN
1	AA	194	ASP
1	AA	198	LEU
1	AA	212	ASN
1	AA	219	VAL
1	AB	37	ARG
1	AB	53	ILE
1	AB	58	LYS
1	AB	73	ARG
1	AB	80	LEU
1	AB	94	GLU
1	AB	116	ARG
1	AB	131	THR
1	AB	158	SER
1	AB	167	LEU
1	AB	170	THR
1	AB	179	LYS
1	AB	180	ARG
1	AB	181	ASN
1	AB	194	ASP
1	AB	198	LEU
1	AB	212	ASN
1	AB	219	VAL
1	AC	37	ARG
1	AC	53	ILE
1	AC	58	LYS
1	AC	73	ARG
1	AC	80	LEU
1	AC	94	GLU
1	AC	116	ARG
1	AC	131	THR
1	AC	158	SER
1	AC	167	LEU
1	AC	170	THR
1	AC	179	LYS
1	AC	180	ARG
1	AC	181	ASN
1	AC	194	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	AC	198	LEU
1	AC	212	ASN
1	AC	219	VAL
1	AD	37	ARG
1	AD	53	ILE
1	AD	58	LYS
1	AD	73	ARG
1	AD	80	LEU
1	AD	94	GLU
1	AD	116	ARG
1	AD	131	THR
1	AD	158	SER
1	AD	167	LEU
1	AD	170	THR
1	AD	179	LYS
1	AD	180	ARG
1	AD	181	ASN
1	AD	194	ASP
1	AD	198	LEU
1	AD	212	ASN
1	AD	219	VAL
1	AE	37	ARG
1	AE	53	ILE
1	AE	58	LYS
1	AE	73	ARG
1	AE	80	LEU
1	AE	94	GLU
1	AE	116	ARG
1	AE	131	THR
1	AE	158	SER
1	AE	167	LEU
1	AE	170	THR
1	AE	179	LYS
1	AE	180	ARG
1	AE	181	ASN
1	AE	194	ASP
1	AE	198	LEU
1	AE	212	ASN
1	AE	219	VAL
1	AF	37	ARG
1	AF	53	ILE
1	AF	58	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	AF	73	ARG
1	AF	80	LEU
1	AF	94	GLU
1	AF	116	ARG
1	AF	131	THR
1	AF	158	SER
1	AF	167	LEU
1	AF	170	THR
1	AF	179	LYS
1	AF	180	ARG
1	AF	181	ASN
1	AF	194	ASP
1	AF	198	LEU
1	AF	212	ASN
1	AF	219	VAL
1	AG	37	ARG
1	AG	53	ILE
1	AG	58	LYS
1	AG	73	ARG
1	AG	80	LEU
1	AG	94	GLU
1	AG	116	ARG
1	AG	131	THR
1	AG	158	SER
1	AG	167	LEU
1	AG	170	THR
1	AG	179	LYS
1	AG	180	ARG
1	AG	181	ASN
1	AG	194	ASP
1	AG	198	LEU
1	AG	212	ASN
1	AG	219	VAL
1	AH	37	ARG
1	AH	53	ILE
1	AH	58	LYS
1	AH	73	ARG
1	AH	80	LEU
1	AH	94	GLU
1	AH	116	ARG
1	AH	131	THR
1	AH	158	SER

Continued on next page...

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Mol	Chain	Res	Type
1	AH	167	LEU
1	AH	170	THR
1	AH	179	LYS
1	AH	180	ARG
1	AH	181	ASN
1	AH	194	ASP
1	AH	198	LEU
1	AH	212	ASN
1	AH	219	VAL
1	AI	37	ARG
1	AI	53	ILE
1	AI	58	LYS
1	AI	73	ARG
1	AI	80	LEU
1	AI	94	GLU
1	AI	116	ARG
1	AI	131	THR
1	AI	158	SER
1	AI	167	LEU
1	AI	170	THR
1	AI	179	LYS
1	AI	180	ARG
1	AI	181	ASN
1	AI	194	ASP
1	AI	198	LEU
1	AI	212	ASN
1	AI	219	VAL
1	AJ	37	ARG
1	AJ	53	ILE
1	AJ	58	LYS
1	AJ	73	ARG
1	AJ	80	LEU
1	AJ	94	GLU
1	AJ	116	ARG
1	AJ	131	THR
1	AJ	158	SER
1	AJ	167	LEU
1	AJ	170	THR
1	AJ	179	LYS
1	AJ	180	ARG
1	AJ	181	ASN
1	AJ	194	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	AJ	198	LEU
1	AJ	212	ASN
1	AJ	219	VAL
1	AK	37	ARG
1	AK	53	ILE
1	AK	58	LYS
1	AK	73	ARG
1	AK	80	LEU
1	AK	94	GLU
1	AK	116	ARG
1	AK	131	THR
1	AK	158	SER
1	AK	167	LEU
1	AK	170	THR
1	AK	179	LYS
1	AK	180	ARG
1	AK	181	ASN
1	AK	194	ASP
1	AK	198	LEU
1	AK	212	ASN
1	AK	219	VAL
1	AL	37	ARG
1	AL	53	ILE
1	AL	58	LYS
1	AL	73	ARG
1	AL	80	LEU
1	AL	94	GLU
1	AL	116	ARG
1	AL	131	THR
1	AL	158	SER
1	AL	167	LEU
1	AL	170	THR
1	AL	179	LYS
1	AL	180	ARG
1	AL	181	ASN
1	AL	194	ASP
1	AL	198	LEU
1	AL	212	ASN
1	AL	219	VAL
1	AM	37	ARG
1	AM	53	ILE
1	AM	58	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	AM	73	ARG
1	AM	80	LEU
1	AM	94	GLU
1	AM	116	ARG
1	AM	131	THR
1	AM	158	SER
1	AM	167	LEU
1	AM	170	THR
1	AM	179	LYS
1	AM	180	ARG
1	AM	181	ASN
1	AM	194	ASP
1	AM	198	LEU
1	AM	212	ASN
1	AM	219	VAL
1	AN	37	ARG
1	AN	53	ILE
1	AN	58	LYS
1	AN	73	ARG
1	AN	80	LEU
1	AN	94	GLU
1	AN	116	ARG
1	AN	131	THR
1	AN	158	SER
1	AN	167	LEU
1	AN	170	THR
1	AN	179	LYS
1	AN	180	ARG
1	AN	181	ASN
1	AN	194	ASP
1	AN	198	LEU
1	AN	212	ASN
1	AN	219	VAL
1	AO	37	ARG
1	AO	53	ILE
1	AO	58	LYS
1	AO	73	ARG
1	AO	80	LEU
1	AO	94	GLU
1	AO	116	ARG
1	AO	131	THR
1	AO	158	SER

Continued on next page...

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Mol	Chain	Res	Type
1	AO	167	LEU
1	AO	170	THR
1	AO	179	LYS
1	AO	180	ARG
1	AO	181	ASN
1	AO	194	ASP
1	AO	198	LEU
1	AO	212	ASN
1	AO	219	VAL
1	AP	37	ARG
1	AP	53	ILE
1	AP	58	LYS
1	AP	73	ARG
1	AP	80	LEU
1	AP	94	GLU
1	AP	116	ARG
1	AP	131	THR
1	AP	158	SER
1	AP	167	LEU
1	AP	170	THR
1	AP	179	LYS
1	AP	180	ARG
1	AP	181	ASN
1	AP	194	ASP
1	AP	198	LEU
1	AP	212	ASN
1	AP	219	VAL
1	AQ	37	ARG
1	AQ	53	ILE
1	AQ	58	LYS
1	AQ	73	ARG
1	AQ	80	LEU
1	AQ	94	GLU
1	AQ	116	ARG
1	AQ	131	THR
1	AQ	158	SER
1	AQ	167	LEU
1	AQ	170	THR
1	AQ	179	LYS
1	AQ	180	ARG
1	AQ	181	ASN
1	AQ	194	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	AQ	198	LEU
1	AQ	212	ASN
1	AQ	219	VAL
1	AR	37	ARG
1	AR	53	ILE
1	AR	58	LYS
1	AR	73	ARG
1	AR	80	LEU
1	AR	94	GLU
1	AR	116	ARG
1	AR	131	THR
1	AR	158	SER
1	AR	167	LEU
1	AR	170	THR
1	AR	179	LYS
1	AR	180	ARG
1	AR	181	ASN
1	AR	194	ASP
1	AR	198	LEU
1	AR	212	ASN
1	AR	219	VAL
1	AS	37	ARG
1	AS	53	ILE
1	AS	58	LYS
1	AS	73	ARG
1	AS	80	LEU
1	AS	94	GLU
1	AS	116	ARG
1	AS	131	THR
1	AS	158	SER
1	AS	167	LEU
1	AS	170	THR
1	AS	179	LYS
1	AS	180	ARG
1	AS	181	ASN
1	AS	194	ASP
1	AS	198	LEU
1	AS	212	ASN
1	AS	219	VAL
1	AT	37	ARG
1	AT	53	ILE
1	AT	58	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	AT	73	ARG
1	AT	80	LEU
1	AT	94	GLU
1	AT	116	ARG
1	AT	131	THR
1	AT	158	SER
1	AT	167	LEU
1	AT	170	THR
1	AT	179	LYS
1	AT	180	ARG
1	AT	181	ASN
1	AT	194	ASP
1	AT	198	LEU
1	AT	212	ASN
1	AT	219	VAL
1	AU	37	ARG
1	AU	53	ILE
1	AU	58	LYS
1	AU	73	ARG
1	AU	80	LEU
1	AU	94	GLU
1	AU	116	ARG
1	AU	131	THR
1	AU	158	SER
1	AU	167	LEU
1	AU	170	THR
1	AU	179	LYS
1	AU	180	ARG
1	AU	181	ASN
1	AU	194	ASP
1	AU	198	LEU
1	AU	212	ASN
1	AU	219	VAL
1	AV	37	ARG
1	AV	53	ILE
1	AV	58	LYS
1	AV	73	ARG
1	AV	80	LEU
1	AV	94	GLU
1	AV	116	ARG
1	AV	131	THR
1	AV	158	SER

Continued on next page...

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Mol	Chain	Res	Type
1	AV	167	LEU
1	AV	170	THR
1	AV	179	LYS
1	AV	180	ARG
1	AV	181	ASN
1	AV	194	ASP
1	AV	198	LEU
1	AV	212	ASN
1	AV	219	VAL
1	AW	37	ARG
1	AW	53	ILE
1	AW	58	LYS
1	AW	73	ARG
1	AW	80	LEU
1	AW	94	GLU
1	AW	116	ARG
1	AW	131	THR
1	AW	158	SER
1	AW	167	LEU
1	AW	170	THR
1	AW	179	LYS
1	AW	180	ARG
1	AW	181	ASN
1	AW	194	ASP
1	AW	198	LEU
1	AW	212	ASN
1	AW	219	VAL
1	AX	37	ARG
1	AX	53	ILE
1	AX	58	LYS
1	AX	73	ARG
1	AX	80	LEU
1	AX	94	GLU
1	AX	116	ARG
1	AX	131	THR
1	AX	158	SER
1	AX	167	LEU
1	AX	170	THR
1	AX	179	LYS
1	AX	180	ARG
1	AX	181	ASN
1	AX	194	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	AX	198	LEU
1	AX	212	ASN
1	AX	219	VAL
1	AY	37	ARG
1	AY	53	ILE
1	AY	58	LYS
1	AY	73	ARG
1	AY	80	LEU
1	AY	94	GLU
1	AY	116	ARG
1	AY	131	THR
1	AY	158	SER
1	AY	167	LEU
1	AY	170	THR
1	AY	179	LYS
1	AY	180	ARG
1	AY	181	ASN
1	AY	194	ASP
1	AY	198	LEU
1	AY	212	ASN
1	AY	219	VAL
1	AZ	37	ARG
1	AZ	53	ILE
1	AZ	58	LYS
1	AZ	73	ARG
1	AZ	80	LEU
1	AZ	94	GLU
1	AZ	116	ARG
1	AZ	131	THR
1	AZ	158	SER
1	AZ	167	LEU
1	AZ	170	THR
1	AZ	179	LYS
1	AZ	180	ARG
1	AZ	181	ASN
1	AZ	194	ASP
1	AZ	198	LEU
1	AZ	212	ASN
1	AZ	219	VAL
1	Aa	37	ARG
1	Aa	53	ILE
1	Aa	58	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	Aa	73	ARG
1	Aa	80	LEU
1	Aa	94	GLU
1	Aa	116	ARG
1	Aa	131	THR
1	Aa	158	SER
1	Aa	167	LEU
1	Aa	170	THR
1	Aa	179	LYS
1	Aa	180	ARG
1	Aa	181	ASN
1	Aa	194	ASP
1	Aa	198	LEU
1	Aa	212	ASN
1	Aa	219	VAL
1	Ab	37	ARG
1	Ab	53	ILE
1	Ab	58	LYS
1	Ab	73	ARG
1	Ab	80	LEU
1	Ab	94	GLU
1	Ab	116	ARG
1	Ab	131	THR
1	Ab	158	SER
1	Ab	167	LEU
1	Ab	170	THR
1	Ab	179	LYS
1	Ab	180	ARG
1	Ab	181	ASN
1	Ab	194	ASP
1	Ab	198	LEU
1	Ab	212	ASN
1	Ab	219	VAL
1	Ac	37	ARG
1	Ac	53	ILE
1	Ac	58	LYS
1	Ac	73	ARG
1	Ac	80	LEU
1	Ac	94	GLU
1	Ac	116	ARG
1	Ac	131	THR
1	Ac	158	SER

Continued on next page...

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Mol	Chain	Res	Type
1	Ac	167	LEU
1	Ac	170	THR
1	Ac	179	LYS
1	Ac	180	ARG
1	Ac	181	ASN
1	Ac	194	ASP
1	Ac	198	LEU
1	Ac	212	ASN
1	Ac	219	VAL
1	Ad	37	ARG
1	Ad	53	ILE
1	Ad	58	LYS
1	Ad	73	ARG
1	Ad	80	LEU
1	Ad	94	GLU
1	Ad	116	ARG
1	Ad	131	THR
1	Ad	158	SER
1	Ad	167	LEU
1	Ad	170	THR
1	Ad	179	LYS
1	Ad	180	ARG
1	Ad	181	ASN
1	Ad	194	ASP
1	Ad	198	LEU
1	Ad	212	ASN
1	Ad	219	VAL
1	Ae	37	ARG
1	Ae	53	ILE
1	Ae	58	LYS
1	Ae	73	ARG
1	Ae	80	LEU
1	Ae	94	GLU
1	Ae	116	ARG
1	Ae	131	THR
1	Ae	158	SER
1	Ae	167	LEU
1	Ae	170	THR
1	Ae	179	LYS
1	Ae	180	ARG
1	Ae	181	ASN
1	Ae	194	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	Ae	198	LEU
1	Ae	212	ASN
1	Ae	219	VAL
1	Af	37	ARG
1	Af	53	ILE
1	Af	58	LYS
1	Af	73	ARG
1	Af	80	LEU
1	Af	94	GLU
1	Af	116	ARG
1	Af	131	THR
1	Af	158	SER
1	Af	167	LEU
1	Af	170	THR
1	Af	179	LYS
1	Af	180	ARG
1	Af	181	ASN
1	Af	194	ASP
1	Af	198	LEU
1	Af	212	ASN
1	Af	219	VAL
1	Ag	37	ARG
1	Ag	53	ILE
1	Ag	58	LYS
1	Ag	73	ARG
1	Ag	80	LEU
1	Ag	94	GLU
1	Ag	116	ARG
1	Ag	131	THR
1	Ag	158	SER
1	Ag	167	LEU
1	Ag	170	THR
1	Ag	179	LYS
1	Ag	180	ARG
1	Ag	181	ASN
1	Ag	194	ASP
1	Ag	198	LEU
1	Ag	212	ASN
1	Ag	219	VAL
1	Ah	37	ARG
1	Ah	53	ILE
1	Ah	58	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	Ah	73	ARG
1	Ah	80	LEU
1	Ah	94	GLU
1	Ah	116	ARG
1	Ah	131	THR
1	Ah	158	SER
1	Ah	167	LEU
1	Ah	170	THR
1	Ah	179	LYS
1	Ah	180	ARG
1	Ah	181	ASN
1	Ah	194	ASP
1	Ah	198	LEU
1	Ah	212	ASN
1	Ah	219	VAL
1	Ai	37	ARG
1	Ai	53	ILE
1	Ai	58	LYS
1	Ai	73	ARG
1	Ai	80	LEU
1	Ai	94	GLU
1	Ai	116	ARG
1	Ai	131	THR
1	Ai	158	SER
1	Ai	167	LEU
1	Ai	170	THR
1	Ai	179	LYS
1	Ai	180	ARG
1	Ai	181	ASN
1	Ai	194	ASP
1	Ai	198	LEU
1	Ai	212	ASN
1	Ai	219	VAL
1	Aj	37	ARG
1	Aj	53	ILE
1	Aj	58	LYS
1	Aj	73	ARG
1	Aj	80	LEU
1	Aj	94	GLU
1	Aj	116	ARG
1	Aj	131	THR
1	Aj	158	SER

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Mol	Chain	Res	Type
1	Aj	167	LEU
1	Aj	170	THR
1	Aj	179	LYS
1	Aj	180	ARG
1	Aj	181	ASN
1	Aj	194	ASP
1	Aj	198	LEU
1	Aj	212	ASN
1	Aj	219	VAL
1	Ak	37	ARG
1	Ak	53	ILE
1	Ak	58	LYS
1	Ak	73	ARG
1	Ak	80	LEU
1	Ak	94	GLU
1	Ak	116	ARG
1	Ak	131	THR
1	Ak	158	SER
1	Ak	167	LEU
1	Ak	170	THR
1	Ak	179	LYS
1	Ak	180	ARG
1	Ak	181	ASN
1	Ak	194	ASP
1	Ak	198	LEU
1	Ak	212	ASN
1	Ak	219	VAL
1	Al	37	ARG
1	Al	53	ILE
1	Al	58	LYS
1	Al	73	ARG
1	Al	80	LEU
1	Al	94	GLU
1	Al	116	ARG
1	Al	131	THR
1	Al	158	SER
1	Al	167	LEU
1	Al	170	THR
1	Al	179	LYS
1	Al	180	ARG
1	Al	181	ASN
1	Al	194	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	Al	198	LEU
1	Al	212	ASN
1	Al	219	VAL
1	Am	37	ARG
1	Am	53	ILE
1	Am	58	LYS
1	Am	73	ARG
1	Am	80	LEU
1	Am	94	GLU
1	Am	116	ARG
1	Am	131	THR
1	Am	158	SER
1	Am	167	LEU
1	Am	170	THR
1	Am	179	LYS
1	Am	180	ARG
1	Am	181	ASN
1	Am	194	ASP
1	Am	198	LEU
1	Am	212	ASN
1	Am	219	VAL
1	An	37	ARG
1	An	53	ILE
1	An	58	LYS
1	An	73	ARG
1	An	80	LEU
1	An	94	GLU
1	An	116	ARG
1	An	131	THR
1	An	158	SER
1	An	167	LEU
1	An	170	THR
1	An	179	LYS
1	An	180	ARG
1	An	181	ASN
1	An	194	ASP
1	An	198	LEU
1	An	212	ASN
1	An	219	VAL
1	Ao	37	ARG
1	Ao	53	ILE
1	Ao	58	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	Ao	73	ARG
1	Ao	80	LEU
1	Ao	94	GLU
1	Ao	116	ARG
1	Ao	131	THR
1	Ao	158	SER
1	Ao	167	LEU
1	Ao	170	THR
1	Ao	179	LYS
1	Ao	180	ARG
1	Ao	181	ASN
1	Ao	194	ASP
1	Ao	198	LEU
1	Ao	212	ASN
1	Ao	219	VAL
1	Ap	37	ARG
1	Ap	53	ILE
1	Ap	58	LYS
1	Ap	73	ARG
1	Ap	80	LEU
1	Ap	94	GLU
1	Ap	116	ARG
1	Ap	131	THR
1	Ap	158	SER
1	Ap	167	LEU
1	Ap	170	THR
1	Ap	179	LYS
1	Ap	180	ARG
1	Ap	181	ASN
1	Ap	194	ASP
1	Ap	198	LEU
1	Ap	212	ASN
1	Ap	219	VAL
1	Aq	37	ARG
1	Aq	53	ILE
1	Aq	58	LYS
1	Aq	73	ARG
1	Aq	80	LEU
1	Aq	94	GLU
1	Aq	116	ARG
1	Aq	131	THR
1	Aq	158	SER

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Mol	Chain	Res	Type
1	Aq	167	LEU
1	Aq	170	THR
1	Aq	179	LYS
1	Aq	180	ARG
1	Aq	181	ASN
1	Aq	194	ASP
1	Aq	198	LEU
1	Aq	212	ASN
1	Aq	219	VAL
1	Ar	37	ARG
1	Ar	53	ILE
1	Ar	58	LYS
1	Ar	73	ARG
1	Ar	80	LEU
1	Ar	94	GLU
1	Ar	116	ARG
1	Ar	131	THR
1	Ar	158	SER
1	Ar	167	LEU
1	Ar	170	THR
1	Ar	179	LYS
1	Ar	180	ARG
1	Ar	181	ASN
1	Ar	194	ASP
1	Ar	198	LEU
1	Ar	212	ASN
1	Ar	219	VAL
1	As	37	ARG
1	As	53	ILE
1	As	58	LYS
1	As	73	ARG
1	As	80	LEU
1	As	94	GLU
1	As	116	ARG
1	As	131	THR
1	As	158	SER
1	As	167	LEU
1	As	170	THR
1	As	179	LYS
1	As	180	ARG
1	As	181	ASN
1	As	194	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	As	198	LEU
1	As	212	ASN
1	As	219	VAL
1	At	37	ARG
1	At	53	ILE
1	At	58	LYS
1	At	73	ARG
1	At	80	LEU
1	At	94	GLU
1	At	116	ARG
1	At	131	THR
1	At	158	SER
1	At	167	LEU
1	At	170	THR
1	At	179	LYS
1	At	180	ARG
1	At	181	ASN
1	At	194	ASP
1	At	198	LEU
1	At	212	ASN
1	At	219	VAL
1	Au	37	ARG
1	Au	53	ILE
1	Au	58	LYS
1	Au	73	ARG
1	Au	80	LEU
1	Au	94	GLU
1	Au	116	ARG
1	Au	131	THR
1	Au	158	SER
1	Au	167	LEU
1	Au	170	THR
1	Au	179	LYS
1	Au	180	ARG
1	Au	181	ASN
1	Au	194	ASP
1	Au	198	LEU
1	Au	212	ASN
1	Au	219	VAL
1	Av	37	ARG
1	Av	53	ILE
1	Av	58	LYS

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Mol	Chain	Res	Type
1	Av	73	ARG
1	Av	80	LEU
1	Av	94	GLU
1	Av	116	ARG
1	Av	131	THR
1	Av	158	SER
1	Av	167	LEU
1	Av	170	THR
1	Av	179	LYS
1	Av	180	ARG
1	Av	181	ASN
1	Av	194	ASP
1	Av	198	LEU
1	Av	212	ASN
1	Av	219	VAL
1	Aw	37	ARG
1	Aw	53	ILE
1	Aw	58	LYS
1	Aw	73	ARG
1	Aw	80	LEU
1	Aw	94	GLU
1	Aw	116	ARG
1	Aw	131	THR
1	Aw	158	SER
1	Aw	167	LEU
1	Aw	170	THR
1	Aw	179	LYS
1	Aw	180	ARG
1	Aw	181	ASN
1	Aw	194	ASP
1	Aw	198	LEU
1	Aw	212	ASN
1	Aw	219	VAL
1	Ax	37	ARG
1	Ax	53	ILE
1	Ax	58	LYS
1	Ax	73	ARG
1	Ax	80	LEU
1	Ax	94	GLU
1	Ax	116	ARG
1	Ax	131	THR
1	Ax	158	SER

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Mol	Chain	Res	Type
1	Ax	167	LEU
1	Ax	170	THR
1	Ax	179	LYS
1	Ax	180	ARG
1	Ax	181	ASN
1	Ax	194	ASP
1	Ax	198	LEU
1	Ax	212	ASN
1	Ax	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (262) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	75	ASN
1	A0	192	ASN
1	A0	195	HIS
1	A0	212	ASN
1	A1	75	ASN
1	A1	192	ASN
1	A1	195	HIS
1	A2	75	ASN
1	A2	192	ASN
1	A2	195	HIS
1	A2	212	ASN
1	A3	75	ASN
1	A3	188	GLN
1	A3	192	ASN
1	A3	195	HIS
1	A4	75	ASN
1	A4	188	GLN
1	A4	192	ASN
1	A4	195	HIS
1	A5	75	ASN
1	A5	188	GLN
1	A5	192	ASN
1	A5	195	HIS
1	A5	212	ASN
1	A6	75	ASN
1	A6	188	GLN
1	A6	192	ASN
1	A6	195	HIS
1	A6	212	ASN

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Mol	Chain	Res	Type
1	A7	75	ASN
1	A7	192	ASN
1	A7	195	HIS
1	A7	212	ASN
1	A8	75	ASN
1	A8	182	GLN
1	A8	188	GLN
1	A8	192	ASN
1	A8	195	HIS
1	A9	75	ASN
1	A9	188	GLN
1	A9	192	ASN
1	A9	195	HIS
1	A9	212	ASN
1	AA	75	ASN
1	AA	182	GLN
1	AA	188	GLN
1	AA	192	ASN
1	AA	195	HIS
1	AA	212	ASN
1	AB	75	ASN
1	AB	182	GLN
1	AB	188	GLN
1	AB	192	ASN
1	AB	195	HIS
1	AB	212	ASN
1	AC	75	ASN
1	AC	192	ASN
1	AC	195	HIS
1	AD	75	ASN
1	AD	188	GLN
1	AD	192	ASN
1	AD	212	ASN
1	AE	75	ASN
1	AE	192	ASN
1	AE	195	HIS
1	AE	212	ASN
1	AF	75	ASN
1	AF	192	ASN
1	AF	195	HIS
1	AG	75	ASN
1	AG	188	GLN

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Mol	Chain	Res	Type
1	AG	192	ASN
1	AG	195	HIS
1	AG	212	ASN
1	AH	75	ASN
1	AH	192	ASN
1	AH	195	HIS
1	AH	212	ASN
1	AI	75	ASN
1	AI	188	GLN
1	AI	192	ASN
1	AI	195	HIS
1	AI	212	ASN
1	AJ	75	ASN
1	AJ	192	ASN
1	AJ	195	HIS
1	AJ	212	ASN
1	AK	75	ASN
1	AK	188	GLN
1	AK	192	ASN
1	AK	195	HIS
1	AL	75	ASN
1	AL	192	ASN
1	AL	195	HIS
1	AL	212	ASN
1	AM	75	ASN
1	AM	188	GLN
1	AM	192	ASN
1	AM	195	HIS
1	AM	212	ASN
1	AN	75	ASN
1	AN	188	GLN
1	AN	192	ASN
1	AN	195	HIS
1	AN	212	ASN
1	AO	75	ASN
1	AO	188	GLN
1	AO	192	ASN
1	AO	195	HIS
1	AO	212	ASN
1	AP	75	ASN
1	AP	182	GLN
1	AP	188	GLN

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Mol	Chain	Res	Type
1	AP	192	ASN
1	AP	195	HIS
1	AQ	75	ASN
1	AQ	188	GLN
1	AQ	192	ASN
1	AQ	195	HIS
1	AQ	212	ASN
1	AR	75	ASN
1	AR	192	ASN
1	AR	195	HIS
1	AR	212	ASN
1	AS	75	ASN
1	AS	188	GLN
1	AS	192	ASN
1	AS	195	HIS
1	AT	75	ASN
1	AT	192	ASN
1	AT	195	HIS
1	AT	212	ASN
1	AU	75	ASN
1	AU	188	GLN
1	AU	192	ASN
1	AU	195	HIS
1	AV	75	ASN
1	AV	192	ASN
1	AV	212	ASN
1	AW	75	ASN
1	AW	188	GLN
1	AW	192	ASN
1	AW	195	HIS
1	AW	212	ASN
1	AX	75	ASN
1	AX	182	GLN
1	AX	188	GLN
1	AX	192	ASN
1	AX	195	HIS
1	AX	212	ASN
1	AY	75	ASN
1	AY	182	GLN
1	AY	188	GLN
1	AY	192	ASN
1	AY	195	HIS

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Mol	Chain	Res	Type
1	AZ	75	ASN
1	AZ	188	GLN
1	AZ	192	ASN
1	AZ	195	HIS
1	Aa	75	ASN
1	Aa	188	GLN
1	Aa	192	ASN
1	Aa	195	HIS
1	Aa	212	ASN
1	Ab	75	ASN
1	Ab	182	GLN
1	Ab	192	ASN
1	Ab	195	HIS
1	Ab	212	ASN
1	Ac	75	ASN
1	Ac	188	GLN
1	Ac	192	ASN
1	Ac	195	HIS
1	Ac	212	ASN
1	Ad	75	ASN
1	Ad	188	GLN
1	Ad	192	ASN
1	Ad	195	HIS
1	Ad	212	ASN
1	Ae	75	ASN
1	Ae	192	ASN
1	Ae	195	HIS
1	Af	75	ASN
1	Af	188	GLN
1	Af	192	ASN
1	Af	195	HIS
1	Ag	75	ASN
1	Ag	188	GLN
1	Ag	192	ASN
1	Ag	195	HIS
1	Ah	75	ASN
1	Ah	188	GLN
1	Ah	192	ASN
1	Ah	195	HIS
1	Ai	75	ASN
1	Ai	188	GLN
1	Ai	192	ASN

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Mol	Chain	Res	Type
1	Ai	195	HIS
1	Ai	212	ASN
1	Aj	75	ASN
1	Aj	192	ASN
1	Aj	195	HIS
1	Aj	212	ASN
1	Ak	75	ASN
1	Ak	188	GLN
1	Ak	192	ASN
1	Ak	195	HIS
1	Al	75	ASN
1	Al	188	GLN
1	Al	192	ASN
1	Al	195	HIS
1	Am	75	ASN
1	Am	182	GLN
1	Am	188	GLN
1	Am	192	ASN
1	Am	195	HIS
1	Am	212	ASN
1	An	75	ASN
1	An	188	GLN
1	An	192	ASN
1	An	195	HIS
1	An	212	ASN
1	Ao	75	ASN
1	Ao	192	ASN
1	Ao	195	HIS
1	Ap	75	ASN
1	Ap	192	ASN
1	Ap	195	HIS
1	Ap	212	ASN
1	Aq	75	ASN
1	Aq	188	GLN
1	Aq	192	ASN
1	Ar	75	ASN
1	Ar	188	GLN
1	Ar	192	ASN
1	Ar	195	HIS
1	As	75	ASN
1	As	188	GLN
1	As	192	ASN

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Mol	Chain	Res	Type
1	As	195	HIS
1	At	75	ASN
1	At	188	GLN
1	At	192	ASN
1	At	195	HIS
1	At	212	ASN
1	Au	75	ASN
1	Au	192	ASN
1	Au	195	HIS
1	Au	212	ASN
1	Av	75	ASN
1	Av	188	GLN
1	Av	192	ASN
1	Av	195	HIS
1	Av	212	ASN
1	Aw	75	ASN
1	Aw	192	ASN
1	Aw	195	HIS
1	Aw	212	ASN
1	Ax	75	ASN
1	Ax	188	GLN
1	Ax	192	ASN
1	Ax	195	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

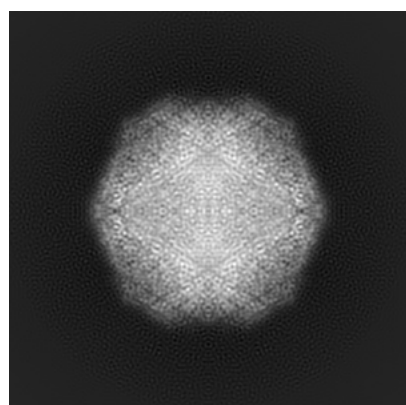
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20113. These allow visual inspection of the internal detail of the map and identification of artifacts.

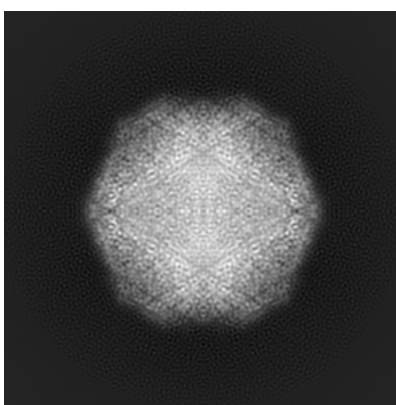
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

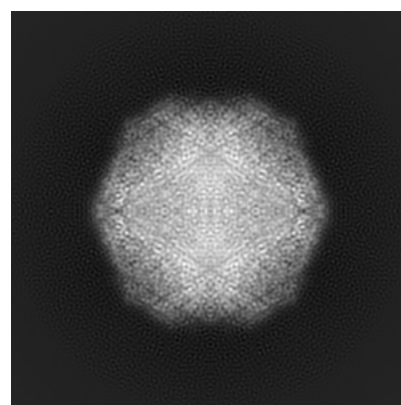
6.1.1 Primary map



X



Y

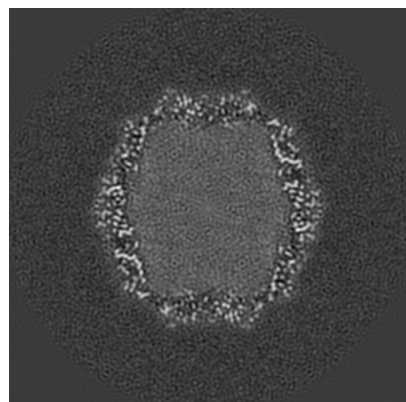


Z

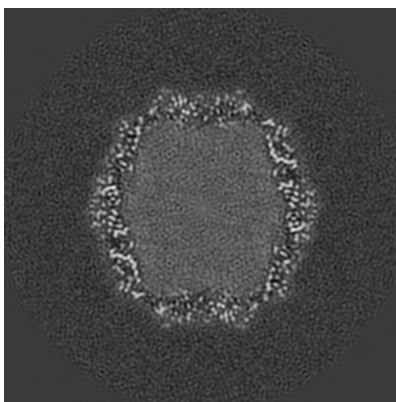
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

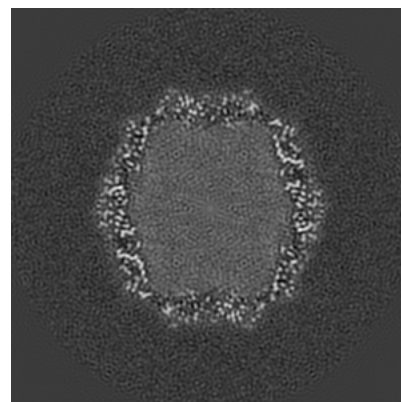
6.2.1 Primary map



X Index: 150



Y Index: 150

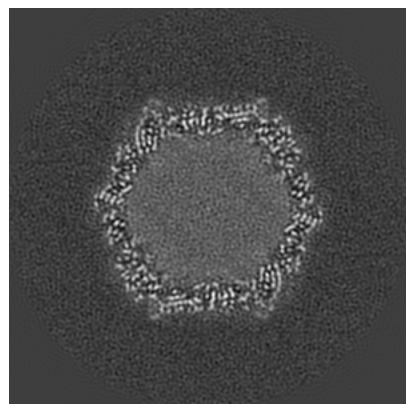


Z Index: 150

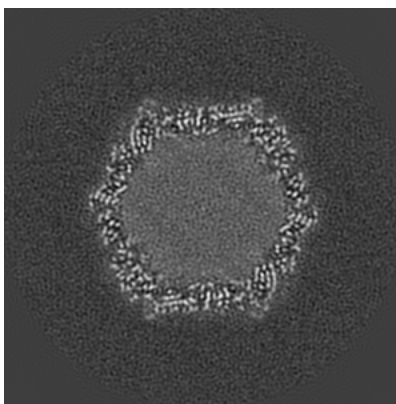
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

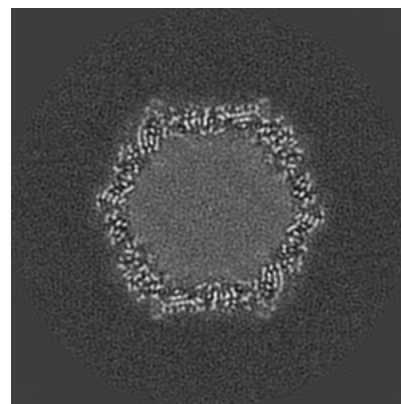
6.3.1 Primary map



X Index: 168



Y Index: 168

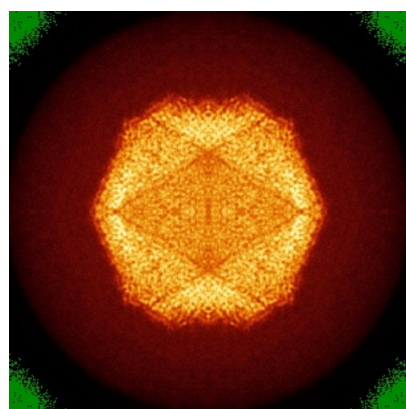


Z Index: 168

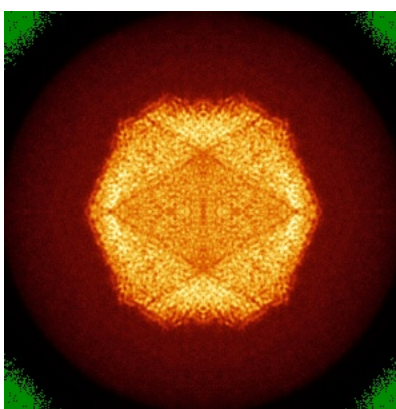
The images above show the largest variance slices of the map in three orthogonal directions.

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

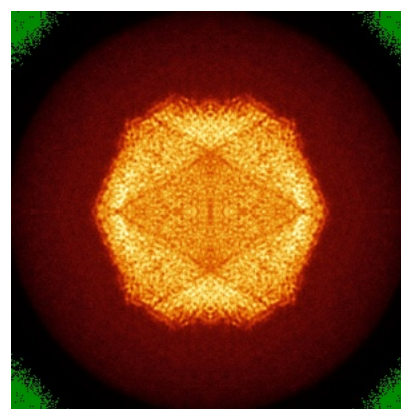
6.4.1 Primary map



X



Y

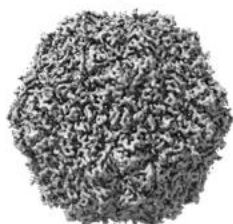


Z

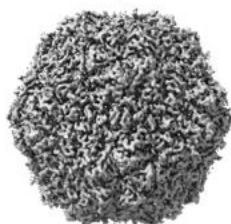
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

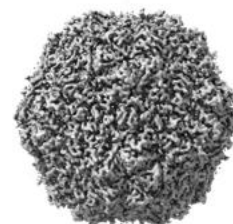
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

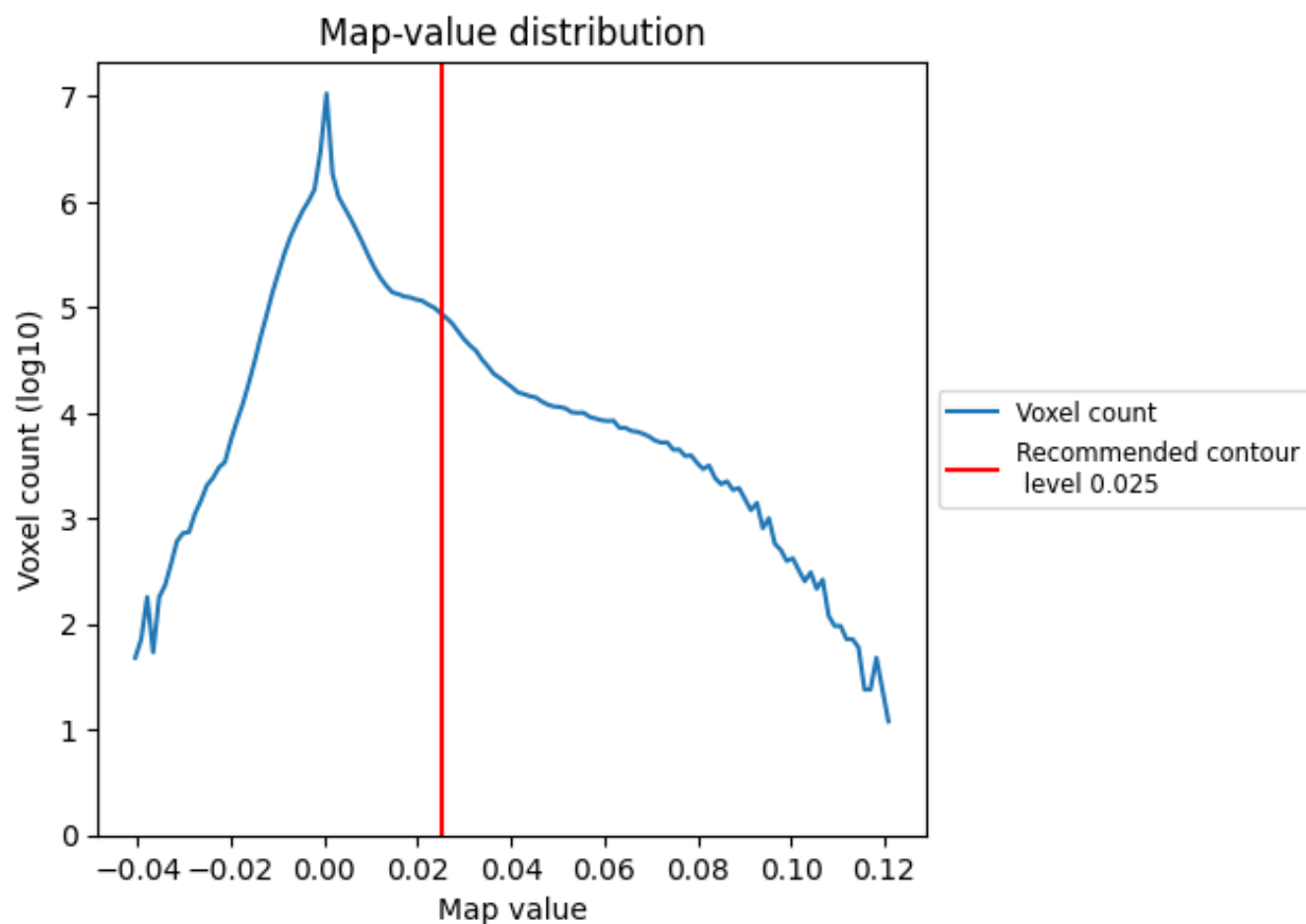
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

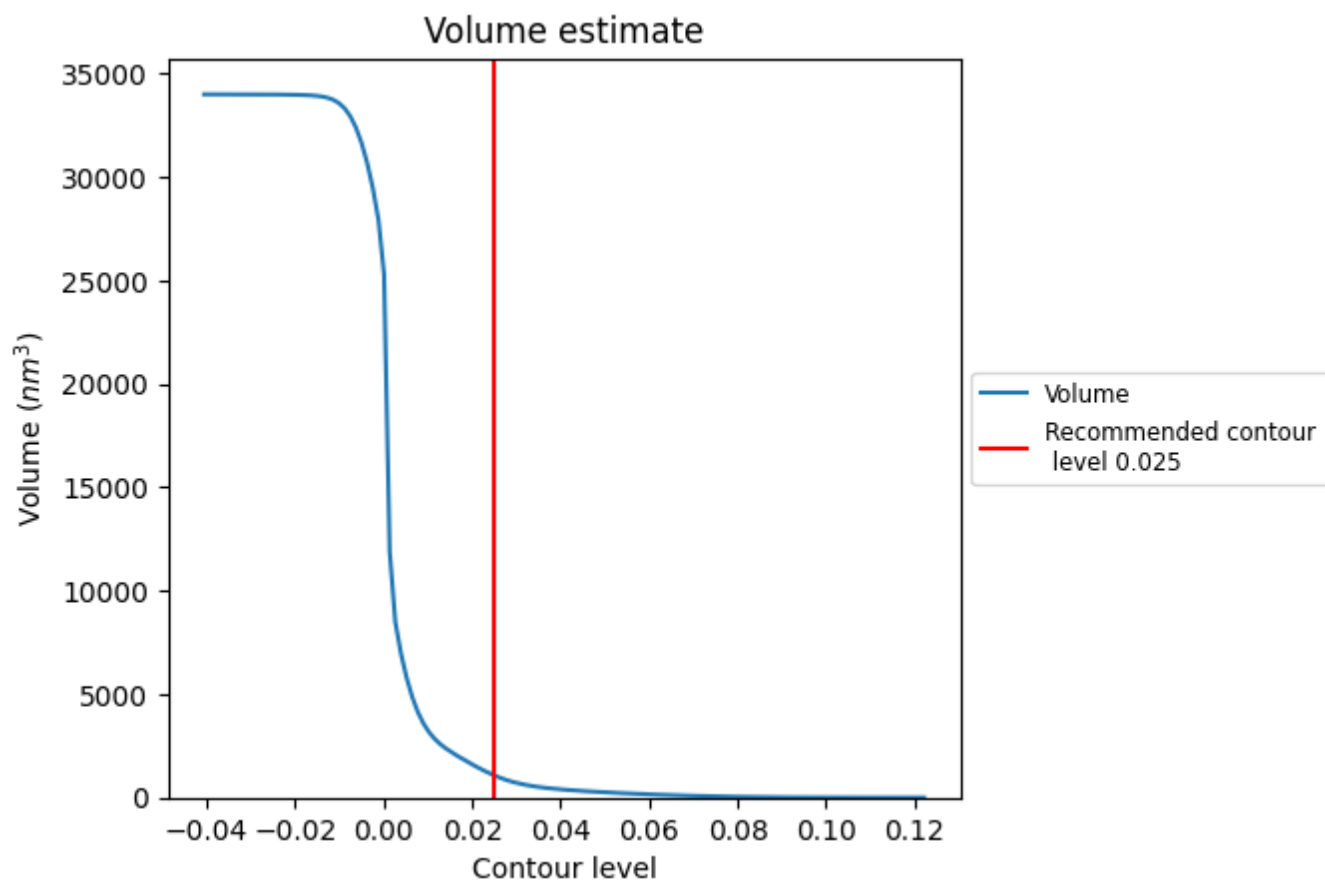
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

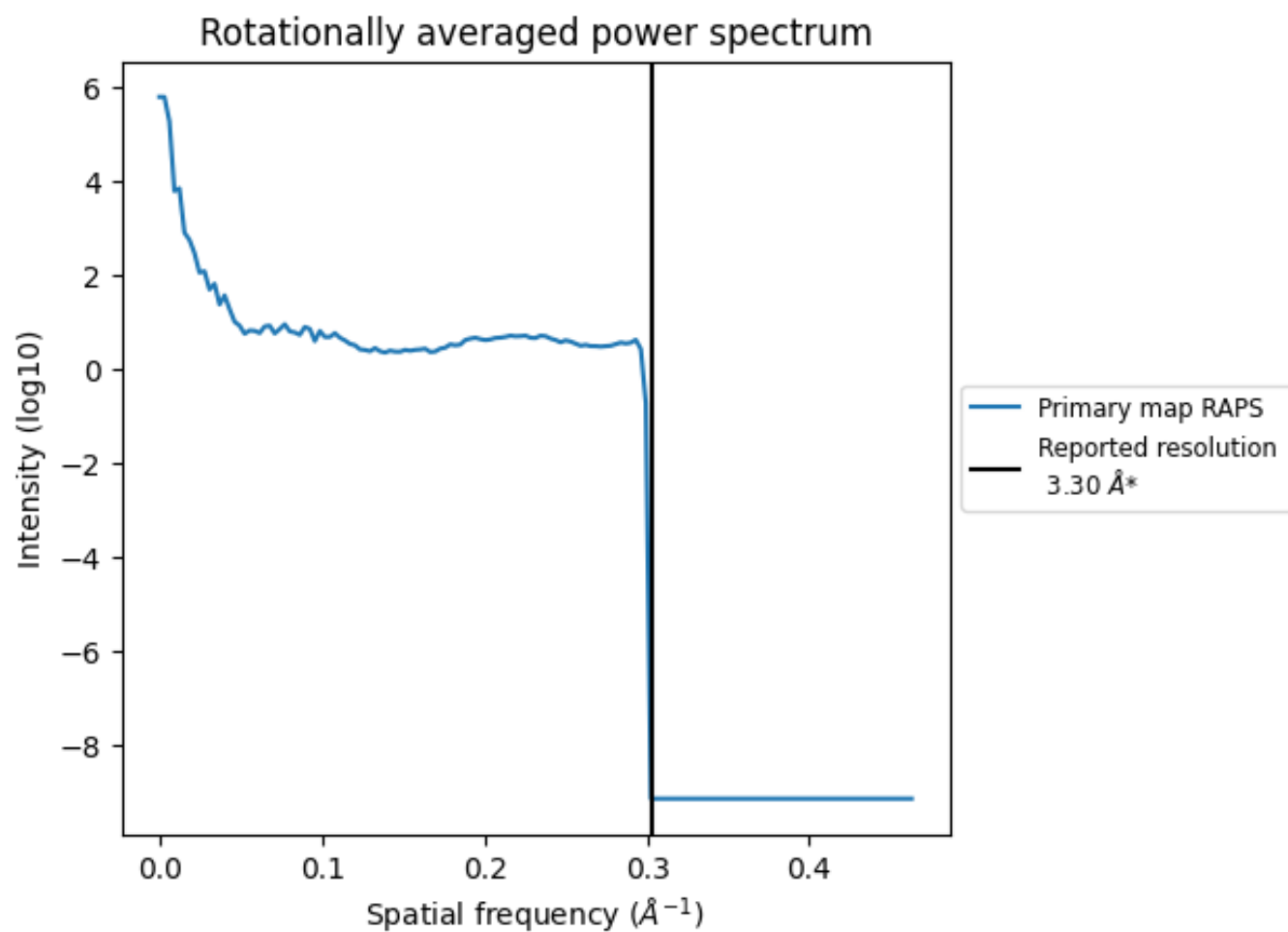
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1078 nm^3 ; this corresponds to an approximate mass of 974 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 0.303 Å⁻¹

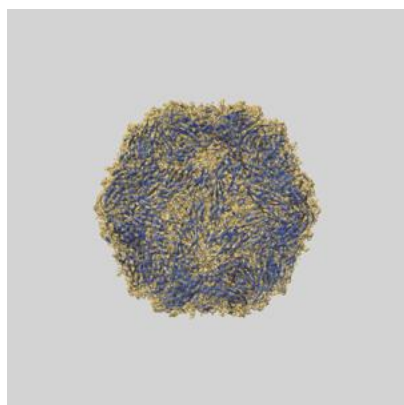
8 Fourier-Shell correlation

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

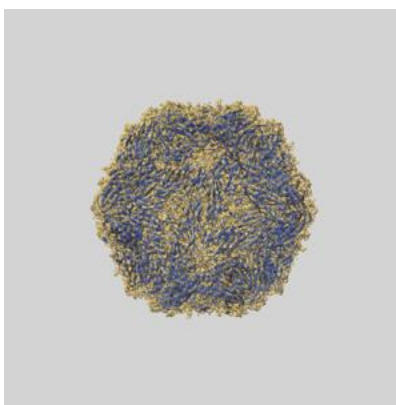
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20113 and PDB model 6OLA. Per-residue inclusion information can be found in section 3 on page 14.

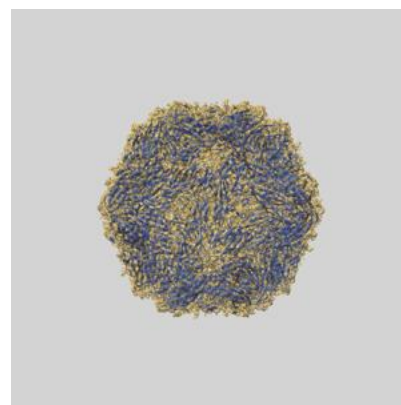
9.1 Map-model overlay [i](#)



X



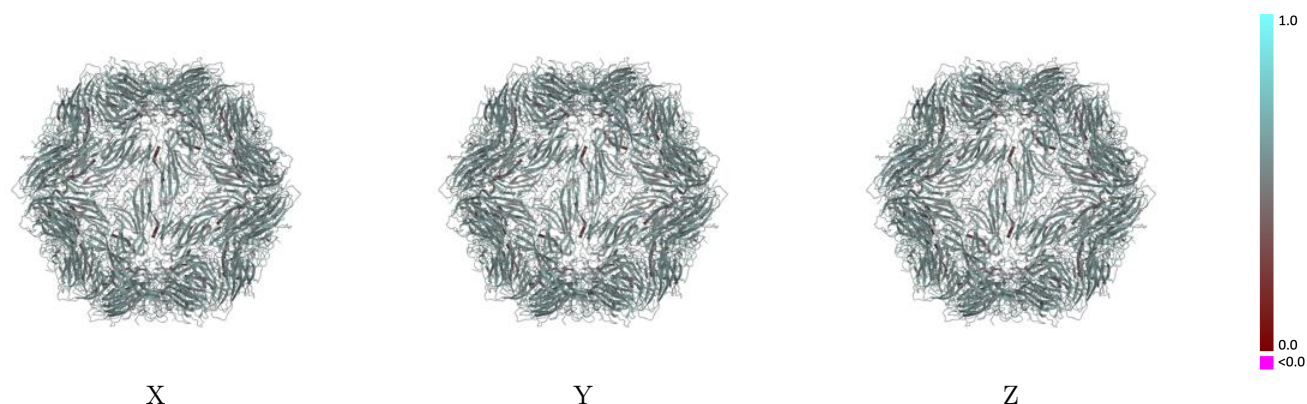
Y



Z

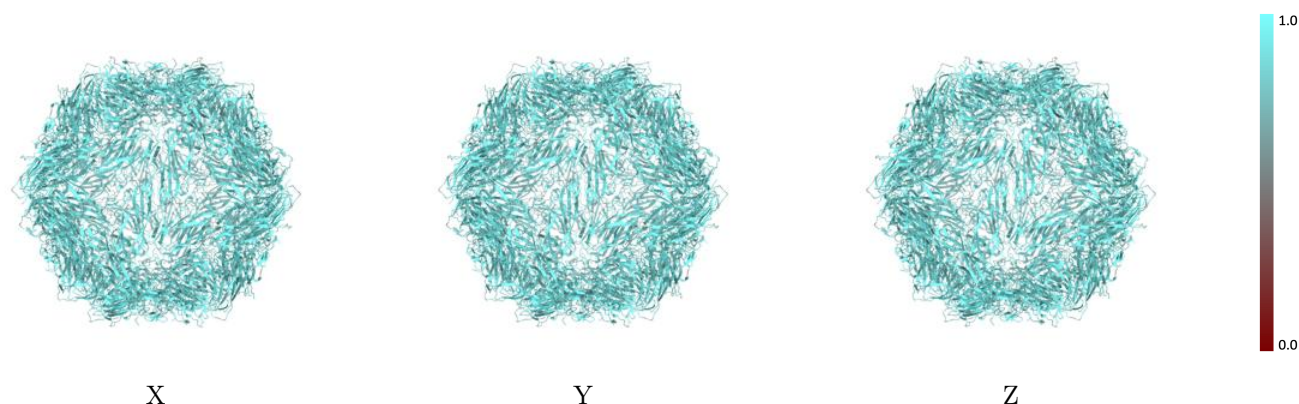
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



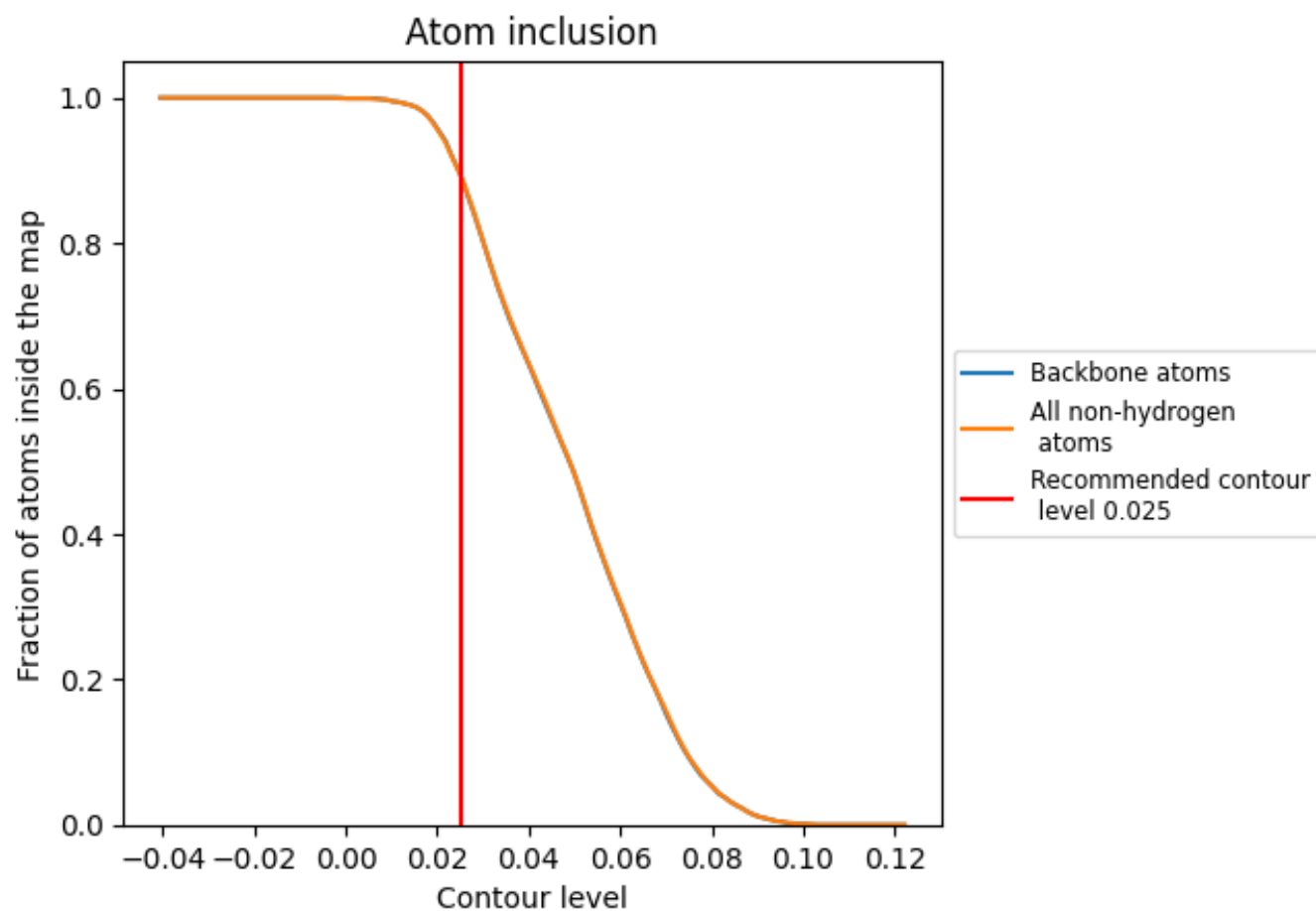
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.5390
A0	 0.9030	 0.5440
A1	 0.9060	 0.5430
A2	 0.9030	 0.5430
A3	 0.9010	 0.5430
A4	 0.9050	 0.5460
A5	 0.9030	 0.5460
A6	 0.9050	 0.5430
A7	 0.9020	 0.5440
A8	 0.9080	 0.5460
A9	 0.9080	 0.5460
AA	 0.9050	 0.5450
AB	 0.9050	 0.5500
AC	 0.9050	 0.5470
AD	 0.9000	 0.5430
AE	 0.9060	 0.5470
AF	 0.9030	 0.5450
AG	 0.9060	 0.5460
AH	 0.9010	 0.5440
AI	 0.9030	 0.5430
AJ	 0.8990	 0.5420
AK	 0.9060	 0.5440
AL	 0.9040	 0.5470
AM	 0.9060	 0.5480
AN	 0.9030	 0.5450
AO	 0.9040	 0.5440
AP	 0.9010	 0.5440
AQ	 0.9060	 0.5450
AR	 0.9050	 0.5460
AS	 0.9050	 0.5470
AT	 0.9010	 0.5460
AU	 0.9060	 0.5460
AV	 0.9060	 0.5470
AW	 0.9030	 0.5460
AX	 0.9040	 0.5460



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Chain	Atom inclusion	Q-score
AY	 0.8980	 0.5480
AZ	 0.9040	 0.5460
Aa	 0.9040	 0.5460
Ab	 0.9010	 0.5470
Ac	 0.9020	 0.5460
Ad	 0.9030	 0.5470
Ae	 0.9010	 0.5450
Af	 0.9060	 0.5450
Ag	 0.9040	 0.5420
Ah	 0.9000	 0.5460
Ai	 0.9050	 0.5460
Aj	 0.9070	 0.5470
Ak	 0.9050	 0.5460
Al	 0.9060	 0.5450
Am	 0.9010	 0.5420
An	 0.9020	 0.5460
Ao	 0.9030	 0.5430
Ap	 0.9040	 0.5470
Aq	 0.9040	 0.5460
Ar	 0.9020	 0.5430
As	 0.9080	 0.5440
At	 0.9080	 0.5430
Au	 0.9030	 0.5430
Av	 0.9070	 0.5450
Aw	 0.9020	 0.5440
Ax	 0.9050	 0.5450
B0	 0.8540	 0.4070
B1	 0.8420	 0.4180
B2	 0.8660	 0.4150
B3	 0.8540	 0.4100
B4	 0.8420	 0.4160
B5	 0.8540	 0.4160
B6	 0.8660	 0.4170
B7	 0.8420	 0.4110
B8	 0.8540	 0.4100
B9	 0.8540	 0.4170
BA	 0.8420	 0.4130
BB	 0.8540	 0.4110
BC	 0.8290	 0.4300
BD	 0.8540	 0.4180
BE	 0.8540	 0.4130
BF	 0.8540	 0.4100

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Chain	Atom inclusion	Q-score
BG	 0.8540	 0.4150
BH	 0.8540	 0.4220
BI	 0.8660	 0.4110
BJ	 0.8540	 0.4140
BK	 0.8540	 0.4110
BL	 0.8540	 0.4210
BM	 0.8540	 0.4220
BN	 0.8660	 0.4210
BO	 0.8660	 0.4190
BP	 0.8540	 0.4190
BQ	 0.8660	 0.4170
BR	 0.8420	 0.4150
BS	 0.8540	 0.4180
BT	 0.8420	 0.4100
BU	 0.8540	 0.4200
BV	 0.8540	 0.4150
BW	 0.8540	 0.4110
BX	 0.8420	 0.4210
BY	 0.8540	 0.4070
BZ	 0.8540	 0.4140
Ba	 0.8540	 0.4140
Bb	 0.8540	 0.4170
Bc	 0.8420	 0.4230
Bd	 0.8420	 0.4190
Be	 0.8420	 0.4200
Bf	 0.8540	 0.4150
Bg	 0.8540	 0.4160
Bh	 0.8540	 0.4130
Bi	 0.8540	 0.4190
Bj	 0.8540	 0.4170
Bk	 0.8540	 0.4170
Bl	 0.8540	 0.4120
Bm	 0.8420	 0.4130
Bn	 0.8540	 0.4210
Bo	 0.8540	 0.4090
Bp	 0.8540	 0.4170
Bq	 0.8540	 0.4170
Br	 0.8540	 0.4170
Bs	 0.8540	 0.4170
Bt	 0.8420	 0.4060
Bu	 0.8540	 0.4050
Bv	 0.8540	 0.4080

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Chain	Atom inclusion	Q-score
Bw	 0.8420	 0.4150
Bx	 0.8540	 0.4230