



Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 05:33 pm GMT

PDB ID : 9RKU / pdb_00009rku
EMDB ID : EMD-54021
Title : Agrobacterium phage 7-7-1 baseplate
Authors : Noteborn, W.E.M.; Hoeksma, T.; Briegel, A.
Deposited on : 2025-06-14
Resolution : 3.44 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:

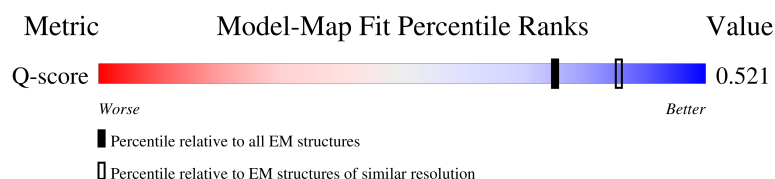
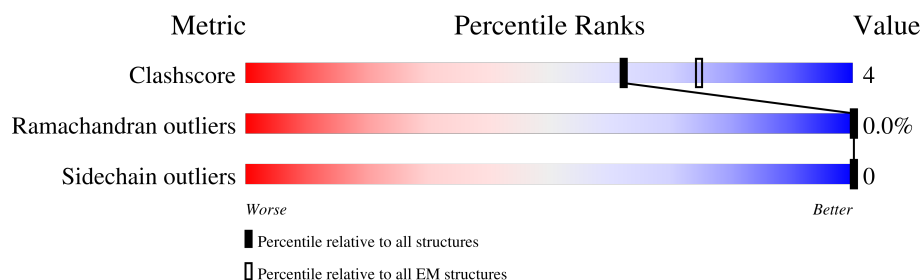
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

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 3.44 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.









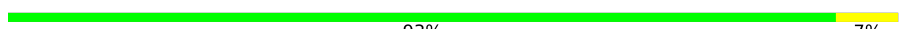

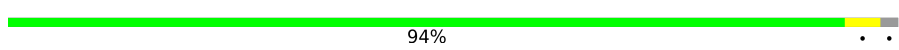
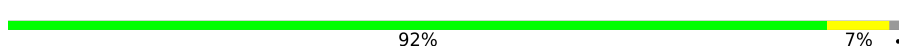
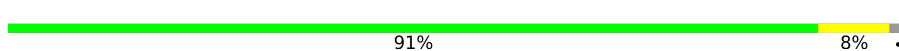
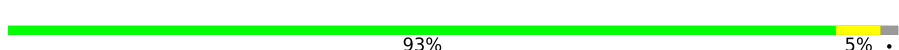
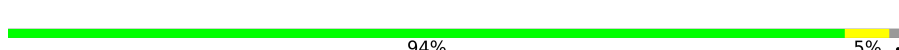
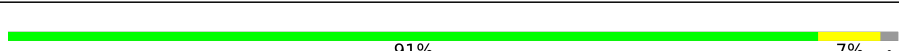
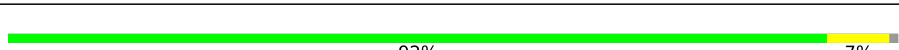
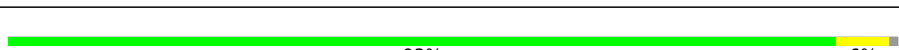
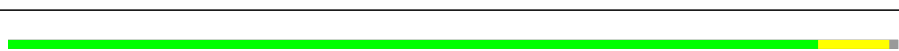

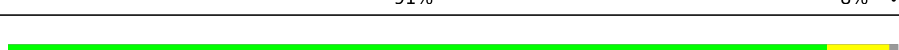
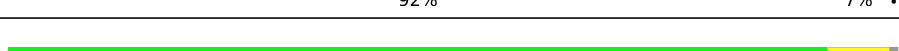
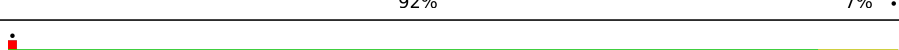
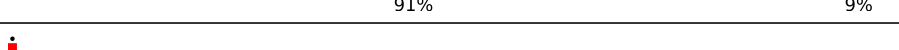
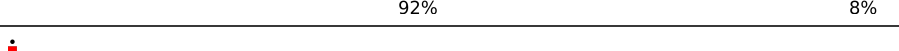
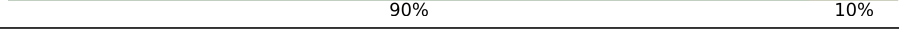
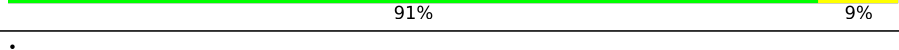
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13877 (2.94 - 3.94)

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	Ac	189	75% 16% 9%
1	Ad	189	70% 21% 9%
1	Ae	189	72% 19% 9%
2	Af	454	58% 14% 28%

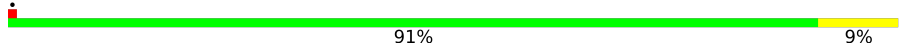


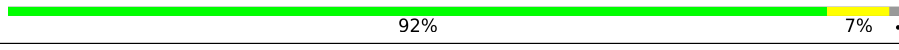

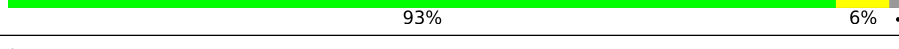
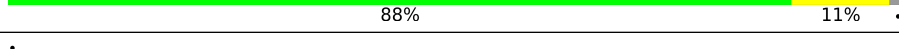
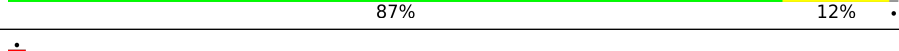
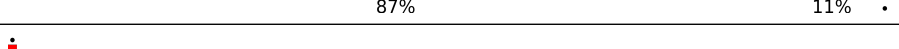
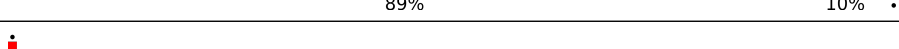
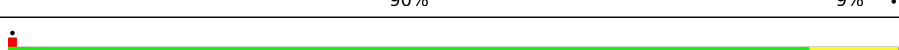
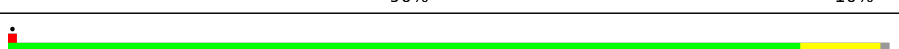
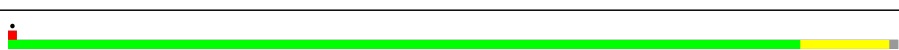

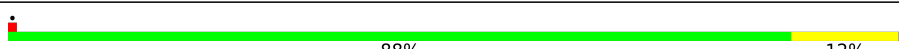


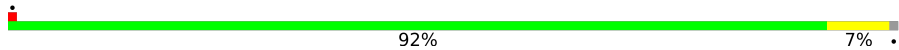


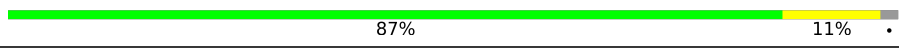
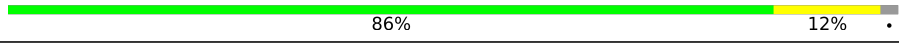



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Mol	Chain	Length	Quality of chain
2	Ag	454	
2	Ah	454	
3	Ai	286	
3	Aj	286	
3	Ak	286	
3	Al	286	
3	Am	286	
3	An	286	
4	Ao	396	
4	Ap	396	
4	Aq	396	
4	Ar	396	
4	As	396	
4	At	396	
4	Au	396	
4	Av	396	
4	Aw	396	
4	Ax	396	
4	Ay	396	
4	Az	396	
5	A1	398	
5	A2	398	
5	A3	398	
5	A4	398	
5	A5	398	

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Mol	Chain	Length	Quality of chain
5	A6	398	 91%9%
6	A0	178	 90%8%
6	A7	178	 88%10%
6	A8	178	 92%7%
6	A9	178	 88%11%
6	BA	178	 93%6%
6	BB	178	 88%11%
7	BC	503	 87%12%
7	BD	503	 87%11%
7	BE	503	 89%10%
7	BF	503	 90%9%
7	BG	503	 90%10%
7	BH	503	 89%9%
7	BI	503	 89%10%
7	BJ	503	 89%10%
7	BK	503	 88%12%
7	BL	503	 90%8%
7	BM	503	 88%11%
7	BN	503	 92%7%
8	BO	136	 88%10%
8	BP	136	 85%12%
8	BQ	136	 87%11%
8	BR	136	 86%12%
8	BS	136	 88%10%
8	BT	136	 86%12%

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Mol	Chain	Length	Quality of chain
8	BU	136	 93% . .
8	BV	136	 79% 18% .
8	BW	136	 85% 13% .
8	BX	136	 79% 19% .
8	BY	136	 88% 10% .
8	BZ	136	 85% 12% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 284548 atoms, of which 140170 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 Baseplate protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ac	172	Total	C	H	N	O	S	0	0
			2580	817	1251	232	277	3		
1	Ad	172	Total	C	H	N	O	S	0	0
			2580	817	1251	232	277	3		
1	Ae	172	Total	C	H	N	O	S	0	0
			2580	817	1251	232	277	3		

- Molecule 2 is a protein called Putative tail biosynthetic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Af	325	Total	C	H	N	O	S	0	0
			5073	1600	2530	442	494	7		
2	Ag	325	Total	C	H	N	O	S	0	0
			5073	1600	2530	442	494	7		
2	Ah	325	Total	C	H	N	O	S	0	0
			5073	1600	2530	442	494	7		

- Molecule 3 is a protein called Structural protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Ai	286	Total	C	H	N	O	S	0	0
			4353	1399	2153	356	423	22		
3	Aj	286	Total	C	H	N	O	S	0	0
			4353	1399	2153	356	423	22		
3	Ak	286	Total	C	H	N	O	S	0	0
			4353	1399	2153	356	423	22		
3	Al	286	Total	C	H	N	O	S	0	0
			4353	1399	2153	356	423	22		
3	Am	286	Total	C	H	N	O	S	0	0
			4353	1399	2153	356	423	22		
3	An	286	Total	C	H	N	O	S	0	0
			4353	1399	2153	356	423	22		

- Molecule 4 is a protein called Baseplate protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ao	390	Total	C	H	N	O	S	0	0
			5910	1889	2904	515	581	21		
4	Ap	390	Total	C	H	N	O	S	0	0
			5910	1889	2904	515	581	21		
4	Aq	390	Total	C	H	N	O	S	0	0
			5910	1889	2904	515	581	21		
4	Ar	390	Total	C	H	N	O	S	0	0
			5910	1889	2904	515	581	21		
4	As	390	Total	C	H	N	O	S	0	0
			5910	1889	2904	515	581	21		
4	At	390	Total	C	H	N	O	S	0	0
			5910	1889	2904	515	581	21		
4	Au	391	Total	C	H	N	O	S	0	0
			5922	1892	2911	516	582	21		
4	Av	391	Total	C	H	N	O	S	0	0
			5922	1892	2911	516	582	21		
4	Aw	391	Total	C	H	N	O	S	0	0
			5922	1892	2911	516	582	21		
4	Ax	391	Total	C	H	N	O	S	0	0
			5922	1892	2911	516	582	21		
4	Ay	391	Total	C	H	N	O	S	0	0
			5922	1892	2911	516	582	21		
4	Az	391	Total	C	H	N	O	S	0	0
			5922	1892	2911	516	582	21		

- Molecule 5 is a protein called Putative tail biosynthetic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A1	398	Total	C	H	N	O	S	0	0
			6053	1944	2969	528	603	9		
5	A2	398	Total	C	H	N	O	S	0	0
			6053	1944	2969	528	603	9		
5	A3	398	Total	C	H	N	O	S	0	0
			6053	1944	2969	528	603	9		
5	A4	398	Total	C	H	N	O	S	0	0
			6053	1944	2969	528	603	9		
5	A5	398	Total	C	H	N	O	S	0	0
			6053	1944	2969	528	603	9		
5	A6	398	Total	C	H	N	O	S	0	0
			6053	1944	2969	528	603	9		

- Molecule 6 is a protein called Putative structural protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	A7	175	Total	C	H	N	O	S	0	0
			2626	815	1298	244	260	9		
6	A8	175	Total	C	H	N	O	S	0	0
			2626	815	1298	244	260	9		
6	A9	175	Total	C	H	N	O	S	0	0
			2626	815	1298	244	260	9		
6	A0	175	Total	C	H	N	O	S	0	0
			2626	815	1298	244	260	9		
6	BA	175	Total	C	H	N	O	S	0	0
			2626	815	1298	244	260	9		
6	BB	175	Total	C	H	N	O	S	0	0
			2626	815	1298	244	260	9		

- Molecule 7 is a protein called Tail sheath protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	BN	496	Total	C	H	N	O	S	0	0
			7376	2349	3634	631	742	20		
7	BC	500	Total	C	H	N	O	S	0	0
			7434	2366	3662	636	749	21		
7	BD	496	Total	C	H	N	O	S	0	0
			7376	2349	3634	631	742	20		
7	BE	500	Total	C	H	N	O	S	0	0
			7434	2366	3662	636	749	21		
7	BF	496	Total	C	H	N	O	S	0	0
			7376	2349	3634	631	742	20		
7	BG	500	Total	C	H	N	O	S	0	0
			7434	2366	3662	636	749	21		
7	BH	496	Total	C	H	N	O	S	0	0
			7376	2349	3634	631	742	20		
7	BI	500	Total	C	H	N	O	S	0	0
			7434	2366	3662	636	749	21		
7	BJ	496	Total	C	H	N	O	S	0	0
			7376	2349	3634	631	742	20		
7	BK	500	Total	C	H	N	O	S	0	0
			7434	2366	3662	636	749	21		
7	BL	496	Total	C	H	N	O	S	0	0
			7376	2349	3634	631	742	20		
7	BM	500	Total	C	H	N	O	S	0	0
			7434	2366	3662	636	749	21		

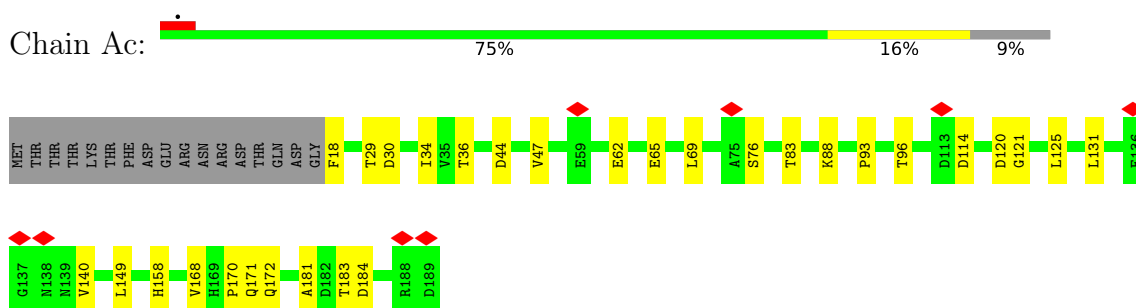
- Molecule 8 is a protein called Structural protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	BO	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BP	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BQ	133	Total 1963	C 616	H 971	N 166	O 202	S 8	0	0
8	BR	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BS	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BT	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BU	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BV	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BW	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BX	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BY	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0
8	BZ	133	Total 1962	C 616	H 970	N 166	O 202	S 8	0	0

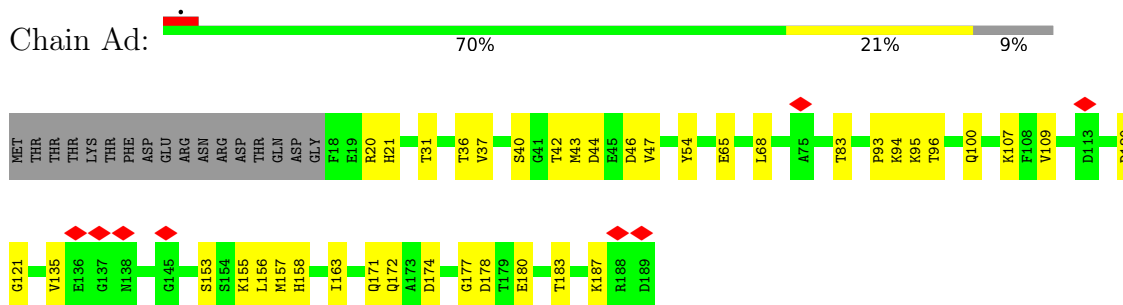
3 Residue-property plots

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.

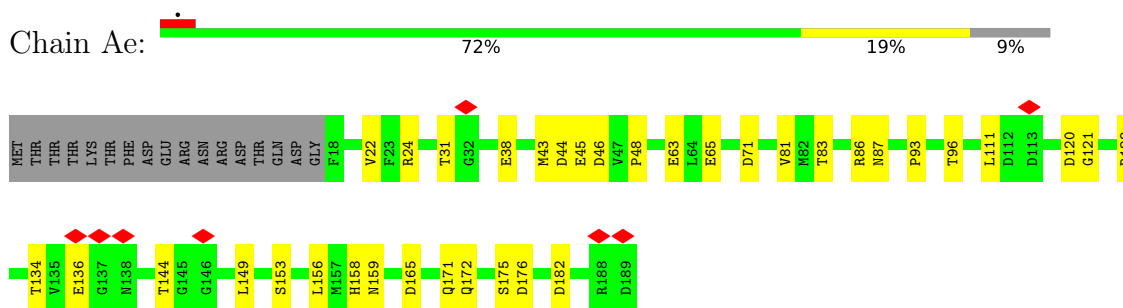
- Molecule 1: Baseplate protein



- Molecule 1: Baseplate protein



- Molecule 1: Baseplate protein



- Molecule 2: Putative tail biosynthetic protein





SER	GLY	LEU	ASN	GLU	LEU	SER	SER	ILE	SER	ASN	SER	LEU	GLN	ALA	ASP	ILE	GLY	VAL	ALA	ARG	VAL	GLN	ALA	GLY	ILE	LYS	LEU	ILE	ALA	GLY	GLN	TYR	PRO	SER	THR	TRP	THR	SER	ALA	ALA	LEU	SER	ALA	ILE	THR	THR	PRO	VAL	ASN	VAL	ILE	ALA	VAL	VAL	ASN	SER	SER	LEU
LEU	LEU	ASN	GLU	GLU	ASP	GLU	SER	THR	THR	PRO	PRO	LYS	GLN	PRO	PRO	LEU	ARG	GLY	LEU	PRO	PRO	PRO	GLU																																			

• Molecule 3: Structural protein

Chain Ai:  89% 11%



• Molecule 3: Structural protein

Chain Aj:  91% 9%



• Molecule 3: Structural protein

Chain Ak:  92% 8%



• Molecule 3: Structural protein

Chain Al:  92% 8%



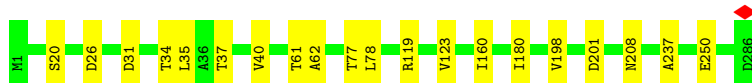
• Molecule 3: Structural protein

Chain Am:  93% 7%



• Molecule 3: Structural protein

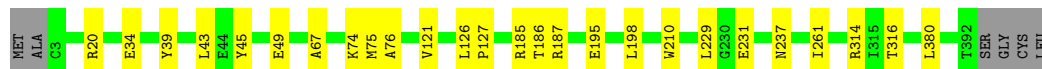
Chain An:  93% 7%



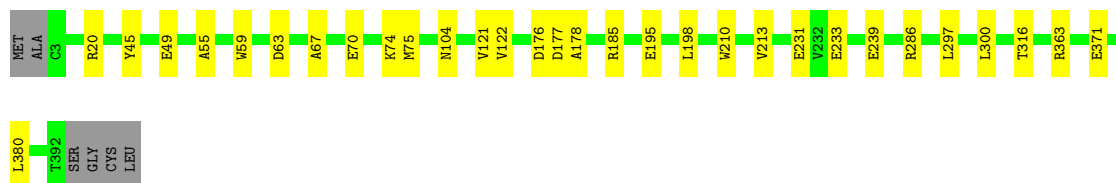
• Molecule 4: Baseplate protein

Chain Ao:  94% . .

• Molecule 4: Baseplate protein

Chain Ap:  92% 7% .

• Molecule 4: Baseplate protein

Chain Aq:  91% 8% .

• Molecule 4: Baseplate protein

Chain Ar:  93% 5% .

• Molecule 4: Baseplate protein

Chain As:  94% 5% .

• Molecule 4: Baseplate protein

Chain At:  91% 7% .

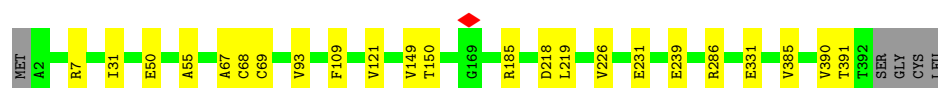
• Molecule 4: Baseplate protein

Chain Au:  92% 7%



- Molecule 4: Baseplate protein

Chain Av:  93% 6%



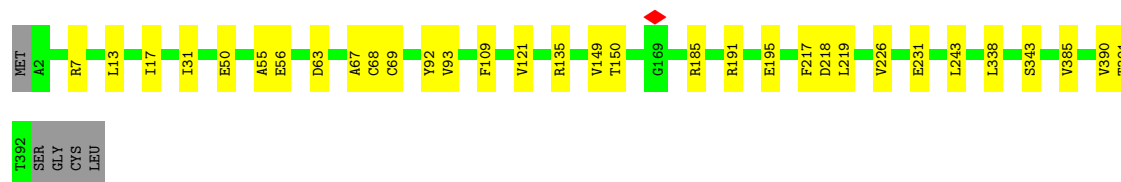
- Molecule 4: Baseplate protein

Chain Aw:  91% 8%



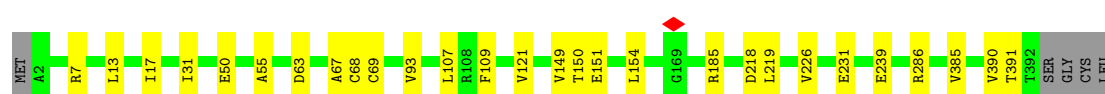
- Molecule 4: Baseplate protein

Chain Ax:  91% 8%



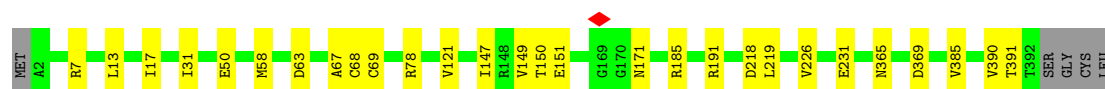
- Molecule 4: Baseplate protein

Chain Ay:  92% 7%




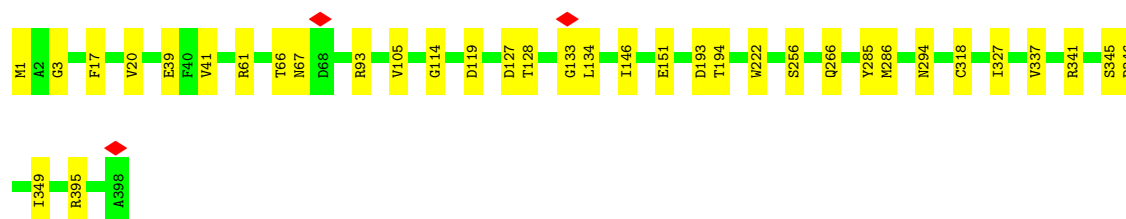
- Molecule 4: Baseplate protein

Chain Az:  92% 7%



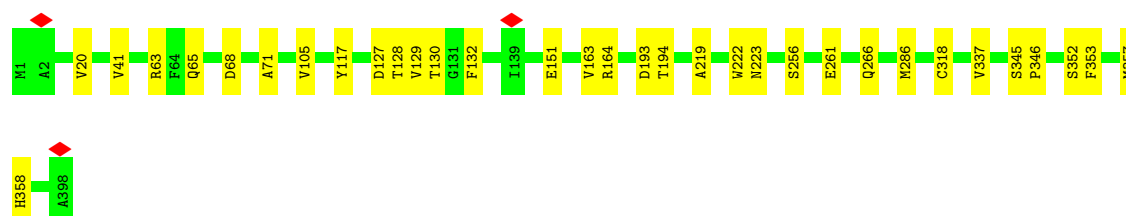
- Molecule 5: Putative tail biosynthetic protein

Chain A1:  91% 9%




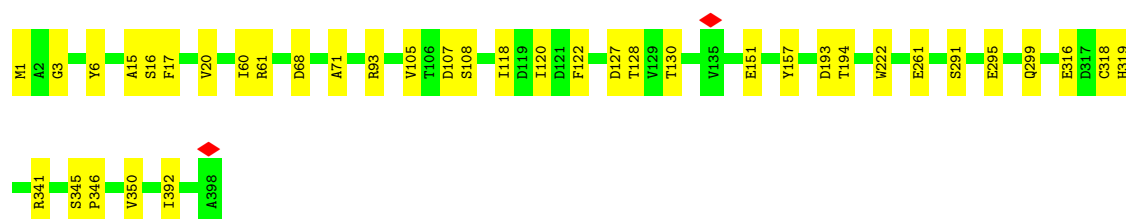
- Molecule 5: Putative tail biosynthetic protein

Chain A2:  92% 8%



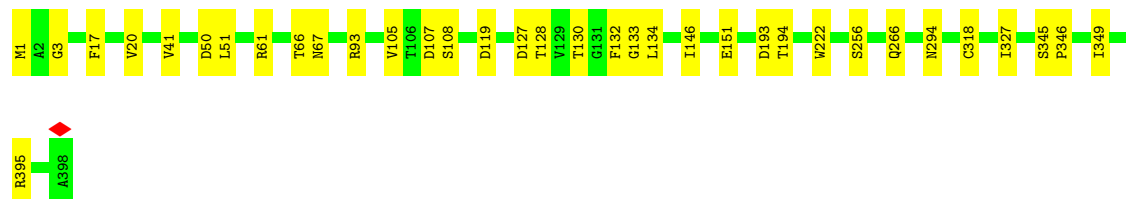
- Molecule 5: Putative tail biosynthetic protein

Chain A3:  90% 10%



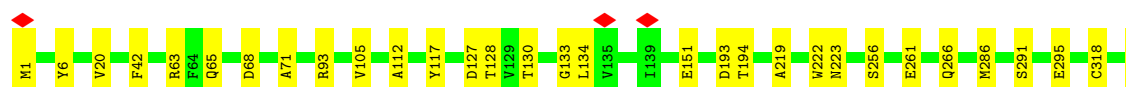
- Molecule 5: Putative tail biosynthetic protein

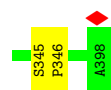
Chain A4:  91% 9%



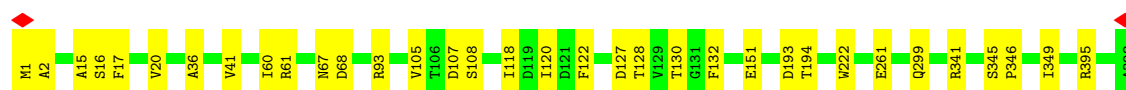
- Molecule 5: Putative tail biosynthetic protein

Chain A5:  92% 8%

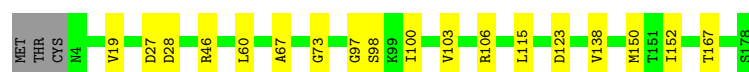




- Molecule 5: Putative tail biosynthetic protein



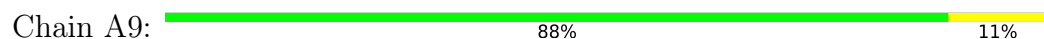
- Molecule 6: Putative structural protein



- Molecule 6: Putative structural protein



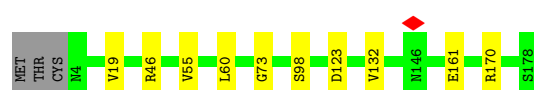
- Molecule 6: Putative structural protein




- Molecule 6: Putative structural protein



- Molecule 6: Putative structural protein



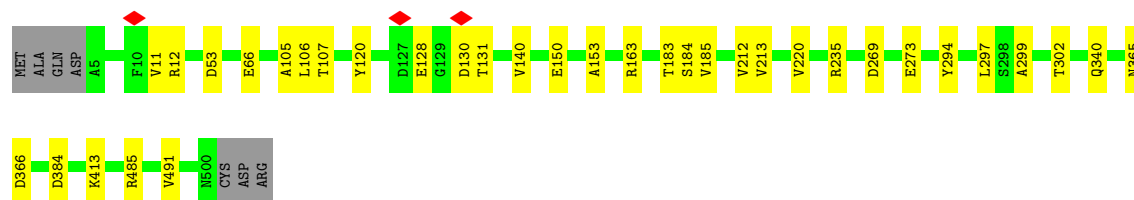
- Molecule 6: Putative structural protein

Chain BB:  88% 11% .



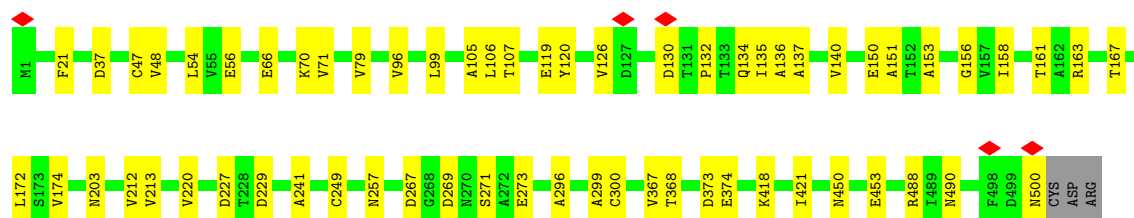
- Molecule 7: Tail sheath protein

Chain BN:  92% 7% .



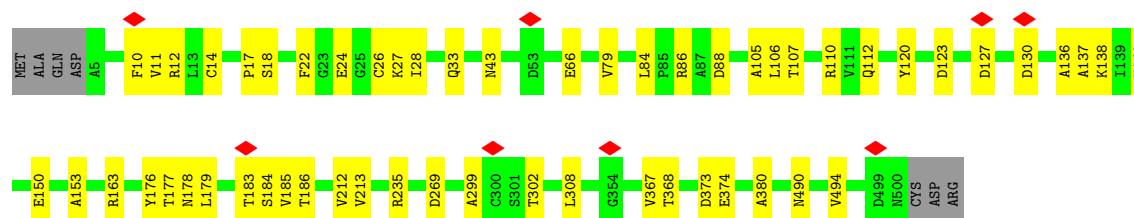
- Molecule 7: Tail sheath protein

Chain BC:  87% 12% .



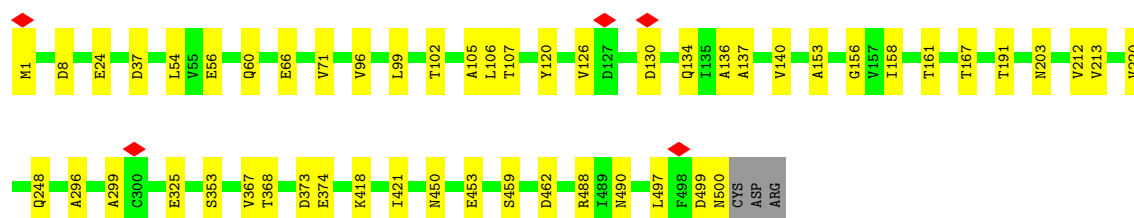
- Molecule 7: Tail sheath protein

Chain BD:  87% 11% .

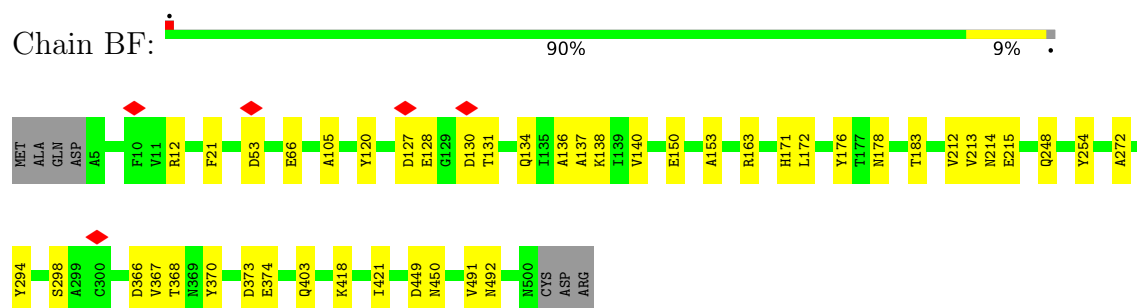


- Molecule 7: Tail sheath protein

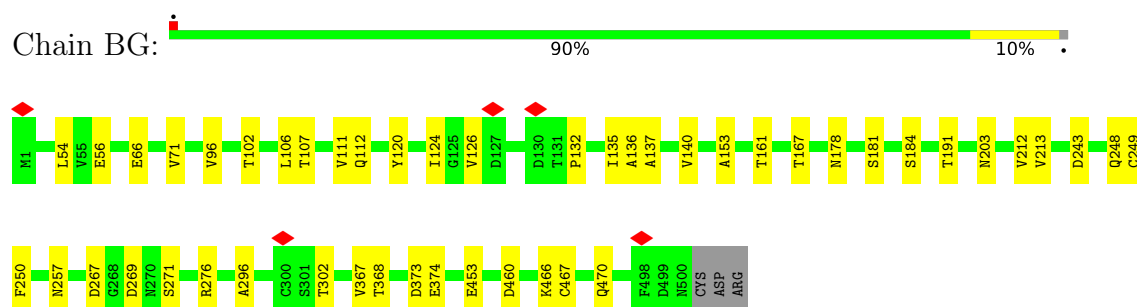
Chain BE:  89% 10% .



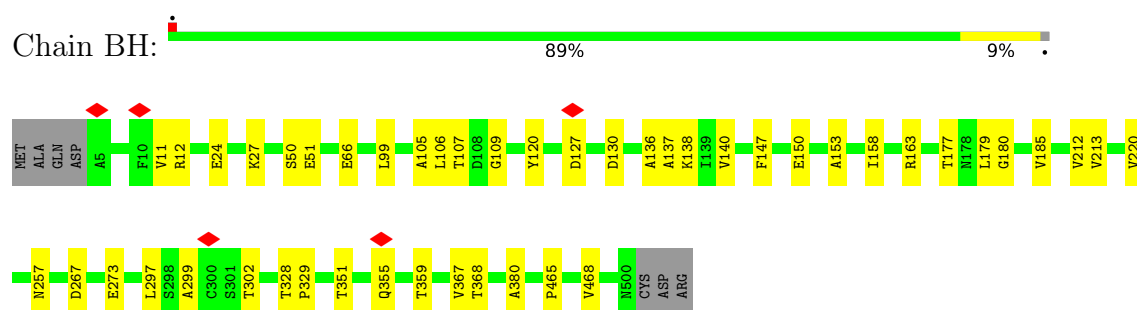
- Molecule 7: Tail sheath protein



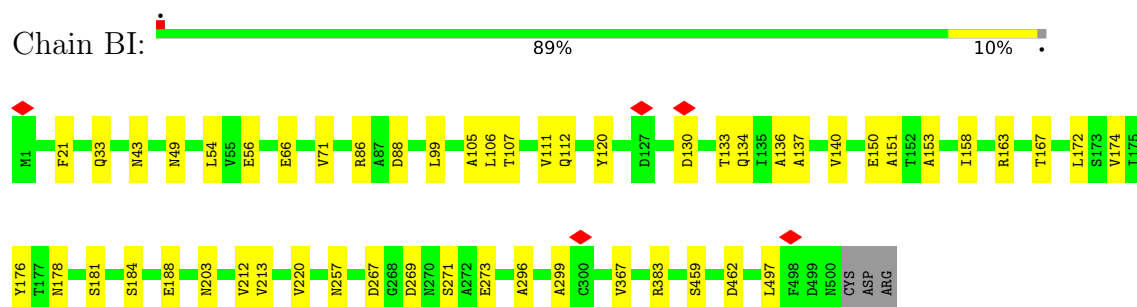
- Molecule 7: Tail sheath protein



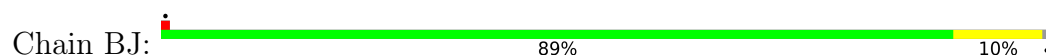
- Molecule 7: Tail sheath protein

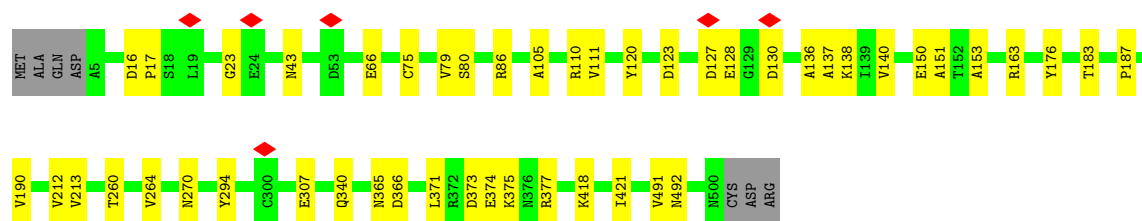


- Molecule 7: Tail sheath protein

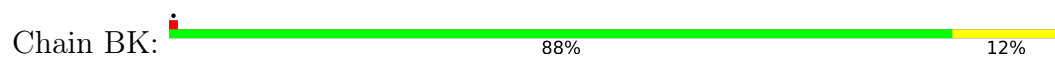


- Molecule 7: Tail sheath protein

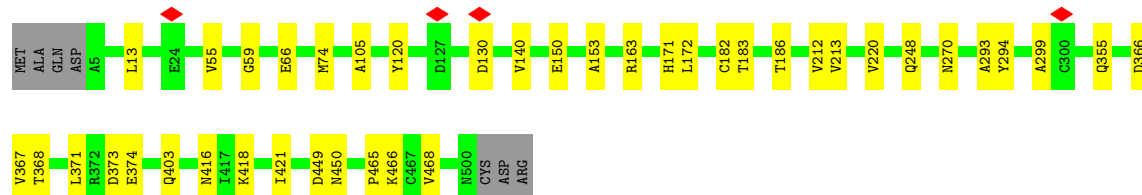
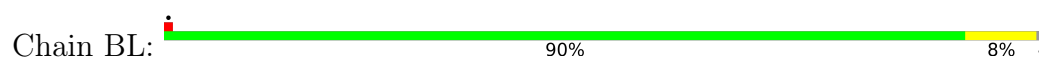




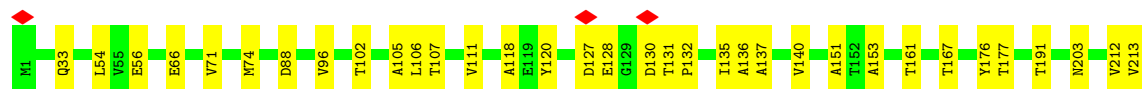
- Molecule 7: Tail sheath protein



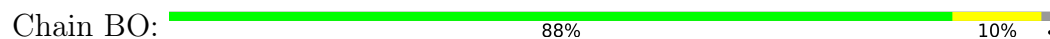
- Molecule 7: Tail sheath protein




- Molecule 7: Tail sheath protein

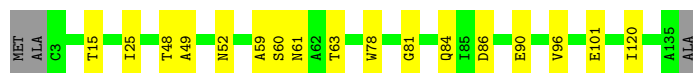


- Molecule 8: Structural protein




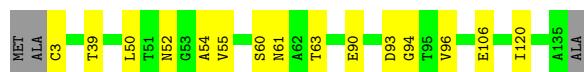
- Molecule 8: Structural protein

Chain BP:  85% 12%




• Molecule 8: Structural protein

Chain BQ:  87% 11%




• Molecule 8: Structural protein

Chain BR:  86% 12%




• Molecule 8: Structural protein

Chain BS:  88% 10%



• Molecule 8: Structural protein

Chain BT:  86% 12%




• Molecule 8: Structural protein

Chain BU:  93%




• Molecule 8: Structural protein

Chain BV:  79% 18%




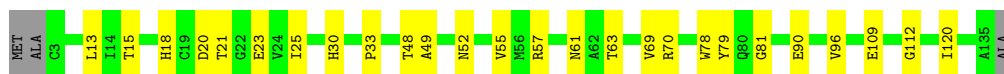
• Molecule 8: Structural protein

Chain BW:  85% 13% .




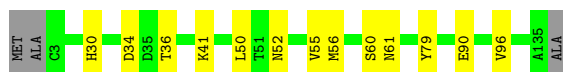
• Molecule 8: Structural protein

Chain BX:  79% 19% .




• Molecule 8: Structural protein

Chain BY:  88% 10% .



• Molecule 8: Structural protein

Chain BZ:  85% 12% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	8161	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.304	Depositor
Minimum map value	-1.208	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	767.2, 767.2, 767.2	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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	Ac	0.10	0/1355	0.29	0/1831
1	Ad	0.11	0/1355	0.32	0/1831
1	Ae	0.10	0/1355	0.30	0/1831
2	Af	0.10	0/2587	0.27	0/3502
2	Ag	0.10	0/2587	0.29	0/3502
2	Ah	0.10	0/2587	0.28	0/3502
3	Ai	0.10	0/2255	0.23	0/3083
3	Aj	0.10	0/2255	0.24	0/3083
3	Ak	0.09	0/2255	0.23	0/3083
3	Al	0.10	0/2255	0.23	0/3083
3	Am	0.10	0/2255	0.22	0/3083
3	An	0.09	0/2255	0.23	0/3083
4	Ao	0.10	0/3071	0.25	0/4183
4	Ap	0.10	0/3071	0.25	0/4183
4	Aq	0.09	0/3071	0.24	0/4183
4	Ar	0.10	0/3071	0.25	0/4183
4	As	0.10	0/3071	0.25	0/4183
4	At	0.09	0/3071	0.24	0/4183
4	Au	0.09	0/3076	0.21	0/4190
4	Av	0.09	0/3076	0.22	0/4190
4	Aw	0.10	0/3076	0.23	0/4190
4	Ax	0.09	0/3076	0.21	0/4190
4	Ay	0.09	0/3076	0.22	0/4190
4	Az	0.10	0/3076	0.23	0/4190
5	A1	0.10	0/3151	0.22	0/4285
5	A2	0.10	0/3151	0.23	0/4285
5	A3	0.10	0/3151	0.22	0/4285
5	A4	0.11	0/3151	0.23	0/4285
5	A5	0.10	0/3151	0.22	0/4285
5	A6	0.10	0/3151	0.23	0/4285
6	A0	0.09	0/1347	0.23	0/1818
6	A7	0.09	0/1347	0.23	0/1818
6	A8	0.09	0/1347	0.23	0/1818
6	A9	0.09	0/1347	0.22	0/1818

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	BA	0.09	0/1347	0.22	0/1818
6	BB	0.09	0/1347	0.22	0/1818
7	BC	0.09	0/3847	0.22	0/5253
7	BD	0.11	0/3817	0.27	0/5213
7	BE	0.10	0/3847	0.24	0/5253
7	BF	0.10	0/3817	0.25	0/5213
7	BG	0.09	0/3847	0.23	0/5253
7	BH	0.10	0/3817	0.25	0/5213
7	BI	0.09	0/3847	0.23	0/5253
7	BJ	0.10	0/3817	0.27	0/5213
7	BK	0.10	0/3847	0.24	0/5253
7	BL	0.10	0/3817	0.25	0/5213
7	BM	0.09	0/3847	0.24	0/5253
7	BN	0.10	0/3817	0.24	0/5213
8	BO	0.10	0/1010	0.25	0/1383
8	BP	0.12	0/1010	0.26	0/1383
8	BQ	0.12	0/1010	0.26	0/1383
8	BR	0.12	0/1010	0.23	0/1383
8	BS	0.10	0/1010	0.24	0/1383
8	BT	0.13	0/1010	0.22	0/1383
8	BU	0.13	0/1010	0.25	0/1383
8	BV	0.12	0/1010	0.24	0/1383
8	BW	0.14	0/1010	0.24	0/1383
8	BX	0.12	0/1010	0.22	0/1383
8	BY	0.12	0/1010	0.25	0/1383
8	BZ	0.12	0/1010	0.23	0/1383
All	All	0.10	0/147330	0.24	0/200745

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
7	BJ	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	BJ	375	LYS	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	Ac	1329	1251	1250	22	0
1	Ad	1329	1251	1250	34	0
1	Ae	1329	1251	1250	32	0
2	Af	2543	2530	2527	50	0
2	Ag	2543	2530	2527	58	0
2	Ah	2543	2530	2527	57	0
3	Ai	2200	2153	2153	23	0
3	Aj	2200	2153	2153	20	0
3	Ak	2200	2153	2153	17	0
3	Al	2200	2153	2153	17	0
3	Am	2200	2153	2153	15	0
3	An	2200	2153	2153	15	0
4	Ao	3006	2904	2903	10	0
4	Ap	3006	2904	2903	19	0
4	Aq	3006	2904	2903	23	0
4	Ar	3006	2904	2903	12	0
4	As	3006	2904	2903	14	0
4	At	3006	2904	2903	22	0
4	Au	3011	2911	2910	18	0
4	Av	3011	2911	2910	18	0
4	Aw	3011	2911	2910	26	0
4	Ax	3011	2911	2910	24	0
4	Ay	3011	2911	2910	23	0
4	Az	3011	2911	2910	22	0
5	A1	3084	2969	2969	30	0
5	A2	3084	2969	2969	25	0
5	A3	3084	2969	2969	27	0
5	A4	3084	2969	2969	31	0
5	A5	3084	2969	2969	26	0
5	A6	3084	2969	2969	29	0
6	A0	1328	1298	1297	11	0
6	A7	1328	1298	1297	13	0
6	A8	1328	1298	1297	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A9	1328	1298	1297	13	0
6	BA	1328	1298	1297	6	0
6	BB	1328	1298	1297	14	0
7	BC	3772	3662	3662	36	0
7	BD	3742	3634	3633	38	0
7	BE	3772	3662	3662	32	0
7	BF	3742	3634	3633	30	0
7	BG	3772	3662	3662	26	0
7	BH	3742	3634	3633	30	0
7	BI	3772	3662	3662	33	0
7	BJ	3742	3634	3633	28	0
7	BK	3772	3662	3662	39	0
7	BL	3742	3634	3633	26	0
7	BM	3772	3662	3662	31	0
7	BN	3742	3634	3633	22	0
8	BO	992	970	969	12	0
8	BP	992	970	971	13	0
8	BQ	992	971	970	15	0
8	BR	992	970	970	13	0
8	BS	992	970	969	10	0
8	BT	992	970	969	12	0
8	BU	992	970	969	7	0
8	BV	992	970	969	20	0
8	BW	992	970	969	13	0
8	BX	992	970	969	25	0
8	BY	992	970	969	10	0
8	BZ	992	970	969	14	0
All	All	144378	140170	140125	1169	0

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

All (1169) 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)
8:BX:30:HIS:HE2	8:BX:79:TYR:HH	1.03	1.00
8:BR:30:HIS:HE2	8:BR:79:TYR:HH	0.98	0.98
8:BV:30:HIS:HE2	8:BV:79:TYR:HH	1.02	0.91
7:BI:107:THR:OG1	7:BI:188:GLU:OE1	1.88	0.90
8:BV:44:ALA:O	8:BV:60:SER:OG	1.89	0.90
1:Ae:63:GLU:OE1	1:Ae:87:ASN:ND2	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A7:98:SER:OG	6:A7:123:ASP:OD2	1.93	0.85
7:BI:66:GLU:OE1	7:BI:120:TYR:OH	1.95	0.85
8:BR:81:GLY:O	8:BT:57:ARG:NH2	2.11	0.83
7:BC:66:GLU:OE1	7:BC:120:TYR:OH	1.95	0.82
3:An:26:ASP:OD1	7:BF:183:THR:OG1	1.97	0.82
5:A1:1:MET:N	8:BU:55:VAL:O	2.11	0.82
8:BZ:70:ARG:NH2	8:BZ:74:VAL:O	2.13	0.82
3:Aj:26:ASP:OD2	3:Aj:27:PHE:N	2.12	0.82
2:Af:218:GLU:OE2	2:Af:225:ASN:ND2	2.14	0.81
7:BJ:270:ASN:ND2	7:BJ:371:LEU:O	2.13	0.81
7:BM:66:GLU:OE1	7:BM:120:TYR:OH	1.98	0.81
7:BI:181:SER:OG	7:BI:184:SER:O	1.98	0.81
1:Ac:181:ALA:O	1:Ae:172:GLN:NE2	2.14	0.81
7:BL:270:ASN:ND2	7:BL:371:LEU:O	2.14	0.80
7:BD:373:ASP:OD1	7:BD:374:GLU:N	2.14	0.80
7:BJ:66:GLU:OE1	7:BJ:120:TYR:OH	1.99	0.79
7:BE:325:GLU:OE2	7:BE:353:SER:OG	1.99	0.79
7:BG:373:ASP:OD1	7:BG:374:GLU:N	2.16	0.79
7:BD:66:GLU:OE1	7:BD:120:TYR:OH	2.02	0.78
7:BD:12:ARG:NH1	7:BD:14:CYS:SG	2.57	0.78
2:Af:129:LYS:NZ	2:Ag:235:GLU:OE2	2.16	0.78
7:BJ:373:ASP:OD1	7:BJ:374:GLU:N	2.17	0.77
1:Ae:65:GLU:OE1	1:Ae:86:ARG:NH2	2.15	0.77
7:BG:66:GLU:OE1	7:BG:120:TYR:OH	2.03	0.76
7:BE:450:ASN:ND2	7:BE:453:GLU:OE2	2.19	0.76
2:Af:336:GLU:OE1	2:Ah:110:VAL:HG11	1.86	0.76
7:BG:106:LEU:HD12	7:BG:107:THR:HG23	1.67	0.76
5:A1:286:MET:CE	5:A1:337:VAL:HG12	2.16	0.75
7:BE:106:LEU:HD12	7:BE:107:THR:HG23	1.68	0.75
7:BE:488:ARG:NH1	7:BE:490:ASN:OD1	2.20	0.75
1:Ad:93:PRO:O	1:Ad:96:THR:OG1	2.04	0.75
1:Ac:171:GLN:NE2	1:Ad:180:GLU:OE1	2.21	0.74
4:Aw:67:ALA:O	4:Aw:185:ARG:NH2	2.20	0.74
1:Ac:170:PRO:O	1:Ad:183:THR:OG1	2.05	0.74
1:Ad:107:LYS:NZ	1:Ad:120:ASP:OD1	2.15	0.74
7:BD:106:LEU:HD12	7:BD:107:THR:HG23	1.68	0.74
7:BC:257:ASN:ND2	7:BC:267:ASP:OD2	2.20	0.74
7:BM:106:LEU:HD12	7:BM:107:THR:HG23	1.70	0.74
1:Ad:65:GLU:O	1:Ad:83:THR:HG22	1.87	0.74
4:Az:67:ALA:O	4:Az:185:ARG:NH2	2.21	0.73
7:BK:450:ASN:ND2	7:BK:453:GLU:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A3:107:ASP:OD1	5:A3:108:SER:N	2.22	0.73
7:BE:1:MET:N	7:BF:215:GLU:OE2	2.18	0.73
4:Av:67:ALA:O	4:Av:185:ARG:NH2	2.22	0.73
7:BC:106:LEU:HD12	7:BC:107:THR:HG23	1.71	0.73
6:BA:161:GLU:OE1	6:BA:170:ARG:NH1	2.22	0.73
7:BE:66:GLU:OE1	7:BE:120:TYR:OH	2.07	0.73
7:BK:325:GLU:OE1	7:BK:353:SER:OG	2.05	0.72
4:Ao:363:ARG:NH2	4:Ao:371:GLU:OE1	2.22	0.72
7:BE:212:VAL:HG23	7:BE:213:VAL:HG23	1.71	0.72
4:Ao:314:ARG:NH2	5:A3:261:GLU:OE2	2.23	0.72
7:BK:66:GLU:OE1	7:BK:120:TYR:OH	2.06	0.72
2:Af:239:ASN:OD1	2:Af:301:ARG:NH1	2.22	0.72
4:Ar:314:ARG:NH2	5:A6:261:GLU:OE2	2.23	0.72
4:Ay:67:ALA:O	4:Ay:185:ARG:NH2	2.22	0.72
2:Ah:150:LYS:NZ	2:Ah:169:GLU:OE2	2.23	0.71
6:BB:146:ASN:OD1	6:BB:147:LYS:N	2.23	0.71
2:Af:235:GLU:OE2	2:Ah:129:LYS:NZ	2.23	0.71
4:Ax:195:GLU:N	4:Ax:195:GLU:OE1	2.22	0.71
7:BI:106:LEU:HD12	7:BI:107:THR:HG23	1.70	0.71
4:Ar:363:ARG:NH2	4:Ar:371:GLU:OE1	2.22	0.71
4:Au:67:ALA:O	4:Au:185:ARG:NH2	2.24	0.71
7:BH:106:LEU:HD12	7:BH:107:THR:HG23	1.73	0.71
7:BH:150:GLU:OE2	7:BH:163:ARG:NH2	2.24	0.71
3:An:119:ARG:NH1	4:Az:63:ASP:OD1	2.24	0.71
2:Ag:40:ASN:OD1	2:Ag:41:TYR:N	2.24	0.70
2:Ah:40:ASN:OD1	2:Ah:41:TYR:N	2.24	0.70
7:BJ:150:GLU:OE2	7:BJ:163:ARG:NH2	2.23	0.70
2:Ag:128:THR:OG1	2:Ag:200:GLU:OE2	2.02	0.70
7:BD:150:GLU:OE2	7:BD:163:ARG:NH2	2.25	0.70
8:BX:81:GLY:O	8:BZ:57:ARG:NH2	2.24	0.70
7:BL:150:GLU:OE2	7:BL:163:ARG:NH2	2.24	0.70
6:A0:98:SER:OG	6:A0:123:ASP:OD2	2.05	0.70
6:BA:98:SER:OG	6:BA:123:ASP:OD2	2.06	0.70
4:Ax:67:ALA:O	4:Ax:185:ARG:NH2	2.25	0.69
5:A1:1:MET:O	8:BU:55:VAL:N	2.25	0.69
4:As:314:ARG:NH2	5:A5:261:GLU:OE2	2.25	0.69
4:Aw:107:LEU:HD21	4:Aw:109:PHE:CE1	2.27	0.69
2:Ah:324:ASP:OD1	2:Ah:325:ILE:N	2.25	0.69
7:BF:150:GLU:OE2	7:BF:163:ARG:NH2	2.25	0.69
1:Ad:40:SER:OG	2:Ah:140:THR:O	2.08	0.69
2:Af:150:LYS:NZ	2:Af:169:GLU:OE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A4:1:MET:O	8:BO:55:VAL:N	2.25	0.69
7:BN:150:GLU:OE2	7:BN:163:ARG:NH2	2.24	0.69
7:BJ:105:ALA:O	7:BJ:130:ASP:N	2.26	0.69
1:Ad:20:ARG:O	1:Ad:21:HIS:ND1	2.26	0.68
2:Af:249:VAL:N	2:Af:284:ASP:OD1	2.26	0.68
4:Ap:126:LEU:HD12	4:Ap:127:PRO:HD2	1.75	0.68
7:BK:212:VAL:HG23	7:BK:213:VAL:HG23	1.75	0.68
7:BL:171:HIS:O	7:BL:172:LEU:HD22	1.93	0.68
4:Ap:314:ARG:NH2	5:A2:261:GLU:OE2	2.26	0.68
5:A4:1:MET:N	8:BO:55:VAL:O	2.20	0.68
7:BM:257:ASN:ND2	7:BM:267:ASP:OD2	2.26	0.68
7:BC:212:VAL:HG23	7:BC:213:VAL:HG23	1.74	0.68
8:BR:63:THR:HG22	8:BR:120:ILE:HG22	1.74	0.68
5:A3:1:MET:N	8:BQ:55:VAL:O	2.23	0.68
2:Ag:324:ASP:OD1	2:Ag:325:ILE:N	2.27	0.68
4:Au:298:ASN:OD1	4:Au:386:ILE:HD11	1.94	0.68
4:Ay:151:GLU:N	4:Ay:151:GLU:OE1	2.27	0.67
6:A8:161:GLU:OE2	6:A8:170:ARG:NH1	2.27	0.67
8:BT:93:ASP:OD1	8:BT:94:GLY:N	2.28	0.67
2:Ag:202:ARG:NH2	2:Ag:324:ASP:OD2	2.27	0.67
7:BI:212:VAL:HG23	7:BI:213:VAL:HG23	1.75	0.67
7:BN:294:TYR:OH	7:BN:366:ASP:OD1	2.12	0.67
8:BZ:4:ASN:OD1	8:BZ:5:LYS:N	2.28	0.67
2:Af:128:THR:HG22	2:Af:200:GLU:OE2	1.94	0.67
4:At:316:THR:HG22	4:At:380:LEU:CD2	2.25	0.66
6:A9:25:SER:OG	6:A9:32:CYS:SG	2.52	0.66
7:BG:257:ASN:ND2	7:BG:267:ASP:OD2	2.27	0.66
7:BD:24:GLU:OE2	7:BD:27:LYS:NZ	2.19	0.66
5:A1:93:ARG:NH2	5:A2:105:VAL:HG11	2.09	0.66
5:A5:1:MET:N	8:BY:55:VAL:O	2.27	0.66
1:Ad:31:THR:OG1	2:Ah:252:ASP:OD1	2.06	0.66
7:BG:212:VAL:HG23	7:BG:213:VAL:HG23	1.77	0.66
5:A4:93:ARG:NH2	5:A5:105:VAL:HG11	2.10	0.66
2:Ag:129:LYS:NZ	2:Ah:235:GLU:OE2	2.22	0.66
2:Af:40:ASN:OD1	2:Af:41:TYR:N	2.29	0.65
7:BM:212:VAL:HG23	7:BM:213:VAL:HG23	1.78	0.65
1:Ae:65:GLU:O	1:Ae:83:THR:HG22	1.95	0.65
7:BF:171:HIS:O	7:BF:172:LEU:HD22	1.95	0.65
8:BZ:93:ASP:OD1	8:BZ:94:GLY:N	2.30	0.65
7:BN:106:LEU:HD12	7:BN:107:THR:HG23	1.78	0.65
7:BF:176:TYR:OH	7:BF:178:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ak:37:THR:O	3:Ak:40:VAL:HG12	1.97	0.65
8:BQ:61:ASN:OD1	8:BS:52:ASN:N	2.30	0.65
2:Ag:150:LYS:NZ	2:Ag:169:GLU:OE2	2.30	0.64
7:BF:294:TYR:OH	7:BF:366:ASP:OD1	2.15	0.64
8:BS:61:ASN:OD1	8:BU:52:ASN:N	2.29	0.64
3:Am:204:ASN:ND2	3:Am:205:ALA:O	2.30	0.64
5:A3:1:MET:O	8:BQ:55:VAL:N	2.31	0.64
3:An:37:THR:O	3:An:40:VAL:HG12	1.98	0.64
7:BF:213:VAL:HG12	7:BF:213:VAL:O	1.96	0.64
7:BH:177:THR:HG23	7:BH:177:THR:O	1.98	0.64
3:Aj:204:ASN:ND2	3:Aj:205:ALA:O	2.31	0.64
2:Ag:249:VAL:N	2:Ag:284:ASP:OD1	2.30	0.64
7:BL:294:TYR:OH	7:BL:366:ASP:OD1	2.14	0.64
1:Ad:135:VAL:HG12	1:Ad:135:VAL:O	1.97	0.63
6:A9:98:SER:OG	6:A9:123:ASP:OD2	2.09	0.63
8:BW:61:ASN:OD1	8:BY:52:ASN:N	2.31	0.63
2:Af:9:ILE:HG22	2:Af:14:LEU:HD11	1.81	0.63
7:BE:105:ALA:O	7:BE:130:ASP:N	2.30	0.63
7:BH:105:ALA:O	7:BH:130:ASP:N	2.31	0.63
8:BX:120:ILE:HD11	8:BZ:55:VAL:CG1	2.29	0.63
8:BX:18:HIS:HD1	8:BX:21:THR:HG22	1.63	0.63
7:BM:127:ASP:OD1	7:BM:128:GLU:N	2.31	0.63
1:Ae:120:ASP:OD1	1:Ae:121:GLY:N	2.32	0.63
3:Ai:34:THR:HG23	7:BH:355:GLN:HG3	1.80	0.63
7:BG:140:VAL:HG21	7:BG:153:ALA:HB2	1.81	0.63
2:Ag:143:PHE:CE2	2:Ag:151:VAL:HG22	2.34	0.63
4:Ay:107:LEU:HD11	4:Ay:154:LEU:HD11	1.81	0.62
8:BO:52:ASN:N	8:BY:61:ASN:OD1	2.31	0.62
2:Ag:176:THR:HG23	2:Ag:176:THR:O	1.99	0.62
4:Ap:20:ARG:NH2	4:Au:50:GLU:OE2	2.33	0.62
1:Ac:62:GLU:OE2	1:Ac:88:LYS:NZ	2.29	0.62
8:BW:61:ASN:ND2	8:BY:50:LEU:O	2.31	0.62
5:A2:256:SER:OG	5:A2:266:GLN:OE1	2.13	0.62
7:BN:384:ASP:OD2	7:BN:485:ARG:NH1	2.33	0.62
4:Ax:92:TYR:OH	4:Ax:135:ARG:NH2	2.33	0.62
7:BH:380:ALA:O	7:BI:497:LEU:HD22	1.99	0.62
2:Af:143:PHE:CE2	2:Af:151:VAL:HG22	2.35	0.62
4:As:20:ARG:NH2	4:Ax:50:GLU:OE2	2.32	0.62
8:BT:30:HIS:NE2	8:BT:79:TYR:OH	2.31	0.61
2:Ag:353:ALA:HA	5:A1:41:VAL:HG12	1.82	0.61
7:BH:212:VAL:HG23	7:BH:213:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ak:34:THR:O	7:BL:355:GLN:NE2	2.33	0.61
7:BN:105:ALA:O	7:BN:130:ASP:N	2.33	0.61
8:BT:61:ASN:ND2	8:BV:50:LEU:O	2.32	0.61
5:A3:151:GLU:OE1	5:A3:222:TRP:NE1	2.34	0.61
8:BP:81:GLY:O	8:BR:57:ARG:NH2	2.31	0.61
8:BQ:61:ASN:ND2	8:BS:50:LEU:O	2.30	0.61
4:At:55:ALA:HB1	4:Aw:58:MET:HE1	1.83	0.61
1:Ad:172:GLN:NE2	1:Ae:182:ASP:O	2.33	0.61
4:Aq:177:ASP:OD1	4:Aq:178:ALA:N	2.31	0.61
7:BC:488:ARG:NE	7:BC:490:ASN:OD1	2.34	0.60
3:Ak:250:GLU:N	3:Ak:250:GLU:OE1	2.35	0.60
7:BN:212:VAL:HG23	7:BN:213:VAL:HG23	1.81	0.60
1:Ad:172:GLN:N	1:Ad:172:GLN:OE1	2.34	0.60
3:An:250:GLU:OE1	3:An:250:GLU:N	2.34	0.60
5:A6:107:ASP:OD1	5:A6:108:SER:N	2.34	0.60
7:BD:183:THR:HA	7:BD:186:THR:HG22	1.83	0.60
8:BV:93:ASP:OD1	8:BV:94:GLY:N	2.35	0.60
4:At:177:ASP:OD1	4:At:178:ALA:N	2.31	0.60
7:BK:254:TYR:HH	7:BK:298:SER:HG	1.48	0.60
3:Aj:16:LYS:NZ	7:BJ:128:GLU:OE2	2.29	0.60
6:BB:146:ASN:ND2	7:BC:500:ASN:OD1	2.34	0.60
8:BP:63:THR:HG22	8:BP:120:ILE:HG22	1.84	0.60
7:BF:212:VAL:HG23	7:BF:213:VAL:HG23	1.84	0.60
8:BU:61:ASN:OD1	8:BW:52:ASN:N	2.34	0.60
7:BH:99:LEU:HD23	7:BH:158:ILE:HD11	1.84	0.60
3:Ai:31:ASP:OD1	3:Ai:32:GLU:N	2.34	0.59
4:At:363:ARG:NH2	4:At:371:GLU:OE1	2.35	0.59
5:A4:151:GLU:OE1	5:A4:222:TRP:NE1	2.35	0.59
2:Ah:143:PHE:CE2	2:Ah:151:VAL:HG22	2.37	0.59
3:Ai:204:ASN:ND2	3:Ai:205:ALA:O	2.35	0.59
5:A6:151:GLU:OE1	5:A6:222:TRP:NE1	2.34	0.59
3:Ai:63:THR:O	3:Ai:65:ASN:ND2	2.34	0.59
4:At:20:ARG:NH2	4:Aw:50:GLU:OE2	2.35	0.59
3:Ak:31:ASP:HB3	3:Ak:34:THR:HG22	1.85	0.59
7:BH:127:ASP:OD1	7:BH:138:LYS:NZ	2.22	0.59
7:BJ:111:VAL:HG23	7:BJ:176:TYR:OH	2.02	0.59
5:A2:353:PHE:HD2	5:A2:357:MET:HE2	1.66	0.59
4:Ar:20:ARG:NH2	4:Ay:50:GLU:OE2	2.36	0.59
7:BM:105:ALA:O	7:BM:130:ASP:N	2.36	0.59
1:Ac:65:GLU:O	1:Ac:83:THR:HG22	2.03	0.59
2:Ah:249:VAL:HG12	2:Ah:249:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Ap:195:GLU:OE2	4:Au:191:ARG:NH2	2.36	0.59
8:BW:31:GLU:OE1	8:BZ:52:ASN:ND2	2.35	0.59
5:A1:286:MET:HE1	5:A1:337:VAL:HG12	1.84	0.58
5:A2:151:GLU:OE1	5:A2:222:TRP:NE1	2.36	0.58
5:A5:256:SER:OG	5:A5:266:GLN:OE1	2.12	0.58
7:BC:134:GLN:OE1	7:BC:156:GLY:N	2.36	0.58
8:BV:61:ASN:OD1	8:BX:52:ASN:N	2.36	0.58
1:Ac:120:ASP:OD1	1:Ac:121:GLY:N	2.35	0.58
4:Aw:93:VAL:HG21	4:Aw:109:PHE:HE2	1.68	0.58
8:BU:90:GLU:HG3	8:BU:96:VAL:HG22	1.84	0.58
7:BM:140:VAL:HG21	7:BM:153:ALA:HB2	1.86	0.58
3:Al:226:ASN:ND2	3:Al:230:CYS:O	2.35	0.58
4:Aq:63:ASP:OD1	4:Az:78:ARG:NH1	2.36	0.58
5:A5:151:GLU:OE1	5:A5:222:TRP:NE1	2.36	0.58
8:BS:90:GLU:HG3	8:BS:96:VAL:HG22	1.86	0.58
7:BH:328:THR:HG22	7:BH:329:PRO:HD2	1.85	0.58
4:Aq:363:ARG:NH2	4:Aq:371:GLU:OE1	2.37	0.58
4:As:195:GLU:OE2	4:Ax:191:ARG:NH2	2.37	0.58
1:Ac:93:PRO:O	1:Ac:96:THR:OG1	2.18	0.58
4:Ao:20:ARG:NH2	4:Av:50:GLU:OE2	2.36	0.58
4:Ar:67:ALA:O	4:Ar:185:ARG:NH2	2.37	0.58
4:Au:385:VAL:O	4:Au:385:VAL:HG13	2.03	0.58
5:A3:93:ARG:NH2	5:A4:105:VAL:HG11	2.19	0.58
7:BM:325:GLU:OE2	7:BM:353:SER:OG	2.20	0.58
2:Ag:9:ILE:HG22	2:Ag:14:LEU:HD11	1.85	0.58
2:Af:112:PHE:HE2	5:A2:41:VAL:HG11	1.68	0.58
7:BH:179:LEU:HD12	7:BH:180:GLY:H	1.68	0.58
3:Ai:127:GLU:OE1	3:Ai:127:GLU:N	2.37	0.58
5:A1:105:VAL:HG11	5:A6:93:ARG:NH2	2.18	0.58
8:BV:63:THR:HG22	8:BV:120:ILE:HG22	1.86	0.58
2:Ah:245:LYS:HG2	2:Ah:263:VAL:HG22	1.84	0.58
4:Ay:93:VAL:HG21	4:Ay:109:PHE:HE2	1.69	0.58
1:Ad:109:VAL:HG23	1:Ae:111:LEU:HD21	1.85	0.57
7:BC:99:LEU:HD23	7:BC:158:ILE:HD11	1.86	0.57
7:BF:254:TYR:HH	7:BF:298:SER:HG	1.52	0.57
7:BI:112:GLN:NE2	7:BI:178:ASN:OD1	2.36	0.57
7:BK:248:GLN:N	7:BK:248:GLN:OE1	2.37	0.57
7:BM:450:ASN:ND2	7:BM:453:GLU:OE1	2.37	0.57
2:Af:249:VAL:HG12	2:Af:249:VAL:O	2.05	0.57
7:BE:140:VAL:HG21	7:BE:153:ALA:HB2	1.86	0.57
8:BV:109:GLU:OE2	8:BX:63:THR:OG1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Aq:20:ARG:NH2	4:Az:50:GLU:OE2	2.38	0.57
6:BB:98:SER:OG	6:BB:123:ASP:OD2	2.10	0.57
8:BO:61:ASN:OD1	8:BQ:52:ASN:N	2.37	0.57
8:BP:90:GLU:HG3	8:BP:96:VAL:HG22	1.86	0.57
3:Aj:96:THR:HG22	4:Ax:55:ALA:HB2	1.86	0.57
7:BI:140:VAL:HG13	7:BI:151:ALA:CB	2.35	0.57
4:Ay:68:CYS:SG	4:Ay:69:CYS:N	2.78	0.57
8:BV:90:GLU:HG3	8:BV:96:VAL:HG22	1.85	0.57
7:BK:102:THR:OG1	7:BK:191:THR:OG1	2.22	0.57
5:A1:151:GLU:OE1	5:A1:222:TRP:NE1	2.38	0.56
8:BO:90:GLU:HG3	8:BO:96:VAL:HG22	1.87	0.56
5:A3:93:ARG:HH21	5:A4:105:VAL:HG11	1.70	0.56
8:BR:120:ILE:HD11	8:BT:55:VAL:CG1	2.35	0.56
7:BJ:140:VAL:HG21	7:BJ:153:ALA:HB2	1.87	0.56
7:BC:140:VAL:HG21	7:BC:153:ALA:HB2	1.88	0.56
7:BE:71:VAL:HG22	7:BE:296:ALA:HB2	1.87	0.56
7:BE:325:GLU:OE2	7:BE:353:SER:N	2.38	0.56
7:BJ:294:TYR:OH	7:BJ:366:ASP:OD1	2.22	0.56
4:Aq:55:ALA:HB1	4:Az:58:MET:HE1	1.87	0.56
4:As:126:LEU:HD12	4:As:127:PRO:HD2	1.87	0.56
4:Ax:385:VAL:O	4:Ax:385:VAL:HG13	2.05	0.56
5:A4:50:ASP:C	5:A4:51:LEU:HD12	2.31	0.56
7:BD:12:ARG:O	7:BD:12:ARG:HD3	2.05	0.56
7:BJ:374:GLU:N	7:BJ:374:GLU:OE2	2.38	0.56
1:Ad:163:ILE:O	1:Ad:163:ILE:HG22	2.06	0.56
7:BI:257:ASN:ND2	7:BI:267:ASP:OD2	2.39	0.56
7:BM:132:PRO:HD2	7:BM:135:ILE:HD12	1.88	0.56
3:Ak:31:ASP:OD1	3:Ak:32:GLU:N	2.38	0.56
4:At:63:ASP:OD1	4:Aw:78:ARG:NH1	2.39	0.56
7:BE:134:GLN:OE1	7:BE:156:GLY:N	2.38	0.56
7:BJ:212:VAL:HG23	7:BJ:213:VAL:HG23	1.88	0.56
2:Ah:344:CYS:HA	2:Ah:363:LEU:HD23	1.88	0.56
8:BP:61:ASN:ND2	8:BR:50:LEU:O	2.31	0.56
8:BW:93:ASP:OD1	8:BW:94:GLY:N	2.39	0.56
7:BL:220:VAL:HG21	7:BL:299:ALA:HA	1.88	0.56
3:Al:26:ASP:OD1	3:Al:27:PHE:N	2.33	0.55
4:Av:68:CYS:SG	4:Av:69:CYS:N	2.78	0.55
5:A6:105:VAL:HG22	5:A6:118:ILE:HD12	1.88	0.55
8:BY:90:GLU:HG3	8:BY:96:VAL:HG22	1.89	0.55
7:BD:140:VAL:HG21	7:BD:153:ALA:HB2	1.88	0.55
8:BZ:108:GLU:N	8:BZ:108:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Af:219:ASP:O	2:Af:221:VAL:HG23	2.07	0.55
4:Aq:316:THR:HG22	4:Aq:380:LEU:HD22	1.88	0.55
5:A1:105:VAL:HG11	5:A6:93:ARG:HH21	1.71	0.55
7:BN:66:GLU:OE1	7:BN:120:TYR:OH	2.21	0.55
8:BQ:106:GLU:O	8:BQ:106:GLU:HG3	2.05	0.55
7:BF:66:GLU:OE1	7:BF:120:TYR:OH	2.18	0.55
7:BE:99:LEU:HD23	7:BE:158:ILE:HD11	1.89	0.55
1:Ae:93:PRO:O	1:Ae:96:THR:OG1	2.17	0.55
2:Af:9:ILE:CG2	2:Af:14:LEU:HD11	2.37	0.55
5:A5:127:ASP:OD1	5:A5:128:THR:N	2.39	0.55
7:BC:450:ASN:ND2	7:BC:453:GLU:OE1	2.40	0.55
8:BP:86:ASP:OD1	8:BP:101:GLU:N	2.37	0.55
7:BJ:140:VAL:HG22	7:BJ:151:ALA:HB1	1.87	0.55
5:A2:353:PHE:CD2	5:A2:357:MET:HE2	2.42	0.55
7:BD:127:ASP:OD1	7:BD:138:LYS:NZ	2.38	0.55
7:BI:99:LEU:HD23	7:BI:158:ILE:HD11	1.89	0.55
2:Af:9:ILE:HG23	2:Af:9:ILE:O	2.06	0.55
7:BE:367:VAL:HG12	7:BE:368:THR:O	2.07	0.55
7:BG:71:VAL:HG22	7:BG:296:ALA:HB2	1.89	0.55
7:BL:66:GLU:OE1	7:BL:120:TYR:OH	2.20	0.55
4:Ay:7:ARG:NH2	5:A1:318:CYS:SG	2.80	0.54
7:BG:181:SER:OG	7:BG:184:SER:O	2.21	0.54
7:BI:150:GLU:OE2	7:BI:163:ARG:NE	2.40	0.54
7:BM:213:VAL:HG12	7:BM:213:VAL:O	2.06	0.54
2:Af:176:THR:O	2:Af:176:THR:HG23	2.07	0.54
2:Ag:174:LYS:HG2	2:Ag:249:VAL:HG11	1.89	0.54
1:Ac:140:VAL:HG21	1:Ae:144:THR:CG2	2.38	0.54
1:Ad:37:VAL:HG21	1:Ad:68:LEU:HD11	1.88	0.54
3:Ai:250:GLU:OE1	3:Ai:250:GLU:N	2.41	0.54
4:Ay:13:LEU:O	4:Ay:17:ILE:HD12	2.08	0.54
8:BV:86:ASP:OD1	8:BV:101:GLU:N	2.38	0.54
3:Am:26:ASP:OD1	3:Am:27:PHE:N	2.37	0.54
4:Aw:391:THR:HG22	4:Aw:391:THR:O	2.07	0.54
6:A7:103:VAL:O	7:BN:11:VAL:HG21	2.07	0.54
8:BX:20:ASP:OD2	7:BL:416:ASN:ND2	2.41	0.54
8:BZ:30:HIS:NE2	8:BZ:79:TYR:OH	2.36	0.54
5:A1:127:ASP:OD1	5:A1:128:THR:N	2.40	0.54
6:A0:101:ARG:HB3	7:BH:11:VAL:HG11	1.90	0.54
7:BF:171:HIS:C	7:BF:172:LEU:HD22	2.33	0.54
3:Al:96:THR:HG22	4:Av:55:ALA:HB2	1.90	0.54
7:BH:24:GLU:OE2	7:BH:27:LYS:NZ	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Al:160:ILE:HD13	3:Al:237:ALA:O	2.07	0.54
2:Ag:52:VAL:HG11	2:Ag:55:LYS:HE3	1.90	0.54
3:Al:160:ILE:HD13	3:Al:237:ALA:O	2.07	0.54
7:BF:418:LYS:HB2	7:BF:421:ILE:HD12	1.90	0.54
7:BK:213:VAL:HG12	7:BK:213:VAL:O	2.07	0.54
7:BK:302:THR:HG22	7:BK:302:THR:O	2.07	0.54
2:Af:62:MET:SD	5:A5:130:THR:HG21	2.48	0.54
8:BS:31:GLU:OE1	8:BV:52:ASN:ND2	2.41	0.54
2:Af:107:ASP:OD1	2:Af:108:VAL:N	2.40	0.54
4:Aq:316:THR:HG22	4:Aq:380:LEU:CD2	2.38	0.54
4:At:45:TYR:OH	4:At:49:GLU:OE1	2.18	0.54
7:BF:248:GLN:N	7:BF:248:GLN:OE1	2.41	0.54
1:Ac:149:LEU:HD23	1:Ae:156:LEU:HD13	1.90	0.53
2:Ag:155:LEU:HD12	2:Ag:177:LEU:CD1	2.39	0.53
4:Au:31:ILE:O	6:A7:46:ARG:NH1	2.41	0.53
2:Af:40:ASN:O	5:A4:130:THR:HG23	2.07	0.53
4:Av:7:ARG:NH2	5:A4:318:CYS:SG	2.81	0.53
4:Az:391:THR:HG22	4:Az:391:THR:O	2.07	0.53
7:BD:184:SER:O	7:BD:185:VAL:HG22	2.09	0.53
7:BG:243:ASP:O	7:BG:248:GLN:NE2	2.41	0.53
2:Ah:110:VAL:O	2:Ah:110:VAL:HG23	2.07	0.53
4:At:334:ARG:NH1	4:Av:331:GLU:OE1	2.41	0.53
4:Au:13:LEU:O	4:Au:17:ILE:HD12	2.08	0.53
4:Ax:13:LEU:O	4:Ax:17:ILE:HD12	2.09	0.53
4:Ax:391:THR:O	4:Ax:391:THR:HG22	2.08	0.53
7:BD:33:GLN:NE2	7:BD:88:ASP:OD1	2.41	0.53
7:BD:176:TYR:CE2	7:BD:178:ASN:HB2	2.43	0.53
7:BH:140:VAL:HG21	7:BH:153:ALA:HB2	1.89	0.53
7:BL:212:VAL:HG23	7:BL:213:VAL:HG23	1.90	0.53
8:BR:61:ASN:OD1	8:BT:52:ASN:N	2.41	0.53
7:BK:140:VAL:HG21	7:BK:153:ALA:HB2	1.91	0.53
1:Ae:65:GLU:OE2	2:Ah:259:ILE:HD11	2.08	0.53
3:Aj:250:GLU:OE1	3:Aj:250:GLU:N	2.42	0.53
4:Av:93:VAL:HG21	4:Av:109:PHE:CE2	2.44	0.53
7:BH:11:VAL:HG12	7:BH:12:ARG:N	2.24	0.53
7:BI:167:THR:OG1	7:BI:203:ASN:ND2	2.41	0.53
1:Ae:46:ASP:O	2:Ag:251:LYS:NZ	2.42	0.53
2:Af:355:SER:HA	5:A4:51:LEU:HD22	1.90	0.53
8:BP:59:ALA:O	8:BP:60:SER:OG	2.23	0.53
7:BD:212:VAL:HG23	7:BD:213:VAL:HG23	1.90	0.53
2:Ah:176:THR:HG23	2:Ah:176:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A9:158:ASP:O	6:A9:170:ARG:NH2	2.42	0.53
7:BL:418:LYS:HB2	7:BL:421:ILE:HD12	1.90	0.53
2:Ag:29:LEU:HD22	2:Ag:132:VAL:CG1	2.39	0.52
2:Ag:112:PHE:HE2	5:A6:41:VAL:HG11	1.74	0.52
3:Al:250:GLU:N	3:Al:250:GLU:OE1	2.42	0.52
7:BI:105:ALA:O	7:BI:130:ASP:N	2.40	0.52
1:Ae:31:THR:HG21	2:Ag:251:LYS:O	2.08	0.52
4:Au:391:THR:O	4:Au:391:THR:HG22	2.09	0.52
7:BN:140:VAL:HG21	7:BN:153:ALA:HB2	1.90	0.52
7:BG:102:THR:OG1	7:BG:191:THR:OG1	2.26	0.52
7:BK:418:LYS:HB2	7:BK:421:ILE:HD12	1.91	0.52
1:Ac:172:GLN:OE1	1:Ac:172:GLN:N	2.42	0.52
3:Ai:141:ILE:HG23	3:Ai:260:MET:HE1	1.90	0.52
5:A3:105:VAL:HG22	5:A3:118:ILE:HD12	1.92	0.52
7:BD:26:CYS:SG	7:BD:79:VAL:HG23	2.49	0.52
2:Ag:9:ILE:CG2	2:Ag:14:LEU:HD11	2.40	0.52
4:Ar:74:LYS:O	4:Ar:75:MET:HG2	2.09	0.52
5:A1:256:SER:OG	5:A1:266:GLN:OE1	2.13	0.52
7:BC:167:THR:OG1	7:BC:203:ASN:ND2	2.42	0.52
1:Ac:18:PHE:CD2	1:Ac:69:LEU:HD21	2.44	0.52
2:Af:324:ASP:OD1	2:Af:325:ILE:N	2.40	0.52
3:Am:250:GLU:OE1	3:Am:250:GLU:N	2.41	0.52
5:A3:127:ASP:OD1	5:A3:128:THR:N	2.42	0.52
6:A9:73:GLY:N	6:A0:167:THR:OG1	2.42	0.52
8:BS:60:SER:OG	8:BS:61:ASN:N	2.42	0.52
8:BV:85:ILE:HD13	8:BV:117:MET:HE1	1.91	0.52
2:Ag:110:VAL:HG21	2:Ah:336:GLU:HG3	1.91	0.52
4:At:239:GLU:OE1	4:At:286:ARG:NH2	2.42	0.52
7:BH:297:LEU:O	7:BH:302:THR:HG22	2.09	0.52
7:BI:71:VAL:HG22	7:BI:296:ALA:HB2	1.91	0.52
1:Ae:175:SER:O	1:Ae:176:ASP:OD1	2.27	0.52
2:Ah:222:LEU:HA	2:Ah:226:ILE:HD12	1.92	0.52
4:Aq:239:GLU:OE1	4:Aq:286:ARG:NH2	2.42	0.52
5:A2:286:MET:CE	5:A2:337:VAL:HG12	2.40	0.52
5:A5:286:MET:CE	5:A5:337:VAL:HG12	2.40	0.52
7:BM:367:VAL:HG12	7:BM:368:THR:O	2.09	0.52
3:Ai:89:LEU:HA	3:Ai:92:VAL:HG12	1.90	0.52
4:Az:31:ILE:O	6:A8:46:ARG:NH1	2.42	0.52
7:BN:220:VAL:HG21	7:BN:299:ALA:HA	1.92	0.52
7:BI:133:THR:OG1	7:BI:134:GLN:NE2	2.43	0.52
5:A1:133:GLY:C	5:A1:134:LEU:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A2:193:ASP:OD1	5:A2:194:THR:N	2.43	0.52
8:BQ:93:ASP:OD1	8:BQ:94:GLY:N	2.42	0.52
7:BG:302:THR:HG22	7:BG:302:THR:O	2.10	0.52
4:Ap:316:THR:HG22	4:Ap:380:LEU:CD2	2.39	0.52
4:Az:13:LEU:O	4:Az:17:ILE:HD12	2.10	0.52
5:A5:193:ASP:OD1	5:A5:194:THR:N	2.43	0.52
6:A9:161:GLU:OE2	6:A9:170:ARG:NH1	2.43	0.52
8:BQ:90:GLU:HG3	8:BQ:96:VAL:HG22	1.91	0.52
1:Ad:120:ASP:OD1	1:Ad:121:GLY:N	2.44	0.51
1:Ad:155:LYS:HD2	1:Ad:157:MET:SD	2.50	0.51
2:Af:29:LEU:HD23	2:Af:29:LEU:O	2.10	0.51
4:Aq:59:TRP:HE1	4:Az:58:MET:HE2	1.75	0.51
4:Aw:13:LEU:O	4:Aw:17:ILE:HD12	2.10	0.51
7:BI:140:VAL:HG11	7:BI:153:ALA:HB2	1.92	0.51
7:BL:140:VAL:HG21	7:BL:153:ALA:HB2	1.93	0.51
7:BM:239:ARG:NE	7:BM:273:GLU:OE2	2.42	0.51
1:Ad:158:HIS:NE2	1:Ae:153:SER:OG	2.43	0.51
5:A4:256:SER:OG	5:A4:266:GLN:OE1	2.13	0.51
7:BC:105:ALA:O	7:BC:130:ASP:N	2.43	0.51
7:BH:66:GLU:OE1	7:BH:120:TYR:OH	2.19	0.51
5:A2:127:ASP:OD1	5:A2:128:THR:N	2.43	0.51
7:BF:134:GLN:OE1	7:BF:134:GLN:HA	2.10	0.51
7:BH:367:VAL:HG12	7:BH:368:THR:O	2.11	0.51
2:Ag:148:ASP:OD1	2:Ag:149:ARG:N	2.43	0.51
3:An:77:THR:HG22	3:An:78:LEU:N	2.26	0.51
5:A1:294:ASN:OD1	6:A9:4:ASN:ND2	2.43	0.51
7:BM:102:THR:OG1	7:BM:191:THR:OG1	2.27	0.51
1:Ac:158:HIS:NE2	1:Ad:153:SER:OG	2.44	0.51
2:Ag:130:TYR:O	2:Ag:134:SER:OG	2.29	0.51
3:Aj:89:LEU:HA	3:Aj:92:VAL:HG12	1.93	0.51
4:Au:226:VAL:HG23	4:Au:231:GLU:C	2.36	0.51
4:Av:226:VAL:HG23	4:Av:231:GLU:C	2.36	0.51
4:Aw:31:ILE:O	6:BA:46:ARG:NH1	2.42	0.51
4:Ay:93:VAL:HG21	4:Ay:109:PHE:CE2	2.45	0.51
4:Ay:226:VAL:HG23	4:Ay:231:GLU:C	2.36	0.51
4:Az:147:ILE:O	4:Az:171:ASN:ND2	2.41	0.51
5:A1:193:ASP:OD1	5:A1:194:THR:N	2.44	0.51
7:BK:182:CYS:SG	7:BK:183:THR:N	2.83	0.51
5:A3:1:MET:HE3	5:A3:6:TYR:HB2	1.91	0.51
7:BE:24:GLU:OE1	7:BE:24:GLU:N	2.43	0.51
8:BR:90:GLU:HG3	8:BR:96:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BS:30:HIS:NE2	8:BS:79:TYR:OH	2.37	0.51
7:BK:499:ASP:OD1	7:BK:500:ASN:N	2.44	0.51
7:BL:171:HIS:C	7:BL:172:LEU:HD22	2.35	0.51
7:BM:118:ALA:HB2	7:BM:322:ASN:OD1	2.10	0.51
1:Ad:171:GLN:NE2	1:Ae:171:GLN:OE1	2.43	0.51
2:Af:155:LEU:HD22	2:Af:183:ILE:CD1	2.41	0.51
4:Aw:226:VAL:HG23	4:Aw:231:GLU:C	2.36	0.51
4:Az:226:VAL:HG23	4:Az:231:GLU:C	2.36	0.51
7:BE:248:GLN:OE1	7:BE:248:GLN:N	2.43	0.51
7:BM:74:MET:SD	7:BM:319:SER:N	2.84	0.51
2:Ah:249:VAL:O	2:Ah:249:VAL:CG1	2.59	0.50
5:A5:1:MET:SD	5:A6:68:ASP:N	2.84	0.50
2:Af:9:ILE:HG22	2:Af:14:LEU:CD1	2.42	0.50
2:Af:47:VAL:HG12	5:A4:130:THR:HG21	1.94	0.50
3:An:201:ASP:OD2	3:An:208:ASN:ND2	2.45	0.50
4:Ao:121:VAL:O	4:Ao:121:VAL:HG23	2.11	0.50
4:Ar:45:TYR:OH	4:Ar:49:GLU:OE1	2.16	0.50
7:BD:494:VAL:O	7:BD:494:VAL:HG13	2.11	0.50
7:BF:491:VAL:HG12	7:BF:491:VAL:O	2.11	0.50
8:BV:120:ILE:HD11	8:BX:55:VAL:HG12	1.91	0.50
4:As:74:LYS:O	4:As:75:MET:HG2	2.11	0.50
6:A7:73:GLY:N	6:A8:167:THR:OG1	2.44	0.50
6:A8:94:MET:HE1	6:A8:129:ALA:HB1	1.94	0.50
7:BC:150:GLU:OE2	7:BC:163:ARG:NE	2.42	0.50
7:BL:248:GLN:OE1	7:BL:248:GLN:N	2.44	0.50
2:Ag:239:ASN:OD1	2:Ag:301:ARG:NH1	2.44	0.50
3:Am:31:ASP:HB3	3:Am:34:THR:HG22	1.92	0.50
3:Am:77:THR:HG22	3:Am:78:LEU:N	2.27	0.50
4:Ax:7:ARG:NH2	4:Ax:56:GLU:OE1	2.44	0.50
4:Ax:226:VAL:HG23	4:Ax:231:GLU:C	2.36	0.50
5:A4:193:ASP:OD1	5:A4:194:THR:N	2.44	0.50
8:BO:61:ASN:ND2	8:BQ:50:LEU:O	2.44	0.50
7:BD:380:ALA:O	7:BE:497:LEU:HD22	2.12	0.50
8:BW:41:LYS:NZ	8:BW:60:SER:OG	2.42	0.50
2:Ag:155:LEU:HD21	2:Ag:183:ILE:HG12	1.93	0.50
2:Ah:148:ASP:OD1	2:Ah:149:ARG:N	2.44	0.50
6:A8:73:GLY:N	6:A9:167:THR:OG1	2.44	0.50
7:BI:220:VAL:HG21	7:BI:299:ALA:HA	1.92	0.50
4:Av:391:THR:HG22	4:Av:391:THR:O	2.10	0.50
5:A3:193:ASP:OD1	5:A3:194:THR:N	2.44	0.50
5:A6:127:ASP:OD1	5:A6:128:THR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A0:138:VAL:HG12	6:A0:152:ILE:HG12	1.94	0.50
7:BE:167:THR:OG1	7:BE:203:ASN:ND2	2.42	0.50
7:BL:465:PRO:HG2	7:BL:468:VAL:HG21	1.94	0.50
3:Ai:96:THR:HG22	4:Ay:55:ALA:HB2	1.94	0.50
3:Am:63:THR:HG23	3:Am:63:THR:O	2.12	0.50
4:Ao:67:ALA:O	4:Ao:185:ARG:NH2	2.45	0.50
7:BE:102:THR:OG1	7:BE:191:THR:OG1	2.29	0.50
7:BL:182:CYS:O	7:BL:183:THR:OG1	2.25	0.50
2:Ag:222:LEU:HA	2:Ag:226:ILE:HD12	1.92	0.50
4:Ar:176:ASP:OD1	4:Ar:177:ASP:N	2.42	0.50
6:A7:167:THR:OG1	6:BB:73:GLY:N	2.45	0.50
1:Ad:174:ASP:OD1	1:Ad:178:ASP:N	2.45	0.50
4:Aq:45:TYR:OH	4:Aq:49:GLU:OE1	2.20	0.50
5:A5:20:VAL:HG23	5:A5:20:VAL:O	2.12	0.49
8:BO:109:GLU:OE1	8:BQ:39:THR:OG1	2.29	0.49
8:BP:61:ASN:OD1	8:BR:52:ASN:N	2.45	0.49
7:BH:109:GLY:HA2	7:BH:185:VAL:HG22	1.93	0.49
2:Af:297:GLU:OE2	2:Af:300:ARG:NH2	2.39	0.49
2:Ah:52:VAL:HG11	2:Ah:55:LYS:HE3	1.93	0.49
4:Ay:391:THR:O	4:Ay:391:THR:HG22	2.11	0.49
8:BX:61:ASN:OD1	8:BZ:52:ASN:N	2.45	0.49
7:BM:71:VAL:HG22	7:BM:296:ALA:HB2	1.93	0.49
7:BM:140:VAL:HG13	7:BM:151:ALA:HB1	1.94	0.49
3:Aj:96:THR:HG22	4:Ax:55:ALA:CB	2.42	0.49
3:Ak:201:ASP:OD2	3:Ak:208:ASN:ND2	2.45	0.49
3:An:160:ILE:HD13	3:An:237:ALA:O	2.12	0.49
7:BF:367:VAL:HG12	7:BF:368:THR:O	2.12	0.49
3:Ak:160:ILE:HD13	3:Ak:237:ALA:O	2.12	0.49
7:BH:136:ALA:O	7:BH:137:ALA:HB3	2.12	0.49
7:BK:112:GLN:NE2	7:BK:178:ASN:OD1	2.39	0.49
3:Ai:215:PHE:O	3:Ai:283:GLN:NE2	2.45	0.49
8:BX:18:HIS:ND1	8:BX:21:THR:HG22	2.26	0.49
4:Ao:176:ASP:OD1	4:Ao:177:ASP:N	2.42	0.49
7:BH:257:ASN:ND2	7:BH:267:ASP:OD2	2.46	0.49
3:Aj:63:THR:HG23	3:Aj:63:THR:O	2.12	0.49
4:Ao:74:LYS:O	4:Ao:75:MET:HG2	2.12	0.49
5:A5:1:MET:HE2	5:A5:6:TYR:CD1	2.47	0.49
6:A0:140:LEU:HD13	6:A0:150:MET:CE	2.43	0.49
7:BD:367:VAL:HG12	7:BD:368:THR:O	2.13	0.49
7:BK:105:ALA:O	7:BK:130:ASP:N	2.42	0.49
2:Ah:29:LEU:HD23	2:Ah:29:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Au:68:CYS:SG	4:Au:69:CYS:N	2.86	0.49
5:A1:114:GLY:O	5:A6:1:MET:N	2.46	0.49
7:BE:220:VAL:HG21	7:BE:299:ALA:HA	1.93	0.49
3:Al:29:ASP:OD1	7:BN:183:THR:N	2.31	0.49
4:Aq:121:VAL:HG23	4:Aq:121:VAL:O	2.13	0.49
4:Ay:218:ASP:OD1	4:Ay:219:LEU:N	2.44	0.49
5:A4:127:ASP:OD1	5:A4:128:THR:N	2.46	0.49
5:A4:349:ILE:HD12	5:A4:395:ARG:HG2	1.94	0.49
5:A6:20:VAL:HG23	5:A6:20:VAL:O	2.12	0.49
7:BE:8:ASP:OD2	7:BF:403:GLN:NE2	2.46	0.49
1:Ad:54:TYR:OH	1:Ad:100:GLN:O	2.31	0.49
3:Al:119:ARG:NH1	4:Ay:63:ASP:OD1	2.44	0.49
4:Ar:121:VAL:HG23	4:Ar:121:VAL:O	2.12	0.49
5:A3:316:GLU:OE2	5:A3:316:GLU:HA	2.13	0.49
7:BD:105:ALA:O	7:BD:130:ASP:N	2.40	0.49
8:BQ:63:THR:HG22	8:BQ:120:ILE:HG22	1.94	0.49
3:Ak:77:THR:HG22	3:Ak:78:LEU:H	1.78	0.48
5:A3:20:VAL:O	5:A3:20:VAL:HG23	2.12	0.48
7:BI:43:ASN:OD1	7:BI:86:ARG:NH1	2.45	0.48
7:BJ:340:GLN:NE2	7:BJ:365:ASN:OD1	2.41	0.48
2:Ah:128:THR:OG1	2:Ah:131:LEU:HD12	2.13	0.48
5:A1:349:ILE:HD12	5:A1:395:ARG:HG2	1.93	0.48
7:BD:43:ASN:OD1	7:BD:86:ARG:NH1	2.43	0.48
8:BY:34:ASP:OD1	8:BY:36:THR:OG1	2.25	0.48
4:Av:149:VAL:HG22	4:Av:150:THR:N	2.29	0.48
5:A1:133:GLY:O	5:A1:134:LEU:HD12	2.13	0.48
5:A6:193:ASP:OD1	5:A6:194:THR:N	2.46	0.48
7:BE:418:LYS:HB2	7:BE:421:ILE:HD12	1.95	0.48
8:BT:86:ASP:OD1	8:BT:101:GLU:N	2.44	0.48
7:BM:373:ASP:OD1	7:BM:374:GLU:N	2.42	0.48
1:Ac:36:THR:OG1	1:Ac:44:ASP:O	2.29	0.48
3:Al:77:THR:HG22	3:Al:78:LEU:N	2.29	0.48
3:Am:191:GLU:HG3	3:Am:192:PRO:HD3	1.96	0.48
4:Av:385:VAL:HG13	4:Av:385:VAL:O	2.13	0.48
7:BC:79:VAL:HG23	7:BC:300:CYS:SG	2.53	0.48
8:BX:90:GLU:HG3	8:BX:96:VAL:HG22	1.93	0.48
7:BE:37:ASP:OD2	7:BE:60:GLN:N	2.43	0.48
2:Ah:255:GLY:O	2:Ah:259:ILE:HD12	2.14	0.48
4:Ax:31:ILE:O	6:A0:46:ARG:NH1	2.46	0.48
6:BA:73:GLY:N	6:BB:167:THR:OG1	2.46	0.48
7:BE:96:VAL:HG13	7:BE:161:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BE:373:ASP:OD1	7:BE:374:GLU:N	2.42	0.48
8:BX:70:ARG:NH2	8:BX:112:GLY:O	2.46	0.48
1:Ad:21:HIS:HB3	1:Ad:37:VAL:O	2.13	0.48
4:Ax:218:ASP:OD1	4:Ax:219:LEU:N	2.46	0.48
5:A1:146:ILE:HD11	5:A1:327:ILE:HD13	1.96	0.48
8:BU:61:ASN:ND2	8:BW:50:LEU:O	2.45	0.48
7:BI:140:VAL:HG13	7:BI:151:ALA:HB1	1.96	0.48
3:Ai:110:VAL:HG22	3:Ai:225:VAL:HB	1.95	0.48
3:Aj:77:THR:HG22	3:Aj:78:LEU:H	1.79	0.48
4:At:121:VAL:HG23	4:At:121:VAL:O	2.13	0.48
7:BC:367:VAL:HG12	7:BC:368:THR:O	2.14	0.48
2:Af:239:ASN:HD22	2:Af:275:ILE:HG22	1.78	0.48
4:Ap:34:GLU:OE2	6:A7:97:GLY:N	2.45	0.48
4:As:45:TYR:OH	4:As:49:GLU:OE1	2.22	0.48
7:BK:126:VAL:HG13	7:BK:126:VAL:O	2.14	0.48
3:Am:198:VAL:HG13	3:Am:198:VAL:O	2.14	0.47
5:A2:63:ARG:NH1	5:A2:117:TYR:OH	2.47	0.47
8:BT:60:SER:OG	8:BT:61:ASN:N	2.47	0.47
8:BT:61:ASN:OD1	8:BV:53:GLY:N	2.38	0.47
7:BM:33:GLN:NE2	7:BM:88:ASP:OD1	2.42	0.47
1:Ae:134:THR:HG22	1:Ae:136:GLU:H	1.79	0.47
2:Ag:39:LEU:HD23	2:Ag:118:TYR:CZ	2.49	0.47
5:A5:1:MET:SD	5:A6:67:ASN:HA	2.55	0.47
6:BA:55:VAL:HG22	6:BA:132:VAL:CG1	2.44	0.47
8:BX:48:THR:HG22	8:BX:49:ALA:H	1.79	0.47
7:BM:54:LEU:O	7:BM:56:GLU:N	2.45	0.47
4:At:74:LYS:O	4:At:75:MET:CG	2.62	0.47
5:A4:146:ILE:HD11	5:A4:327:ILE:HD13	1.95	0.47
6:A8:55:VAL:HG22	6:A8:132:VAL:CG1	2.45	0.47
7:BI:213:VAL:HG12	7:BI:213:VAL:O	2.14	0.47
3:Aj:198:VAL:HG13	3:Aj:198:VAL:O	2.14	0.47
5:A4:93:ARG:HH21	5:A5:105:VAL:HG11	1.78	0.47
5:A6:2:ALA:HA	8:BW:54:ALA:HA	1.97	0.47
8:BP:48:THR:HG22	8:BP:49:ALA:H	1.79	0.47
7:BL:367:VAL:HG12	7:BL:368:THR:O	2.14	0.47
4:Ay:31:ILE:O	6:A9:46:ARG:NH1	2.48	0.47
5:A5:63:ARG:NH1	5:A5:117:TYR:OH	2.47	0.47
5:A5:219:ALA:O	5:A5:223:ASN:ND2	2.48	0.47
6:A9:64:LEU:O	6:A9:65:THR:OG1	2.32	0.47
7:BF:140:VAL:HG21	7:BF:153:ALA:HB2	1.97	0.47
7:BM:241:ALA:HB1	7:BM:249:CYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Af:148:ASP:OD1	2:Af:149:ARG:N	2.47	0.47
4:At:59:TRP:HE1	4:Aw:58:MET:HE2	1.79	0.47
8:BP:52:ASN:N	8:BZ:61:ASN:OD1	2.47	0.47
7:BJ:187:PRO:O	7:BJ:190:VAL:HG22	2.14	0.47
1:Ac:168:VAL:HG23	1:Ad:187:LYS:NZ	2.29	0.47
2:Af:130:TYR:O	2:Af:134:SER:OG	2.30	0.47
3:Aj:191:GLU:HG3	3:Aj:192:PRO:HD3	1.95	0.47
3:Al:61:THR:HG22	3:Al:65:ASN:O	2.15	0.47
3:Al:198:VAL:HG13	3:Al:198:VAL:O	2.15	0.47
6:A7:138:VAL:HG12	6:A7:152:ILE:HG12	1.97	0.47
6:A9:19:VAL:CG1	6:A9:60:LEU:HD11	2.44	0.47
7:BF:214:ASN:C	7:BF:214:ASN:OD1	2.58	0.47
7:BI:459:SER:OG	7:BI:462:ASP:OD2	2.32	0.47
3:Al:215:PHE:O	3:Al:283:GLN:NE2	2.47	0.47
4:Ap:126:LEU:HD12	4:Ap:127:PRO:CD	2.44	0.47
4:Au:156:THR:O	4:Au:156:THR:OG1	2.32	0.47
5:A2:20:VAL:HG23	5:A2:20:VAL:O	2.14	0.47
5:A4:133:GLY:C	5:A4:134:LEU:HD12	2.40	0.47
6:BB:19:VAL:CG1	6:BB:60:LEU:HD11	2.45	0.47
7:BN:340:GLN:NE2	7:BN:365:ASN:OD1	2.44	0.47
7:BL:105:ALA:O	7:BL:130:ASP:N	2.43	0.47
1:Ae:93:PRO:HG2	1:Ae:96:THR:HG21	1.96	0.47
4:Av:31:ILE:O	6:BB:46:ARG:NH1	2.47	0.47
4:Aw:176:ASP:OD1	4:Aw:177:ASP:N	2.48	0.47
4:Az:385:VAL:O	4:Az:385:VAL:HG13	2.15	0.47
5:A5:133:GLY:C	5:A5:134:LEU:HD12	2.40	0.47
6:BB:106:ARG:NH1	6:BB:115:LEU:HD22	2.29	0.47
7:BC:172:LEU:HD21	7:BC:174:VAL:HG23	1.95	0.47
1:Ae:22:VAL:HG13	2:Ah:259:ILE:HD13	1.96	0.47
2:Ag:39:LEU:HD23	2:Ag:118:TYR:OH	2.14	0.47
3:Ai:77:THR:HG22	3:Ai:78:LEU:H	1.80	0.47
7:BD:10:PHE:CD2	7:BD:11:VAL:N	2.83	0.47
7:BH:11:VAL:HG12	7:BH:12:ARG:H	1.80	0.47
3:Am:180:ILE:HD11	4:Ap:198:LEU:HB2	1.97	0.46
3:An:20:SER:N	4:Aq:70:GLU:OE2	2.42	0.46
8:BU:60:SER:OG	8:BU:61:ASN:N	2.48	0.46
7:BK:428:LEU:HD13	8:BX:13:LEU:HD11	1.97	0.46
1:Ad:21:HIS:CD2	1:Ad:68:LEU:HD13	2.50	0.46
2:Ag:29:LEU:HD23	2:Ag:29:LEU:O	2.15	0.46
4:Aq:74:LYS:O	4:Aq:75:MET:CG	2.62	0.46
4:Aw:385:VAL:HG13	4:Aw:385:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A4:20:VAL:HG23	5:A4:20:VAL:O	2.15	0.46
5:A6:349:ILE:HD12	5:A6:395:ARG:HG2	1.96	0.46
7:BK:167:THR:OG1	7:BK:203:ASN:ND2	2.48	0.46
7:BK:439:ASP:C	7:BK:439:ASP:OD2	2.58	0.46
2:Af:334:PRO:N	2:Af:335:PRO:CD	2.78	0.46
3:Ak:119:ARG:NH1	4:Aw:63:ASP:OD1	2.48	0.46
4:Av:149:VAL:HG22	4:Av:150:THR:H	1.81	0.46
5:A1:1:MET:SD	5:A1:3:GLY:O	2.73	0.46
5:A1:20:VAL:HG23	5:A1:20:VAL:O	2.15	0.46
5:A3:1:MET:SD	5:A3:3:GLY:O	2.74	0.46
5:A4:130:THR:HG22	5:A4:130:THR:O	2.16	0.46
6:A7:67:ALA:N	6:A7:98:SER:O	2.44	0.46
8:BV:120:ILE:HD11	8:BX:55:VAL:CG1	2.45	0.46
7:BK:115:MET:HE2	7:BK:122:LEU:HD23	1.98	0.46
3:Ai:198:VAL:O	3:Ai:198:VAL:HG13	2.15	0.46
4:Ap:74:LYS:O	4:Ap:75:MET:HG2	2.15	0.46
4:Aw:390:VAL:HG12	4:Aw:391:THR:N	2.31	0.46
5:A2:219:ALA:O	5:A2:223:ASN:ND2	2.48	0.46
5:A4:1:MET:SD	5:A4:3:GLY:O	2.73	0.46
1:Ac:34:ILE:HG22	1:Ac:47:VAL:HG22	1.96	0.46
2:Af:333:ILE:HD12	2:Af:338:ILE:HD12	1.96	0.46
2:Ag:9:ILE:HG22	2:Ag:14:LEU:CD1	2.46	0.46
2:Ag:110:VAL:HG23	2:Ag:110:VAL:O	2.15	0.46
2:Ah:4:PRO:O	2:Ah:62:MET:N	2.42	0.46
3:An:31:ASP:HB3	3:An:34:THR:HG22	1.96	0.46
4:Av:93:VAL:HG21	4:Av:109:PHE:HE2	1.81	0.46
4:Ax:68:CYS:SG	4:Ax:69:CYS:N	2.88	0.46
4:Az:390:VAL:HG12	4:Az:391:THR:N	2.31	0.46
5:A1:61:ARG:NH1	5:A1:119:ASP:OD2	2.49	0.46
7:BC:241:ALA:HB1	7:BC:249:CYS:O	2.15	0.46
7:BI:273:GLU:N	7:BI:273:GLU:OE1	2.49	0.46
8:BV:59:ALA:O	8:BV:60:SER:OG	2.33	0.46
7:BL:449:ASP:OD1	7:BL:450:ASN:N	2.48	0.46
2:Ag:286:THR:O	2:Ag:289:SER:OG	2.31	0.46
3:Aj:191:GLU:N	3:Aj:192:PRO:CD	2.79	0.46
4:Aq:231:GLU:N	4:Aq:231:GLU:OE1	2.48	0.46
4:Aq:233:GLU:N	4:Aq:233:GLU:OE1	2.49	0.46
4:Av:218:ASP:OD1	4:Av:219:LEU:N	2.44	0.46
8:BV:25:ILE:HD12	8:BV:78:TRP:CZ3	2.50	0.46
8:BV:85:ILE:HD13	8:BV:117:MET:CE	2.45	0.46
8:BY:41:LYS:NZ	8:BY:61:ASN:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Af:236:ASP:OD1	2:Af:236:ASP:O	2.34	0.46
4:Ap:231:GLU:N	4:Ap:231:GLU:OE1	2.49	0.46
7:BC:132:PRO:HD2	7:BC:135:ILE:HD12	1.97	0.46
7:BF:21:PHE:O	7:BF:21:PHE:CD2	2.68	0.46
7:BF:449:ASP:OD1	7:BF:450:ASN:N	2.47	0.46
7:BH:220:VAL:HG21	7:BH:299:ALA:HA	1.97	0.46
7:BK:71:VAL:HG22	7:BK:296:ALA:HB2	1.98	0.46
2:Ah:39:LEU:HD23	2:Ah:118:TYR:OH	2.16	0.46
4:Aq:67:ALA:O	4:Aq:185:ARG:NH2	2.49	0.46
7:BC:126:VAL:O	7:BC:126:VAL:HG13	2.16	0.46
2:Af:344:CYS:HA	2:Af:363:LEU:HD23	1.96	0.46
3:Aj:180:ILE:HD11	4:As:198:LEU:HB2	1.97	0.46
5:A4:294:ASN:OD1	6:BB:4:ASN:ND2	2.47	0.46
7:BM:118:ALA:HB3	7:BM:321:ILE:HG22	1.98	0.46
2:Ah:3:LYS:NZ	2:Ah:17:TYR:OH	2.48	0.45
4:Ap:45:TYR:OH	4:Ap:49:GLU:OE1	2.19	0.45
6:A8:19:VAL:HG13	6:A8:60:LEU:HD11	1.98	0.45
8:BQ:60:SER:OG	8:BQ:61:ASN:N	2.50	0.45
7:BI:140:VAL:HG13	7:BI:151:ALA:HB3	1.97	0.45
7:BK:8:ASP:OD2	7:BL:403:GLN:NE2	2.48	0.45
1:Ae:44:ASP:OD1	1:Ae:45:GLU:N	2.49	0.45
2:Ag:334:PRO:N	2:Ag:335:PRO:CD	2.79	0.45
2:Ah:120:VAL:HG12	2:Ah:121:THR:N	2.31	0.45
3:Am:42:LEU:HD21	5:A2:358:HIS:ND1	2.31	0.45
5:A3:350:VAL:HG22	5:A3:392:ILE:HG12	1.98	0.45
5:A6:17:PHE:O	5:A6:20:VAL:HG22	2.17	0.45
2:Ah:249:VAL:N	2:Ah:284:ASP:OD1	2.45	0.45
5:A2:68:ASP:OD2	5:A2:71:ALA:HB3	2.17	0.45
7:BE:54:LEU:O	7:BE:56:GLU:N	2.47	0.45
7:BF:12:ARG:HG3	7:BF:12:ARG:HH11	1.80	0.45
8:BW:90:GLU:HG3	8:BW:96:VAL:HG22	1.97	0.45
1:Ad:174:ASP:OD1	1:Ad:177:GLY:N	2.50	0.45
6:A7:106:ARG:NH1	6:A7:115:LEU:HD22	2.31	0.45
7:BD:84:LEU:HD23	7:BD:84:LEU:O	2.16	0.45
8:BV:15:THR:HG23	8:BV:25:ILE:O	2.16	0.45
2:Ag:236:ASP:OD1	2:Ag:236:ASP:O	2.35	0.45
3:Al:77:THR:HG22	3:Al:78:LEU:H	1.82	0.45
4:Ar:231:GLU:OE1	4:Ar:231:GLU:N	2.50	0.45
7:BD:110:ARG:NH2	7:BD:123:ASP:OD1	2.50	0.45
7:BG:269:ASP:OD1	7:BG:271:SER:OG	2.30	0.45
7:BH:351:THR:HG22	7:BH:359:THR:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:49:ASN:O	7:BJ:377:ARG:NH2	2.50	0.45
8:BX:25:ILE:HD12	8:BX:78:TRP:CZ3	2.52	0.45
8:BY:30:HIS:NE2	8:BY:79:TYR:OH	2.38	0.45
2:Af:120:VAL:HG12	2:Af:121:THR:N	2.32	0.45
3:Aj:77:THR:HG22	3:Aj:78:LEU:N	2.32	0.45
4:Av:390:VAL:HG12	4:Av:391:THR:N	2.32	0.45
8:BO:41:LYS:NZ	8:BO:60:SER:OG	2.49	0.45
2:Ag:62:MET:O	2:Ag:62:MET:HG3	2.16	0.45
2:Ah:9:ILE:HG23	2:Ah:9:ILE:O	2.17	0.45
2:Ah:351:VAL:HG12	2:Ah:352:ASP:N	2.31	0.45
4:Aw:147:ILE:O	4:Aw:171:ASN:ND2	2.42	0.45
2:Ag:351:VAL:HG22	2:Ag:352:ASP:N	2.32	0.45
4:At:297:LEU:HD13	4:At:300:LEU:HD11	1.99	0.45
7:BD:213:VAL:HG12	7:BD:213:VAL:O	2.16	0.45
7:BE:499:ASP:OD1	7:BE:500:ASN:N	2.49	0.45
7:BK:54:LEU:O	7:BK:56:GLU:N	2.45	0.45
7:BK:373:ASP:OD1	7:BK:374:GLU:N	2.44	0.45
3:Ak:226:ASN:ND2	3:Ak:230:CYS:O	2.44	0.45
4:As:231:GLU:N	4:As:231:GLU:OE1	2.49	0.45
4:Au:149:VAL:HG22	4:Au:150:THR:H	1.81	0.45
4:Ax:121:VAL:HG23	4:Ax:121:VAL:O	2.17	0.45
8:BP:48:THR:HG22	8:BP:49:ALA:N	2.32	0.45
2:Af:29:LEU:HD22	2:Af:132:VAL:HG22	1.99	0.45
4:Ax:149:VAL:HG22	4:Ax:150:THR:H	1.82	0.45
4:Ax:390:VAL:HG12	4:Ax:391:THR:N	2.32	0.45
5:A6:1:MET:HE3	5:A6:2:ALA:O	2.16	0.45
7:BN:491:VAL:HG21	7:BL:13:LEU:HD12	1.98	0.45
7:BH:273:GLU:OE1	7:BH:273:GLU:N	2.49	0.45
3:Ak:173:GLU:OE2	3:Ak:173:GLU:HA	2.18	0.44
4:As:74:LYS:O	4:As:75:MET:CG	2.66	0.44
5:A6:132:PHE:O	5:A6:132:PHE:CD2	2.70	0.44
1:Ad:36:THR:OG1	1:Ad:44:ASP:O	2.36	0.44
2:Ag:333:ILE:HD12	2:Ag:338:ILE:HD12	1.99	0.44
3:Ak:180:ILE:HD11	4:At:198:LEU:HB2	1.99	0.44
4:Aw:151:GLU:OE1	4:Aw:151:GLU:N	2.51	0.44
6:BA:19:VAL:CG1	6:BA:60:LEU:HD11	2.47	0.44
7:BC:140:VAL:HG13	7:BC:151:ALA:CB	2.47	0.44
1:Ae:43:MET:HE2	2:Ag:174:LYS:NZ	2.33	0.44
2:Af:25:THR:HG22	2:Af:27:LYS:H	1.82	0.44
2:Ah:110:VAL:HG12	2:Ah:120:VAL:HG22	1.99	0.44
3:Am:34:THR:HG23	3:Am:35:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A4:61:ARG:NH1	5:A4:119:ASP:OD2	2.49	0.44
6:BB:138:VAL:HG12	6:BB:152:ILE:HG12	1.99	0.44
8:BO:63:THR:HG22	8:BO:64:MET:N	2.33	0.44
7:BH:147:PHE:O	7:BH:163:ARG:NH1	2.50	0.44
7:BJ:43:ASN:OD1	7:BJ:86:ARG:NH1	2.48	0.44
2:Ag:331:VAL:HG12	2:Ag:332:GLU:N	2.32	0.44
2:Ah:334:PRO:N	2:Ah:335:PRO:CD	2.81	0.44
3:Am:179:ILE:HD13	3:Am:189:VAL:HG21	1.99	0.44
5:A4:107:ASP:OD1	5:A4:108:SER:N	2.49	0.44
7:BE:136:ALA:O	7:BE:137:ALA:HB3	2.17	0.44
8:BV:81:GLY:O	8:BX:57:ARG:NH1	2.49	0.44
7:BM:167:THR:OG1	7:BM:203:ASN:ND2	2.46	0.44
3:Al:29:ASP:OD1	7:BN:183:THR:HG22	2.16	0.44
4:Av:239:GLU:OE1	4:Av:286:ARG:NE	2.41	0.44
5:A5:68:ASP:OD2	5:A5:71:ALA:HB3	2.17	0.44
6:A0:150:MET:HG2	7:BJ:491:VAL:HG23	2.00	0.44
8:BT:63:THR:HG22	8:BT:120:ILE:HG22	2.00	0.44
1:Ae:175:SER:O	1:Ae:176:ASP:CG	2.61	0.44
2:Ah:143:PHE:CD2	2:Ah:146:THR:HG21	2.52	0.44
4:Aq:297:LEU:HD13	4:Aq:300:LEU:HD11	1.99	0.44
5:A6:299:GLN:OE1	5:A6:341:ARG:NH2	2.50	0.44
7:BK:99:LEU:HD23	7:BK:158:ILE:HD11	2.00	0.44
8:BZ:86:ASP:OD1	8:BZ:101:GLU:N	2.43	0.44
8:BS:63:THR:HG22	8:BS:120:ILE:HG22	2.00	0.44
7:BM:111:VAL:HG23	7:BM:176:TYR:CZ	2.53	0.44
1:Ac:125:LEU:HD12	1:Ac:131:LEU:HD22	2.00	0.44
1:Ad:156:LEU:HD13	1:Ae:149:LEU:HD23	1.98	0.44
2:Ag:176:THR:O	2:Ag:176:THR:CG2	2.65	0.44
3:An:34:THR:HG23	3:An:35:LEU:N	2.33	0.44
6:A9:19:VAL:HG13	6:A9:60:LEU:HD11	2.00	0.44
8:BS:34:ASP:OD1	8:BS:36:THR:OG1	2.30	0.44
1:Ad:46:ASP:OD1	1:Ad:47:VAL:N	2.51	0.44
5:A1:285:TYR:O	5:A1:341:ARG:NH1	2.50	0.44
6:A8:19:VAL:CG1	6:A8:60:LEU:HD11	2.48	0.44
7:BC:418:LYS:HB2	7:BC:421:ILE:HD12	2.00	0.44
7:BF:127:ASP:OD1	7:BF:138:LYS:NZ	2.46	0.44
8:BX:15:THR:HG23	8:BX:25:ILE:O	2.18	0.44
2:Ah:29:LEU:HD22	2:Ah:132:VAL:HG12	2.00	0.43
4:Au:218:ASP:OD1	4:Au:219:LEU:N	2.46	0.43
4:Au:239:GLU:OE1	4:Au:286:ARG:NE	2.43	0.43
5:A3:17:PHE:O	5:A3:20:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:136:ALA:O	7:BG:137:ALA:HB3	2.17	0.43
7:BJ:418:LYS:HB2	7:BJ:421:ILE:HD12	1.99	0.43
7:BL:55:VAL:O	7:BL:59:GLY:N	2.51	0.43
7:BL:213:VAL:O	7:BL:213:VAL:HG12	2.18	0.43
2:Af:47:VAL:CG1	5:A4:130:THR:HG21	2.48	0.43
4:Az:149:VAL:HG22	4:Az:150:THR:H	1.83	0.43
4:Az:218:ASP:OD1	4:Az:219:LEU:N	2.46	0.43
6:A7:150:MET:N	7:BD:490:ASN:O	2.45	0.43
8:BQ:106:GLU:O	8:BQ:106:GLU:CG	2.66	0.43
1:Ae:71:ASP:OD2	2:Ag:247:HIS:ND1	2.46	0.43
2:Ah:355:SER:O	5:A6:36:ALA:HB2	2.18	0.43
3:Aj:119:ARG:NH1	4:Ax:63:ASP:OD1	2.50	0.43
4:Ao:210:TRP:HB3	4:Ao:213:VAL:HG21	1.99	0.43
4:Au:121:VAL:HG23	4:Au:121:VAL:O	2.17	0.43
6:A8:100:ILE:HD13	7:BD:12:ARG:HE	1.83	0.43
7:BC:220:VAL:HG21	7:BC:299:ALA:CB	2.48	0.43
8:BR:25:ILE:HD12	8:BR:78:TRP:CZ3	2.53	0.43
7:BF:272:ALA:HB2	7:BF:370:TYR:HD1	1.84	0.43
7:BH:50:SER:OG	7:BH:51:GLU:OE1	2.36	0.43
2:Ag:131:LEU:HD22	2:Ag:183:ILE:HD13	1.99	0.43
2:Ag:253:VAL:O	2:Ag:253:VAL:HG23	2.17	0.43
3:Ai:76:PRO:C	3:Ai:77:THR:HG1	2.26	0.43
3:Ak:61:THR:OG1	3:Ak:62:ALA:N	2.52	0.43
4:Au:390:VAL:HG12	4:Au:391:THR:N	2.33	0.43
6:A0:146:ASN:OD1	6:A0:147:LYS:N	2.50	0.43
7:BC:273:GLU:OE1	7:BC:273:GLU:N	2.51	0.43
7:BK:269:ASP:OD1	7:BK:271:SER:OG	2.34	0.43
8:BX:61:ASN:ND2	8:BZ:50:LEU:O	2.39	0.43
2:Af:39:LEU:HD23	2:Af:118:TYR:OH	2.18	0.43
7:BN:273:GLU:OE1	7:BN:273:GLU:N	2.51	0.43
7:BD:302:THR:HG22	7:BD:308:LEU:HD23	2.01	0.43
7:BF:53:ASP:O	7:BF:53:ASP:OD1	2.36	0.43
7:BH:465:PRO:HG2	7:BH:468:VAL:HG21	2.00	0.43
7:BK:254:TYR:OH	7:BK:298:SER:OG	2.22	0.43
3:Aj:29:ASP:OD1	7:BJ:183:THR:N	2.42	0.43
3:Aj:223:ASP:OD1	3:Aj:223:ASP:N	2.51	0.43
3:Ak:198:VAL:HG13	3:Ak:198:VAL:O	2.18	0.43
3:Am:215:PHE:O	3:Am:283:GLN:NE2	2.51	0.43
4:Ay:390:VAL:HG12	4:Ay:391:THR:N	2.34	0.43
5:A1:67:ASN:N	5:A6:1:MET:HE1	2.34	0.43
5:A2:132:PHE:O	5:A2:132:PHE:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A3:299:GLN:OE1	5:A3:341:ARG:NH2	2.50	0.43
5:A6:60:ILE:HG22	5:A6:61:ARG:N	2.34	0.43
7:BC:70:LYS:NZ	7:BC:119:GLU:OE2	2.43	0.43
2:Af:256:LYS:HD2	2:Af:256:LYS:N	2.33	0.43
2:Ah:57:ILE:C	2:Ah:58:LEU:HD12	2.44	0.43
3:Ai:152:VAL:HG11	3:Ai:251:LEU:HD11	2.00	0.43
4:Aq:104:ASN:O	4:Aq:122:VAL:HG21	2.19	0.43
4:At:104:ASN:O	4:At:122:VAL:HG21	2.19	0.43
7:BK:96:VAL:HG13	7:BK:161:THR:HG22	2.00	0.43
7:BK:136:ALA:O	7:BK:137:ALA:HB3	2.18	0.43
7:BM:131:THR:HG22	7:BM:135:ILE:HG21	1.99	0.43
2:Ag:336:GLU:O	2:Ag:336:GLU:HG2	2.17	0.43
2:Ah:123:THR:HG22	2:Ah:124:ALA:N	2.33	0.43
2:Ah:219:ASP:O	2:Ah:221:VAL:HG23	2.18	0.43
3:Aj:31:ASP:HB3	3:Aj:34:THR:HG22	2.00	0.43
4:Ay:385:VAL:HG13	4:Ay:385:VAL:O	2.19	0.43
5:A3:130:THR:O	5:A3:130:THR:HG22	2.18	0.43
7:BN:184:SER:O	7:BN:185:VAL:C	2.61	0.43
7:BN:235:ARG:NH1	7:BN:269:ASP:OD2	2.52	0.43
7:BC:373:ASP:OD1	7:BC:374:GLU:N	2.47	0.43
7:BD:112:GLN:CG	7:BD:177:THR:HG21	2.47	0.43
7:BE:37:ASP:OD1	7:BE:37:ASP:N	2.50	0.43
7:BE:126:VAL:O	7:BE:126:VAL:HG13	2.18	0.43
7:BJ:16:ASP:OD2	7:BJ:17:PRO:HD2	2.18	0.43
2:Ah:9:ILE:CG2	2:Ah:14:LEU:HD11	2.49	0.43
3:Aj:179:ILE:HD13	3:Aj:189:VAL:HG21	2.01	0.43
4:Ar:129:THR:HG23	4:Ar:131:VAL:HG12	2.00	0.43
6:BB:158:ASP:O	6:BB:170:ARG:NH2	2.52	0.43
7:BD:374:GLU:OE2	7:BD:374:GLU:HA	2.19	0.43
7:BG:126:VAL:HG13	7:BG:126:VAL:O	2.18	0.43
7:BG:269:ASP:OD2	7:BG:276:ARG:NH2	2.51	0.43
7:BJ:110:ARG:NH2	7:BJ:123:ASP:OD1	2.46	0.43
8:BW:34:ASP:OD1	8:BW:36:THR:OG1	2.32	0.43
1:Ac:93:PRO:HG2	1:Ac:96:THR:HG21	2.01	0.43
2:Ag:110:VAL:HG11	2:Ah:336:GLU:OE2	2.19	0.43
3:Am:230:CYS:HA	7:BD:183:THR:HG21	2.01	0.43
5:A1:1:MET:HA	5:A2:65:GLN:O	2.19	0.43
5:A3:157:TYR:OH	5:A3:319:HIS:O	2.34	0.43
5:A3:291:SER:OG	5:A3:295:GLU:OE1	2.36	0.43
6:A7:100:ILE:HB	7:BN:12:ARG:HH22	1.84	0.43
8:BR:15:THR:HG23	8:BR:25:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:167:THR:OG1	7:BG:203:ASN:ND2	2.47	0.43
7:BI:33:GLN:NE2	7:BI:88:ASP:OD1	2.52	0.43
7:BK:134:GLN:OE1	7:BK:134:GLN:HA	2.19	0.43
7:BK:140:VAL:HG13	7:BK:151:ALA:HB3	2.01	0.43
8:BY:60:SER:OG	8:BY:61:ASN:N	2.51	0.43
3:Al:180:ILE:O	3:Al:180:ILE:HG23	2.18	0.42
7:BC:37:ASP:OD1	7:BC:37:ASP:N	2.47	0.42
7:BC:71:VAL:HG22	7:BC:296:ALA:HB2	2.01	0.42
7:BI:54:LEU:O	7:BI:56:GLU:N	2.52	0.42
7:BK:51:GLU:HA	7:BK:54:LEU:HD13	2.00	0.42
2:Ag:253:VAL:O	2:Ag:254:TRP:CD1	2.72	0.42
2:Ah:29:LEU:HD22	2:Ah:132:VAL:CG1	2.49	0.42
3:Ai:77:THR:HG22	3:Ai:78:LEU:N	2.34	0.42
3:Ak:127:GLU:N	3:Ak:127:GLU:OE1	2.52	0.42
6:A7:27:ASP:OD1	6:A7:28:ASP:N	2.51	0.42
8:BP:84:GLN:OE1	8:BQ:3:CYS:N	2.52	0.42
7:BI:172:LEU:HD21	7:BI:174:VAL:HG23	2.01	0.42
8:BW:15:THR:HG23	8:BW:25:ILE:O	2.18	0.42
1:Ae:48:PRO:HD3	2:Ag:254:TRP:CH2	2.54	0.42
2:Ag:226:ILE:HG22	2:Ag:227:LEU:N	2.34	0.42
2:Ah:155:LEU:HD11	2:Ah:183:ILE:HG12	2.01	0.42
4:Aq:59:TRP:NE1	4:Az:58:MET:HE2	2.33	0.42
4:Az:68:CYS:SG	4:Az:69:CYS:N	2.92	0.42
5:A2:352:SER:O	5:A2:352:SER:OG	2.34	0.42
6:A9:138:VAL:HG12	6:A9:152:ILE:HG12	2.01	0.42
7:BC:96:VAL:HG13	7:BC:161:THR:HG22	2.01	0.42
2:Ag:9:ILE:HG23	2:Ag:9:ILE:O	2.18	0.42
2:Ag:37:ILE:HG22	2:Ag:38:PHE:N	2.33	0.42
3:Aj:215:PHE:O	3:Aj:283:GLN:NE2	2.51	0.42
3:An:35:LEU:HD12	3:An:35:LEU:C	2.44	0.42
4:Ap:39:TYR:O	4:Ap:43:LEU:HD13	2.20	0.42
4:At:316:THR:HG22	4:At:380:LEU:HD21	1.98	0.42
7:BJ:307:GLU:OE1	7:BJ:307:GLU:N	2.46	0.42
7:BM:177:THR:HG22	7:BM:177:THR:O	2.19	0.42
1:Ad:163:ILE:HD11	1:Ae:165:ASP:HA	2.01	0.42
2:Af:218:GLU:CG	2:Af:219:ASP:N	2.82	0.42
2:Ah:128:THR:HG22	2:Ah:200:GLU:OE2	2.20	0.42
3:Ai:34:THR:HG23	7:BH:355:GLN:CG	2.47	0.42
3:Al:127:GLU:N	3:Al:127:GLU:OE1	2.53	0.42
3:An:61:THR:OG1	3:An:62:ALA:N	2.52	0.42
3:An:180:ILE:HD11	4:Aq:198:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:An:198:VAL:O	3:An:198:VAL:HG13	2.19	0.42
4:Ax:93:VAL:HG11	4:Ax:109:PHE:CE2	2.54	0.42
6:A0:140:LEU:HD13	6:A0:150:MET:HE2	2.00	0.42
7:BC:54:LEU:O	7:BC:56:GLU:N	2.51	0.42
7:BG:367:VAL:HG12	7:BG:368:THR:O	2.19	0.42
7:BI:140:VAL:HG21	7:BI:153:ALA:HB2	2.01	0.42
8:BX:120:ILE:HD11	8:BZ:55:VAL:HG13	2.00	0.42
7:BM:136:ALA:O	7:BM:137:ALA:HB3	2.20	0.42
2:Af:123:THR:HG22	2:Af:124:ALA:N	2.35	0.42
2:Ag:110:VAL:HG12	2:Ag:120:VAL:HG22	2.02	0.42
3:An:123:VAL:HG23	3:An:123:VAL:O	2.18	0.42
4:Ay:149:VAL:HG22	4:Ay:150:THR:H	1.84	0.42
8:BP:15:THR:HG23	8:BP:25:ILE:O	2.20	0.42
7:BG:132:PRO:HD2	7:BG:135:ILE:HD12	2.02	0.42
2:Ag:155:LEU:C	2:Ag:155:LEU:HD23	2.45	0.42
4:Ax:93:VAL:HG11	4:Ax:109:PHE:HE2	1.83	0.42
4:Ay:239:GLU:OE1	4:Ay:286:ARG:NE	2.41	0.42
5:A1:66:THR:HG22	5:A1:67:ASN:N	2.34	0.42
5:A2:130:THR:O	5:A2:130:THR:HG22	2.20	0.42
5:A2:345:SER:CB	5:A2:346:PRO:CD	2.98	0.42
5:A3:345:SER:CB	5:A3:346:PRO:CD	2.98	0.42
5:A4:132:PHE:CD2	5:A4:132:PHE:O	2.73	0.42
5:A5:345:SER:CB	5:A5:346:PRO:CD	2.98	0.42
1:Ae:158:HIS:CD2	1:Ae:159:ASN:OD1	2.73	0.42
4:As:210:TRP:CD1	4:As:261:ILE:HD11	2.55	0.42
7:BG:111:VAL:HG13	7:BG:124:ILE:HG23	2.02	0.42
7:BG:460:ASP:OD2	7:BG:470:GLN:N	2.46	0.42
1:Ac:29:THR:HG22	1:Ac:30:ASP:H	1.85	0.42
1:Ad:43:MET:SD	2:Ah:174:LYS:HE2	2.60	0.42
4:Ao:129:THR:HG23	4:Ao:131:VAL:HG12	2.02	0.42
4:Aw:7:ARG:NH2	5:A5:318:CYS:SG	2.93	0.42
4:Aw:270:GLN:NE2	4:Aw:283:GLY:O	2.49	0.42
5:A5:93:ARG:NH2	5:A6:105:VAL:HG11	2.35	0.42
7:BC:220:VAL:HG21	7:BC:299:ALA:HA	2.02	0.42
7:BC:269:ASP:OD1	7:BC:271:SER:OG	2.27	0.42
7:BF:105:ALA:O	7:BF:130:ASP:N	2.42	0.42
7:BG:54:LEU:O	7:BG:56:GLU:N	2.48	0.42
7:BJ:260:THR:O	7:BJ:264:VAL:HG23	2.19	0.42
7:BL:466:LYS:O	7:BL:468:VAL:HG23	2.19	0.42
2:Af:110:VAL:HG23	2:Af:110:VAL:O	2.20	0.42
2:Af:143:PHE:CZ	2:Af:151:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ah:39:LEU:HD23	2:Ah:118:TYR:CZ	2.55	0.42
2:Ah:218:GLU:CG	2:Ah:219:ASP:N	2.83	0.42
4:Ap:210:TRP:CD1	4:Ap:261:ILE:HD11	2.55	0.42
4:Aq:210:TRP:HB3	4:Aq:213:VAL:HG21	2.02	0.42
4:As:121:VAL:O	4:As:121:VAL:HG23	2.19	0.42
4:At:67:ALA:O	4:At:185:ARG:NH2	2.52	0.42
5:A1:17:PHE:O	5:A1:20:VAL:HG22	2.20	0.42
7:BC:136:ALA:O	7:BC:137:ALA:HB3	2.19	0.42
8:BR:33:PRO:HB3	8:BR:69:VAL:HG22	2.02	0.42
7:BJ:491:VAL:HG22	7:BJ:492:ASN:N	2.35	0.42
3:Ak:77:THR:HG22	3:Ak:78:LEU:N	2.34	0.41
4:Ap:74:LYS:O	4:Ap:75:MET:CG	2.68	0.41
4:Ap:121:VAL:O	4:Ap:121:VAL:HG23	2.19	0.41
4:Ar:210:TRP:HB3	4:Ar:213:VAL:HG21	2.02	0.41
4:Av:121:VAL:O	4:Av:121:VAL:HG23	2.20	0.41
4:Ay:121:VAL:HG23	4:Ay:121:VAL:O	2.20	0.41
5:A3:60:ILE:HG22	5:A3:61:ARG:N	2.34	0.41
5:A4:345:SER:CB	5:A4:346:PRO:CD	2.98	0.41
6:A0:98:SER:OG	6:A0:99:LYS:N	2.53	0.41
7:BE:459:SER:OG	7:BE:462:ASP:OD2	2.33	0.41
7:BI:136:ALA:O	7:BI:137:ALA:HB3	2.19	0.41
7:BK:428:LEU:HD13	8:BX:13:LEU:CD1	2.50	0.41
1:Ad:42:THR:HG23	1:Ad:43:MET:N	2.35	0.41
2:Af:155:LEU:HD21	2:Af:177:LEU:HD13	2.01	0.41
2:Ag:7:ILE:HD12	2:Ag:59:VAL:HG22	2.01	0.41
2:Ag:310:VAL:HG12	2:Ag:311:THR:N	2.35	0.41
2:Ah:227:LEU:O	2:Ah:228:ASP:OD1	2.37	0.41
3:Ai:61:THR:HG22	3:Ai:64:GLY:O	2.20	0.41
4:Au:338:LEU:HD21	4:Au:343:SER:HA	2.03	0.41
4:Aw:68:CYS:SG	4:Aw:69:CYS:N	2.93	0.41
4:Aw:121:VAL:O	4:Aw:121:VAL:HG23	2.20	0.41
5:A3:68:ASP:OD2	5:A3:71:ALA:HB3	2.20	0.41
5:A4:17:PHE:O	5:A4:20:VAL:HG22	2.20	0.41
5:A5:112:ALA:CB	8:BO:56:MET:HE3	2.49	0.41
6:BB:98:SER:OG	6:BB:99:LYS:N	2.53	0.41
7:BN:183:THR:HG23	7:BN:184:SER:N	2.35	0.41
8:BR:61:ASN:ND2	8:BT:50:LEU:O	2.37	0.41
7:BF:128:GLU:O	7:BF:131:THR:HG23	2.20	0.41
7:BG:249:CYS:O	7:BG:250:PHE:C	2.63	0.41
7:BI:269:ASP:OD1	7:BI:271:SER:OG	2.32	0.41
8:BX:33:PRO:HB3	8:BX:69:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BL:373:ASP:OD1	7:BL:374:GLU:N	2.45	0.41
7:BM:140:VAL:HG13	7:BM:151:ALA:CB	2.50	0.41
1:Ac:140:VAL:HG21	1:Ae:144:THR:HG22	2.01	0.41
2:Ah:9:ILE:HG22	2:Ah:14:LEU:CD1	2.50	0.41
2:Ah:9:ILE:HG22	2:Ah:14:LEU:HD11	2.02	0.41
4:Aq:176:ASP:OD1	4:Aq:177:ASP:N	2.49	0.41
4:Aw:218:ASP:OD1	4:Aw:219:LEU:N	2.46	0.41
4:Az:121:VAL:O	4:Az:121:VAL:HG23	2.20	0.41
5:A6:15:ALA:O	5:A6:16:SER:OG	2.34	0.41
7:BN:297:LEU:O	7:BN:302:THR:HG22	2.20	0.41
7:BD:17:PRO:O	7:BD:18:SER:C	2.63	0.41
7:BD:28:ILE:HD12	7:BD:299:ALA:CB	2.51	0.41
7:BJ:23:GLY:O	7:BJ:80:SER:OG	2.29	0.41
8:BW:48:THR:O	8:BW:55:VAL:HA	2.21	0.41
7:BK:273:GLU:N	7:BK:273:GLU:OE1	2.53	0.41
8:BX:21:THR:HG23	8:BX:23:GLU:H	1.86	0.41
1:Ae:65:GLU:CD	2:Ah:259:ILE:HD11	2.46	0.41
2:Ah:128:THR:HG22	2:Ah:200:GLU:CD	2.45	0.41
4:At:195:GLU:OE2	4:Aw:191:ARG:NH2	2.54	0.41
5:A3:15:ALA:O	5:A3:16:SER:OG	2.35	0.41
5:A4:1:MET:HA	5:A5:65:GLN:O	2.21	0.41
6:A9:106:ARG:NH1	6:A9:115:LEU:HD22	2.35	0.41
8:BO:60:SER:OG	8:BO:61:ASN:N	2.53	0.41
7:BD:136:ALA:O	7:BD:137:ALA:HB3	2.21	0.41
7:BF:491:VAL:O	7:BF:492:ASN:C	2.63	0.41
7:BG:466:LYS:HD2	7:BG:467:CYS:N	2.35	0.41
7:BK:459:SER:OG	7:BK:462:ASP:OD2	2.36	0.41
1:Ac:183:THR:HG22	1:Ac:184:ASP:N	2.35	0.41
2:Af:351:VAL:HG12	2:Af:352:ASP:N	2.34	0.41
4:Ap:67:ALA:O	4:Ap:185:ARG:NH2	2.53	0.41
4:As:67:ALA:O	4:As:185:ARG:NH2	2.52	0.41
5:A5:345:SER:HB3	5:A5:346:PRO:CD	2.51	0.41
8:BP:25:ILE:HD12	8:BP:78:TRP:CZ3	2.56	0.41
7:BE:213:VAL:O	7:BE:213:VAL:HG12	2.20	0.41
4:Ax:338:LEU:HD21	4:Ax:343:SER:HA	2.02	0.41
6:A7:19:VAL:HG13	6:A7:60:LEU:HD11	2.01	0.41
8:BO:93:ASP:OD1	8:BO:94:GLY:N	2.54	0.41
7:BC:47:CYS:SG	7:BC:48:VAL:N	2.93	0.41
7:BH:213:VAL:HG12	7:BH:213:VAL:O	2.19	0.41
7:BI:367:VAL:HG23	7:BI:383:ARG:O	2.20	0.41
7:BJ:127:ASP:OD1	7:BJ:138:LYS:NZ	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BY:50:LEU:HD21	8:BY:56:MET:SD	2.60	0.41
1:Ad:135:VAL:O	1:Ad:135:VAL:CG1	2.68	0.41
2:Af:112:PHE:CE2	5:A2:41:VAL:HG11	2.52	0.41
2:Ag:354:LYS:NZ	5:A1:39:GLU:OE2	2.51	0.41
3:Ak:123:VAL:O	3:Ak:123:VAL:HG23	2.21	0.41
3:Al:110:VAL:HG22	3:Al:225:VAL:HB	2.03	0.41
4:As:186:THR:O	4:As:187:ARG:HB3	2.21	0.41
4:At:74:LYS:C	4:At:76:ALA:H	2.29	0.41
4:Az:151:GLU:N	4:Az:151:GLU:OE2	2.54	0.41
7:BN:128:GLU:O	7:BN:131:THR:HG23	2.21	0.41
7:BC:21:PHE:N	7:BC:21:PHE:CD1	2.87	0.41
1:Ac:114:ASP:OD2	1:Ae:129:ARG:NH1	2.54	0.41
2:Ah:4:PRO:HD2	5:A5:42:PHE:CE2	2.56	0.41
4:Ao:39:TYR:O	4:Ao:43:LEU:HD13	2.20	0.41
5:A6:345:SER:CB	5:A6:346:PRO:CD	2.98	0.41
6:BB:161:GLU:OE2	6:BB:170:ARG:NH1	2.53	0.41
7:BF:136:ALA:O	7:BF:137:ALA:HB3	2.20	0.41
7:BG:96:VAL:HG13	7:BG:161:THR:HG22	2.02	0.41
8:BW:106:GLU:O	8:BW:106:GLU:HG3	2.20	0.41
8:BX:109:GLU:OE2	8:BZ:63:THR:OG1	2.34	0.41
1:Ad:94:LYS:C	1:Ad:95:LYS:HG2	2.46	0.41
1:Ae:24:ARG:NE	1:Ae:38:GLU:OE2	2.53	0.41
2:Ah:143:PHE:CZ	2:Ah:151:VAL:HG22	2.56	0.41
2:Ah:342:MET:HE2	2:Ah:363:LEU:HB3	2.03	0.41
3:Ai:30:MET:HE3	3:Ai:30:MET:HB3	2.00	0.41
3:Ai:123:VAL:O	3:Ai:123:VAL:HG23	2.20	0.41
3:Am:77:THR:HG22	3:Am:78:LEU:H	1.86	0.41
4:Ap:74:LYS:C	4:Ap:76:ALA:H	2.29	0.41
4:Aq:195:GLU:OE2	4:Az:191:ARG:NH2	2.54	0.41
4:At:210:TRP:HB3	4:At:213:VAL:HG21	2.02	0.41
4:Au:7:ARG:NH2	5:A3:318:CYS:SG	2.94	0.41
4:Ax:17:ILE:HD12	4:Ax:17:ILE:H	1.86	0.41
4:Ay:107:LEU:HD11	4:Ay:154:LEU:CD1	2.50	0.41
4:Az:365:ASN:OD1	4:Az:369:ASP:N	2.54	0.41
5:A1:93:ARG:HH21	5:A2:105:VAL:HG11	1.81	0.41
5:A2:129:VAL:HG12	5:A2:130:THR:N	2.35	0.41
7:BC:213:VAL:HG12	7:BC:213:VAL:O	2.21	0.41
7:BC:227:ASP:OD1	7:BC:229:ASP:N	2.53	0.41
7:BF:373:ASP:OD1	7:BF:374:GLU:N	2.46	0.41
8:BS:50:LEU:HD21	8:BS:56:MET:SD	2.60	0.41
7:BG:112:GLN:NE2	7:BG:178:ASN:OD1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:453:GLU:N	7:BG:453:GLU:OE1	2.54	0.41
7:BI:21:PHE:N	7:BI:21:PHE:CD1	2.88	0.41
8:BV:34:ASP:OD1	8:BV:34:ASP:N	2.54	0.41
7:BJ:136:ALA:O	7:BJ:137:ALA:HB3	2.21	0.41
7:BK:12:ARG:HG3	7:BK:12:ARG:NH1	2.36	0.41
7:BK:140:VAL:HG11	7:BK:153:ALA:HB2	2.02	0.41
1:Ac:76:SER:O	2:Af:174:LYS:HD3	2.21	0.41
3:Al:123:VAL:HG23	3:Al:123:VAL:O	2.20	0.41
4:Ay:17:ILE:HD12	4:Ay:17:ILE:H	1.86	0.41
5:A2:163:VAL:HG22	5:A2:164:ARG:N	2.36	0.41
7:BD:22:PHE:CG	7:BD:22:PHE:O	2.74	0.41
7:BM:459:SER:OG	7:BM:462:ASP:OD2	2.37	0.41
1:Ad:95:LYS:O	1:Ad:96:THR:HG23	2.21	0.40
2:Af:155:LEU:HD22	2:Af:183:ILE:HD12	2.03	0.40
3:Ai:180:ILE:O	3:Ai:180:ILE:HG23	2.20	0.40
4:Ap:229:LEU:HD12	4:Ap:237:ASN:CG	2.46	0.40
4:Ar:33:PRO:O	4:Ar:34:GLU:HB2	2.21	0.40
5:A6:130:THR:O	5:A6:130:THR:HG22	2.20	0.40
7:BD:112:GLN:HG3	7:BD:177:THR:HG21	2.03	0.40
8:BT:15:THR:HG23	8:BT:25:ILE:O	2.21	0.40
7:BK:63:VAL:HG21	7:BK:168:ILE:HG21	2.03	0.40
8:BX:48:THR:HG22	8:BX:49:ALA:N	2.36	0.40
2:Af:110:VAL:HG21	2:Ag:336:GLU:OE1	2.20	0.40
2:Ag:110:VAL:HG11	2:Ah:336:GLU:CG	2.52	0.40
4:Ap:186:THR:O	4:Ap:187:ARG:HB3	2.21	0.40
4:At:198:LEU:O	4:At:198:LEU:HG	2.21	0.40
4:Ax:217:PHE:HE2	4:Ax:243:LEU:HD12	1.86	0.40
4:Az:7:ARG:NH2	5:A2:318:CYS:SG	2.94	0.40
5:A1:345:SER:CB	5:A1:346:PRO:CD	2.98	0.40
7:BD:11:VAL:HG12	7:BD:12:ARG:N	2.37	0.40
1:Ae:81:VAL:O	1:Ae:81:VAL:HG13	2.21	0.40
2:Ag:112:PHE:CE2	5:A6:41:VAL:HG11	2.54	0.40
2:Ah:114:LYS:HA	5:A4:41:VAL:HG12	2.04	0.40
4:At:59:TRP:NE1	4:Aw:58:MET:HE2	2.37	0.40
5:A3:120:ILE:HG21	5:A3:122:PHE:CZ	2.57	0.40
5:A4:66:THR:HG22	5:A4:67:ASN:N	2.37	0.40
5:A5:291:SER:OG	5:A5:295:GLU:OE1	2.36	0.40
6:BB:153:MET:HE3	6:BB:153:MET:HB3	2.00	0.40
7:BN:53:ASP:OD1	7:BN:53:ASP:O	2.39	0.40
7:BJ:75:CYS:HB3	7:BJ:79:VAL:HG12	2.03	0.40
7:BL:74:MET:HE3	7:BL:293:ALA:HB1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BM:96:VAL:HG13	7:BM:161:THR:HG22	2.02	0.40
3:Al:35:LEU:C	3:Al:35:LEU:HD12	2.46	0.40
4:Aw:302:CYS:SG	4:Aw:390:VAL:HG11	2.61	0.40
5:A6:1:MET:HG3	5:A6:2:ALA:O	2.22	0.40
6:A0:48:THR:HG22	6:A0:49:ILE:N	2.36	0.40
7:BI:111:VAL:HG23	7:BI:176:TYR:CE1	2.57	0.40
7:BK:269:ASP:O	7:BK:270:ASN:C	2.65	0.40
7:BL:183:THR:O	7:BL:186:THR:N	2.40	0.40
4:As:74:LYS:C	4:As:76:ALA:H	2.29	0.40
4:Aw:17:ILE:HD12	4:Aw:17:ILE:H	1.87	0.40
4:Ay:226:VAL:HG23	4:Ay:231:GLU:O	2.21	0.40
5:A3:1:MET:O	8:BQ:54:ALA:HB1	2.21	0.40
5:A6:120:ILE:HG21	5:A6:122:PHE:CZ	2.56	0.40
7:BD:178:ASN:O	7:BD:179:LEU:HB3	2.22	0.40
7:BD:235:ARG:NH1	7:BD:269:ASP:OD2	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	Ac	170/189 (90%)	157 (92%)	13 (8%)	0	100	100
1	Ad	170/189 (90%)	157 (92%)	13 (8%)	0	100	100
1	Ae	170/189 (90%)	159 (94%)	11 (6%)	0	100	100
2	Af	319/454 (70%)	299 (94%)	20 (6%)	0	100	100
2	Ag	319/454 (70%)	300 (94%)	19 (6%)	0	100	100
2	Ah	319/454 (70%)	295 (92%)	24 (8%)	0	100	100
3	Ai	284/286 (99%)	271 (95%)	13 (5%)	0	100	100
3	Aj	284/286 (99%)	274 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ak	284/286 (99%)	270 (95%)	14 (5%)	0	100	100
3	Al	284/286 (99%)	272 (96%)	12 (4%)	0	100	100
3	Am	284/286 (99%)	273 (96%)	11 (4%)	0	100	100
3	An	284/286 (99%)	270 (95%)	14 (5%)	0	100	100
4	Ao	388/396 (98%)	374 (96%)	14 (4%)	0	100	100
4	Ap	388/396 (98%)	378 (97%)	10 (3%)	0	100	100
4	Aq	388/396 (98%)	376 (97%)	12 (3%)	0	100	100
4	Ar	388/396 (98%)	373 (96%)	15 (4%)	0	100	100
4	As	388/396 (98%)	377 (97%)	11 (3%)	0	100	100
4	At	388/396 (98%)	378 (97%)	10 (3%)	0	100	100
4	Au	389/396 (98%)	384 (99%)	5 (1%)	0	100	100
4	Av	389/396 (98%)	385 (99%)	4 (1%)	0	100	100
4	Aw	389/396 (98%)	384 (99%)	5 (1%)	0	100	100
4	Ax	389/396 (98%)	386 (99%)	3 (1%)	0	100	100
4	Ay	389/396 (98%)	386 (99%)	3 (1%)	0	100	100
4	Az	389/396 (98%)	382 (98%)	7 (2%)	0	100	100
5	A1	396/398 (100%)	387 (98%)	9 (2%)	0	100	100
5	A2	396/398 (100%)	385 (97%)	11 (3%)	0	100	100
5	A3	396/398 (100%)	385 (97%)	11 (3%)	0	100	100
5	A4	396/398 (100%)	386 (98%)	10 (2%)	0	100	100
5	A5	396/398 (100%)	384 (97%)	12 (3%)	0	100	100
5	A6	396/398 (100%)	385 (97%)	11 (3%)	0	100	100
6	A0	173/178 (97%)	166 (96%)	7 (4%)	0	100	100
6	A7	173/178 (97%)	168 (97%)	5 (3%)	0	100	100
6	A8	173/178 (97%)	165 (95%)	8 (5%)	0	100	100
6	A9	173/178 (97%)	166 (96%)	7 (4%)	0	100	100
6	BA	173/178 (97%)	166 (96%)	7 (4%)	0	100	100
6	BB	173/178 (97%)	165 (95%)	8 (5%)	0	100	100
7	BC	498/503 (99%)	481 (97%)	17 (3%)	0	100	100
7	BD	494/503 (98%)	460 (93%)	34 (7%)	0	100	100
7	BE	498/503 (99%)	477 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BF	494/503 (98%)	459 (93%)	35 (7%)	0	100	100
7	BG	498/503 (99%)	480 (96%)	18 (4%)	0	100	100
7	BH	494/503 (98%)	459 (93%)	35 (7%)	0	100	100
7	BI	498/503 (99%)	480 (96%)	18 (4%)	0	100	100
7	BJ	494/503 (98%)	464 (94%)	30 (6%)	0	100	100
7	BK	498/503 (99%)	479 (96%)	19 (4%)	0	100	100
7	BL	494/503 (98%)	464 (94%)	30 (6%)	0	100	100
7	BM	498/503 (99%)	469 (94%)	28 (6%)	1 (0%)	44	74
7	BN	494/503 (98%)	469 (95%)	24 (5%)	1 (0%)	44	74
8	BO	131/136 (96%)	123 (94%)	8 (6%)	0	100	100
8	BP	131/136 (96%)	122 (93%)	9 (7%)	0	100	100
8	BQ	131/136 (96%)	124 (95%)	7 (5%)	0	100	100
8	BR	131/136 (96%)	126 (96%)	5 (4%)	0	100	100
8	BS	131/136 (96%)	121 (92%)	10 (8%)	0	100	100
8	BT	131/136 (96%)	124 (95%)	7 (5%)	0	100	100
8	BU	131/136 (96%)	123 (94%)	8 (6%)	0	100	100
8	BV	131/136 (96%)	121 (92%)	10 (8%)	0	100	100
8	BW	131/136 (96%)	124 (95%)	7 (5%)	0	100	100
8	BX	131/136 (96%)	124 (95%)	7 (5%)	0	100	100
8	BY	131/136 (96%)	123 (94%)	8 (6%)	0	100	100
8	BZ	131/136 (96%)	125 (95%)	6 (5%)	0	100	100
All	All	18771/19521 (96%)	17989 (96%)	780 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	BM	499	ASP
7	BN	413	LYS

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	Ac	148/164 (90%)	148 (100%)	0	100	100
1	Ad	148/164 (90%)	148 (100%)	0	100	100
1	Ae	148/164 (90%)	148 (100%)	0	100	100
2	Af	280/383 (73%)	280 (100%)	0	100	100
2	Ag	280/383 (73%)	280 (100%)	0	100	100
2	Ah	280/383 (73%)	280 (100%)	0	100	100
3	Ai	248/248 (100%)	248 (100%)	0	100	100
3	Aj	248/248 (100%)	248 (100%)	0	100	100
3	Ak	248/248 (100%)	248 (100%)	0	100	100
3	Al	248/248 (100%)	248 (100%)	0	100	100
3	Am	248/248 (100%)	248 (100%)	0	100	100
3	An	248/248 (100%)	248 (100%)	0	100	100
4	Ao	326/330 (99%)	326 (100%)	0	100	100
4	Ap	326/330 (99%)	326 (100%)	0	100	100
4	Aq	326/330 (99%)	326 (100%)	0	100	100
4	Ar	326/330 (99%)	326 (100%)	0	100	100
4	As	326/330 (99%)	326 (100%)	0	100	100
4	At	326/330 (99%)	326 (100%)	0	100	100
4	Au	326/330 (99%)	326 (100%)	0	100	100
4	Av	326/330 (99%)	326 (100%)	0	100	100
4	Aw	326/330 (99%)	326 (100%)	0	100	100
4	Ax	326/330 (99%)	326 (100%)	0	100	100
4	Ay	326/330 (99%)	326 (100%)	0	100	100
4	Az	326/330 (99%)	326 (100%)	0	100	100
5	A1	325/325 (100%)	325 (100%)	0	100	100
5	A2	325/325 (100%)	325 (100%)	0	100	100
5	A3	325/325 (100%)	325 (100%)	0	100	100
5	A4	325/325 (100%)	325 (100%)	0	100	100
5	A5	325/325 (100%)	325 (100%)	0	100	100
5	A6	325/325 (100%)	325 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A0	138/141 (98%)	138 (100%)	0	100	100
6	A7	138/141 (98%)	138 (100%)	0	100	100
6	A8	138/141 (98%)	138 (100%)	0	100	100
6	A9	138/141 (98%)	138 (100%)	0	100	100
6	BA	138/141 (98%)	138 (100%)	0	100	100
6	BB	138/141 (98%)	138 (100%)	0	100	100
7	BC	412/415 (99%)	412 (100%)	0	100	100
7	BD	409/415 (99%)	409 (100%)	0	100	100
7	BE	412/415 (99%)	412 (100%)	0	100	100
7	BF	409/415 (99%)	409 (100%)	0	100	100
7	BG	412/415 (99%)	412 (100%)	0	100	100
7	BH	409/415 (99%)	409 (100%)	0	100	100
7	BI	412/415 (99%)	412 (100%)	0	100	100
7	BJ	409/415 (99%)	409 (100%)	0	100	100
7	BK	412/415 (99%)	412 (100%)	0	100	100
7	BL	409/415 (99%)	409 (100%)	0	100	100
7	BM	412/415 (99%)	412 (100%)	0	100	100
7	BN	409/415 (99%)	409 (100%)	0	100	100
8	BO	110/111 (99%)	110 (100%)	0	100	100
8	BP	110/111 (99%)	110 (100%)	0	100	100
8	BQ	110/111 (99%)	110 (100%)	0	100	100
8	BR	110/111 (99%)	110 (100%)	0	100	100
8	BS	110/111 (99%)	110 (100%)	0	100	100
8	BT	110/111 (99%)	110 (100%)	0	100	100
8	BU	110/111 (99%)	110 (100%)	0	100	100
8	BV	110/111 (99%)	110 (100%)	0	100	100
8	BW	110/111 (99%)	110 (100%)	0	100	100
8	BX	110/111 (99%)	110 (100%)	0	100	100
8	BY	110/111 (99%)	110 (100%)	0	100	100
8	BZ	110/111 (99%)	110 (100%)	0	100	100
All	All	15708/16197 (97%)	15708 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ac	51	ASN
1	Ac	167	HIS
1	Ad	167	HIS
1	Ae	21	HIS
2	Af	329	HIS
2	Ag	329	HIS
3	Ai	162	GLN
3	Aj	204	ASN
3	Ak	283	GLN
3	Am	204	ASN
3	An	283	GLN
4	Ao	71	ASN
4	Ao	110	GLN
4	Ao	313	GLN
4	Ao	359	GLN
4	Aq	359	GLN
4	Ar	110	GLN
4	Ar	359	GLN
4	As	110	GLN
4	At	57	GLN
4	At	359	GLN
4	Au	106	ASN
4	Au	222	ASN
4	Au	270	GLN
4	Au	320	ASN
4	Av	320	ASN
4	Av	322	HIS
4	Aw	222	ASN
4	Ax	222	ASN
4	Ax	270	GLN
4	Ay	322	HIS
4	Az	222	ASN
4	Az	270	GLN
5	A1	11	HIS
5	A1	31	HIS
5	A2	31	HIS
5	A3	302	GLN
5	A3	319	HIS
5	A4	31	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A4	65	GLN
5	A5	31	HIS
5	A6	302	GLN
5	A6	319	HIS
7	BN	33	GLN
7	BN	257	ASN
8	BO	11	ASN
7	BC	369	ASN
7	BC	450	ASN
7	BD	257	ASN
7	BE	164	ASN
7	BE	291	ASN
7	BE	369	ASN
8	BR	18	HIS
7	BF	60	GLN
7	BF	178	ASN
7	BF	309	ASN
7	BF	369	ASN
7	BF	450	ASN
7	BF	477	ASN
8	BS	18	HIS
7	BG	450	ASN
7	BG	492	ASN
8	BT	6	GLN
8	BT	84	GLN
8	BT	88	GLN
7	BH	257	ASN
7	BI	134	GLN
7	BI	291	ASN
7	BI	369	ASN
7	BJ	164	ASN
7	BJ	257	ASN
7	BJ	452	ASN
7	BJ	492	ASN
7	BJ	500	ASN
7	BK	3	GLN
7	BK	291	ASN
7	BK	369	ASN
7	BK	450	ASN
7	BL	369	ASN
7	BL	477	ASN
7	BM	112	GLN

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Mol	Chain	Res	Type
7	BM	291	ASN
7	BM	340	GLN
7	BM	369	ASN
7	BM	450	ASN
7	BM	492	ASN
8	BZ	84	GLN

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

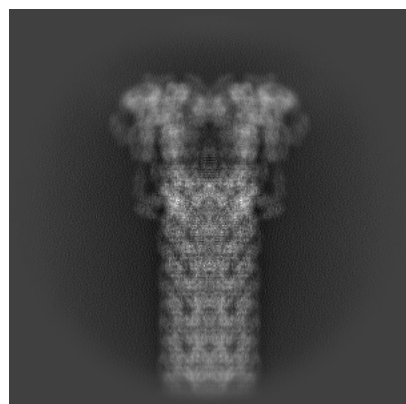
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54021. These allow visual inspection of the internal detail of the map and identification of artifacts.

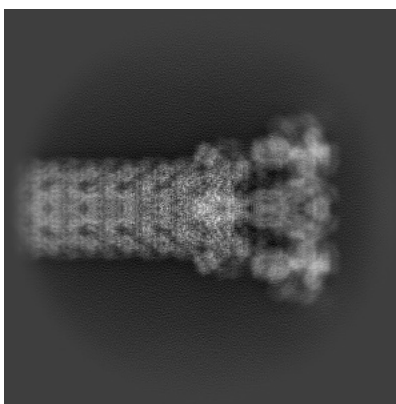
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

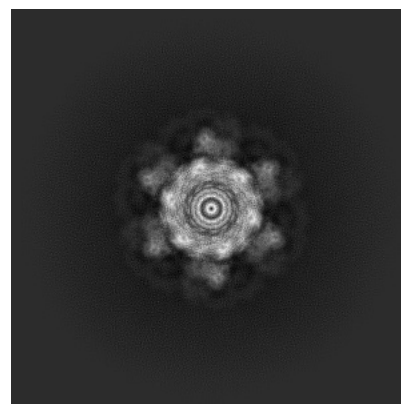
6.1.1 Primary map



X

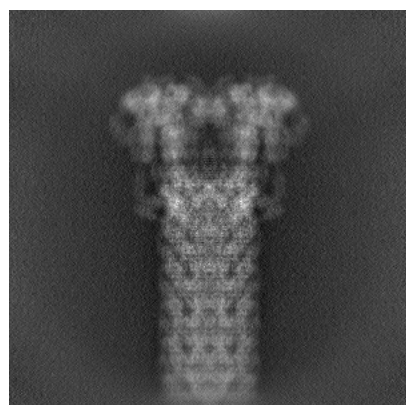


Y

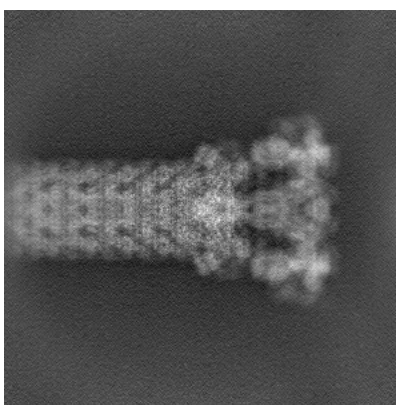


Z

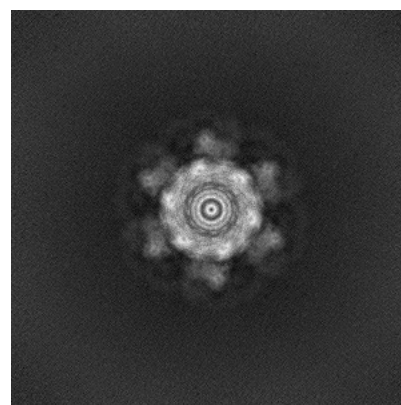
6.1.2 Raw map



X



Y

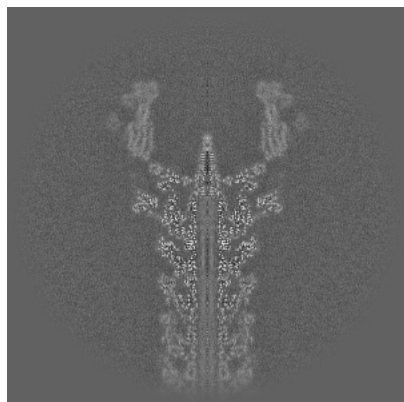


Z

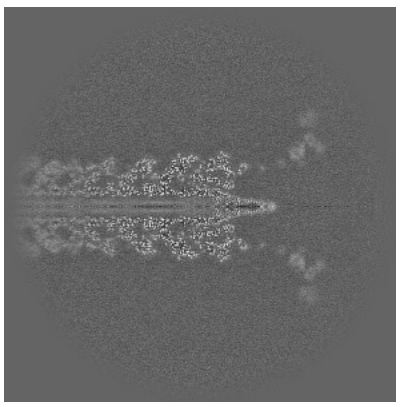
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

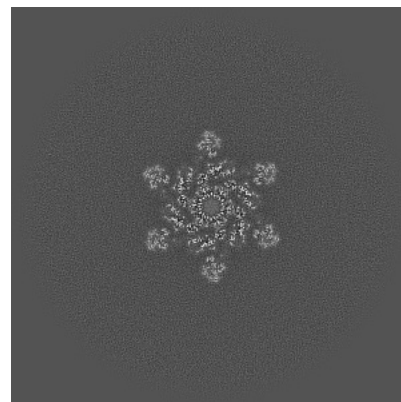
6.2.1 Primary map



X Index: 280

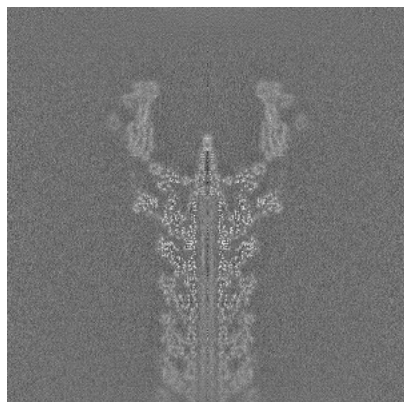


Y Index: 280

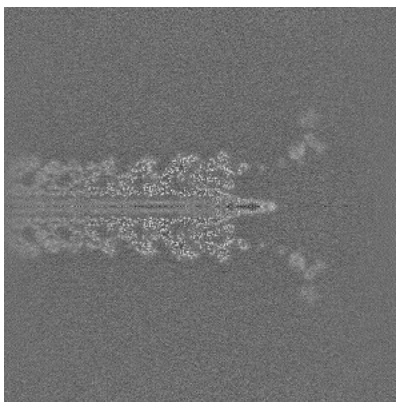


Z Index: 280

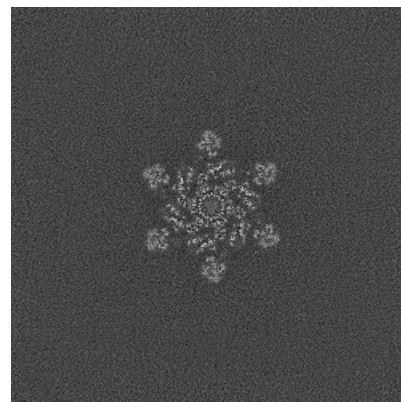
6.2.2 Raw map



X Index: 280



Y Index: 280

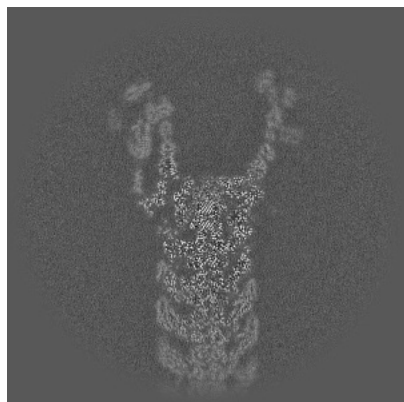


Z Index: 280

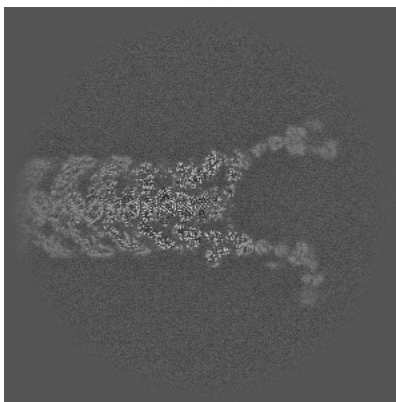
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

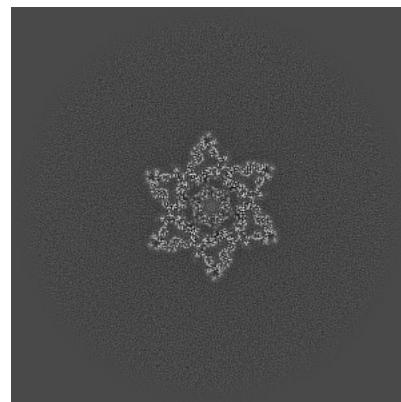
6.3.1 Primary map



X Index: 296

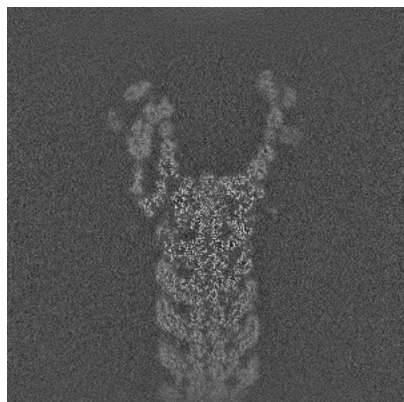


Y Index: 298

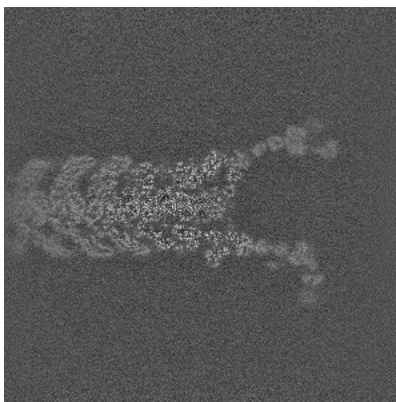


Z Index: 288

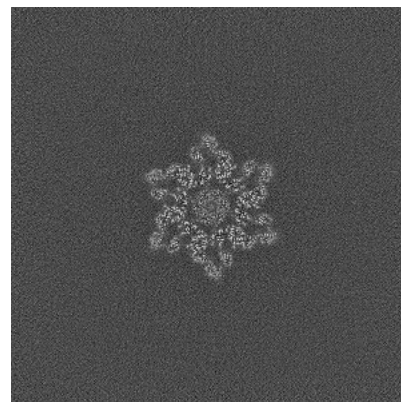
6.3.2 Raw map



X Index: 295



Y Index: 298

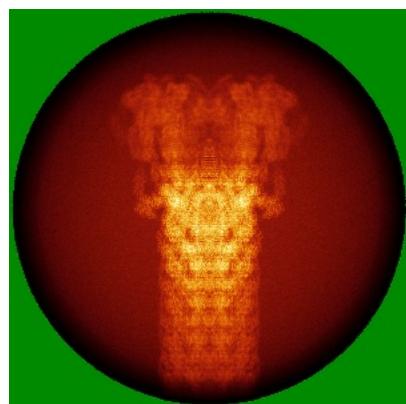


Z Index: 293

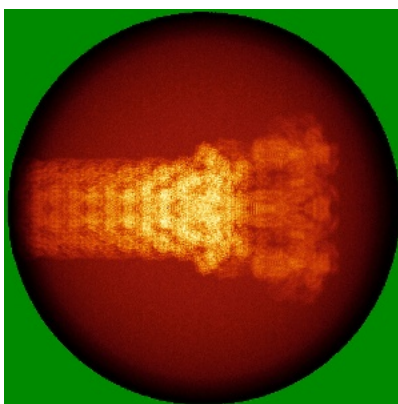
The images above show the largest variance slices of the map in three orthogonal directions.

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

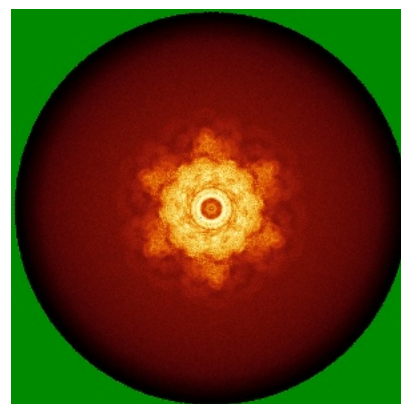
6.4.1 Primary map



X

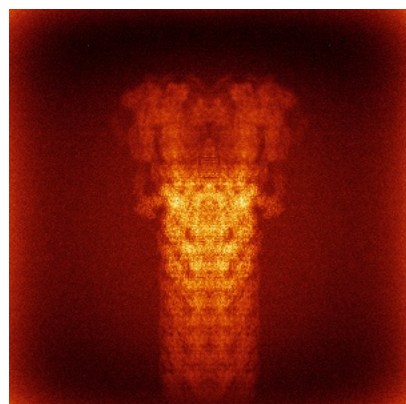


Y

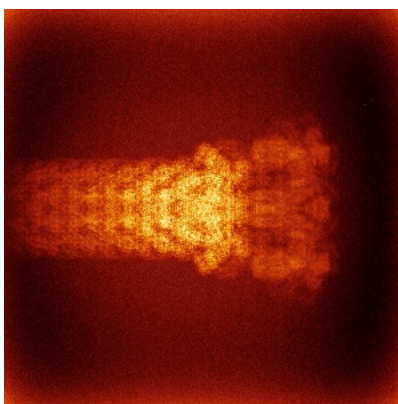


Z

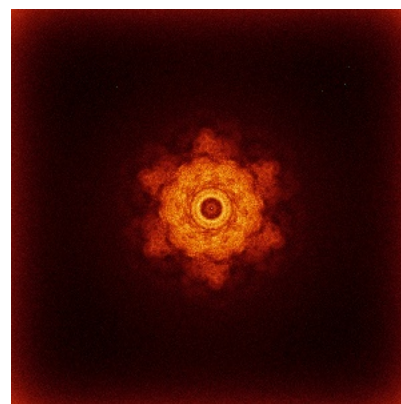
6.4.2 Raw map



X



Y

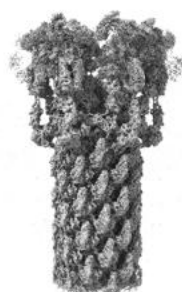


Z

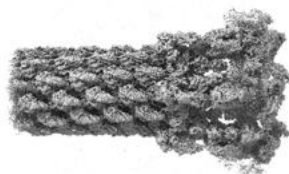
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

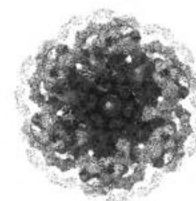
6.5.1 Primary map



X



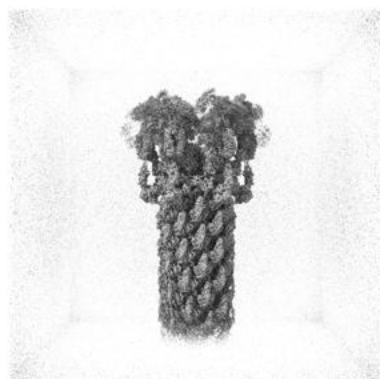
Y



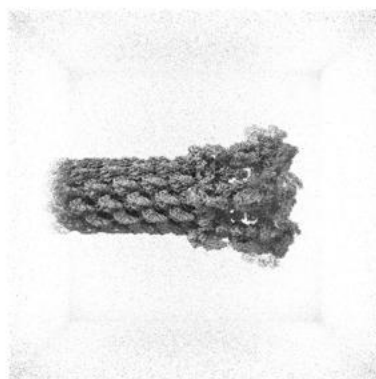
Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

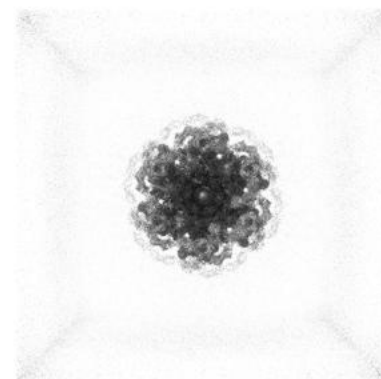
6.5.2 Raw map



X



Y



Z

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

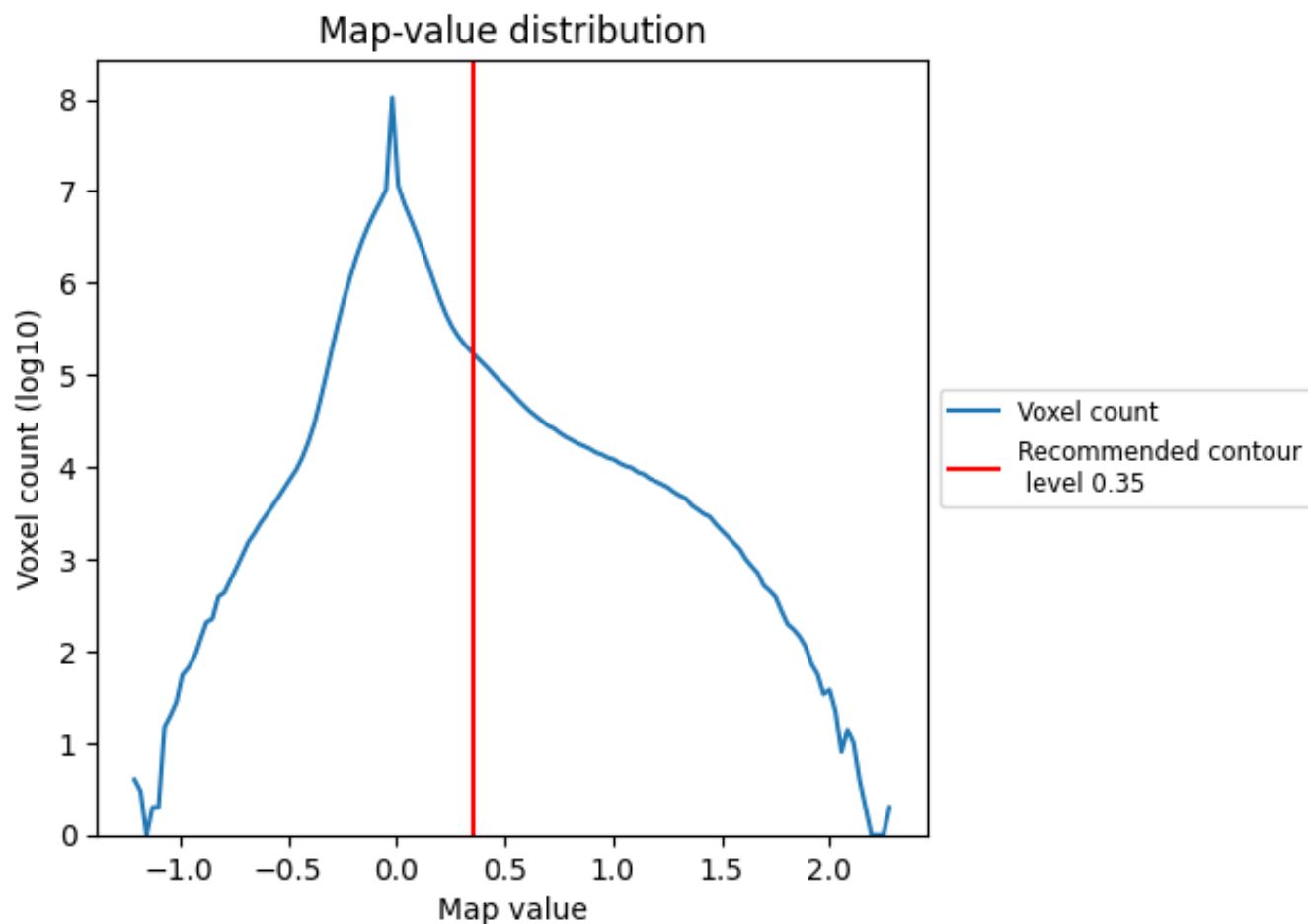
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

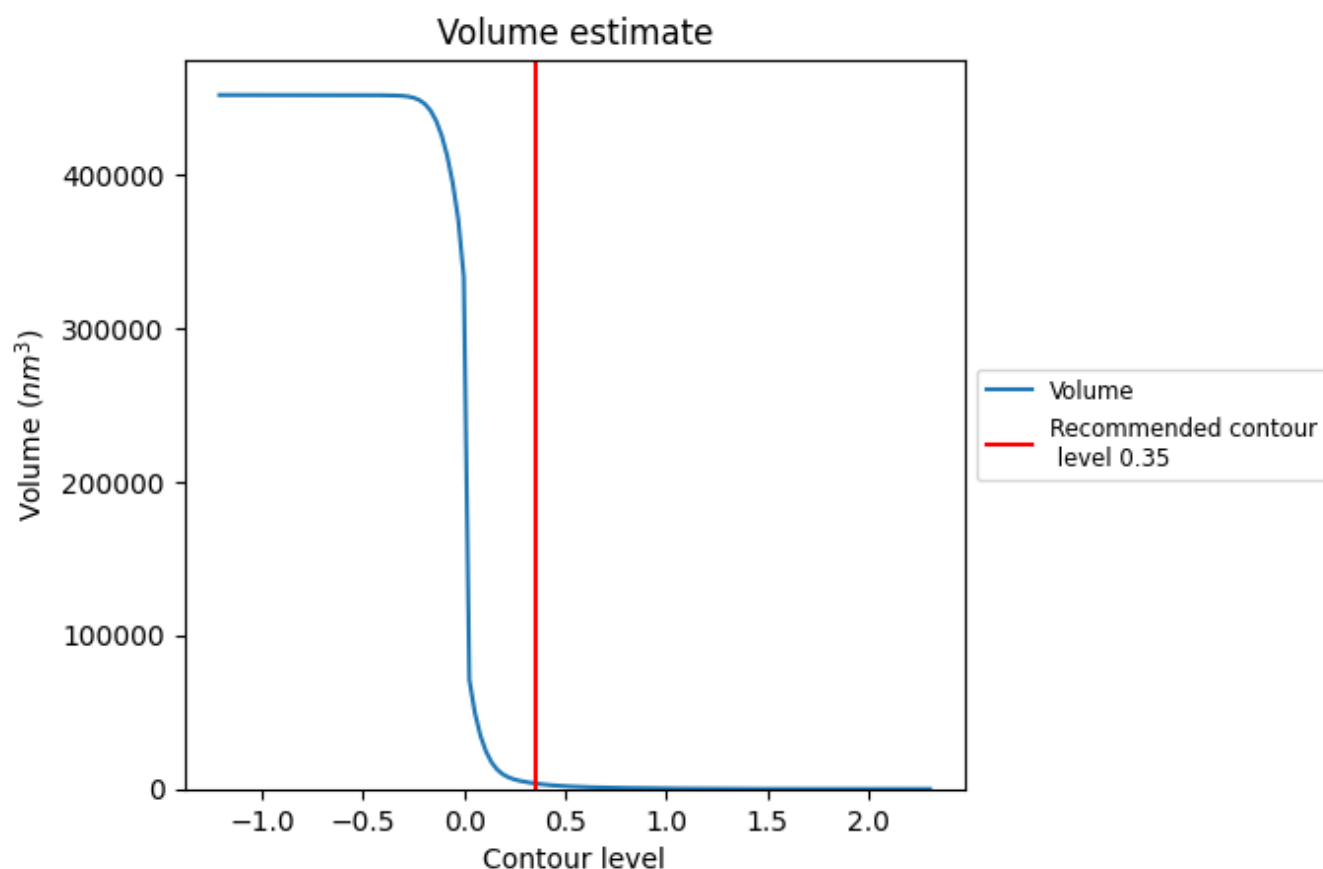
This section contains the results of statistical analysis of the map.

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.

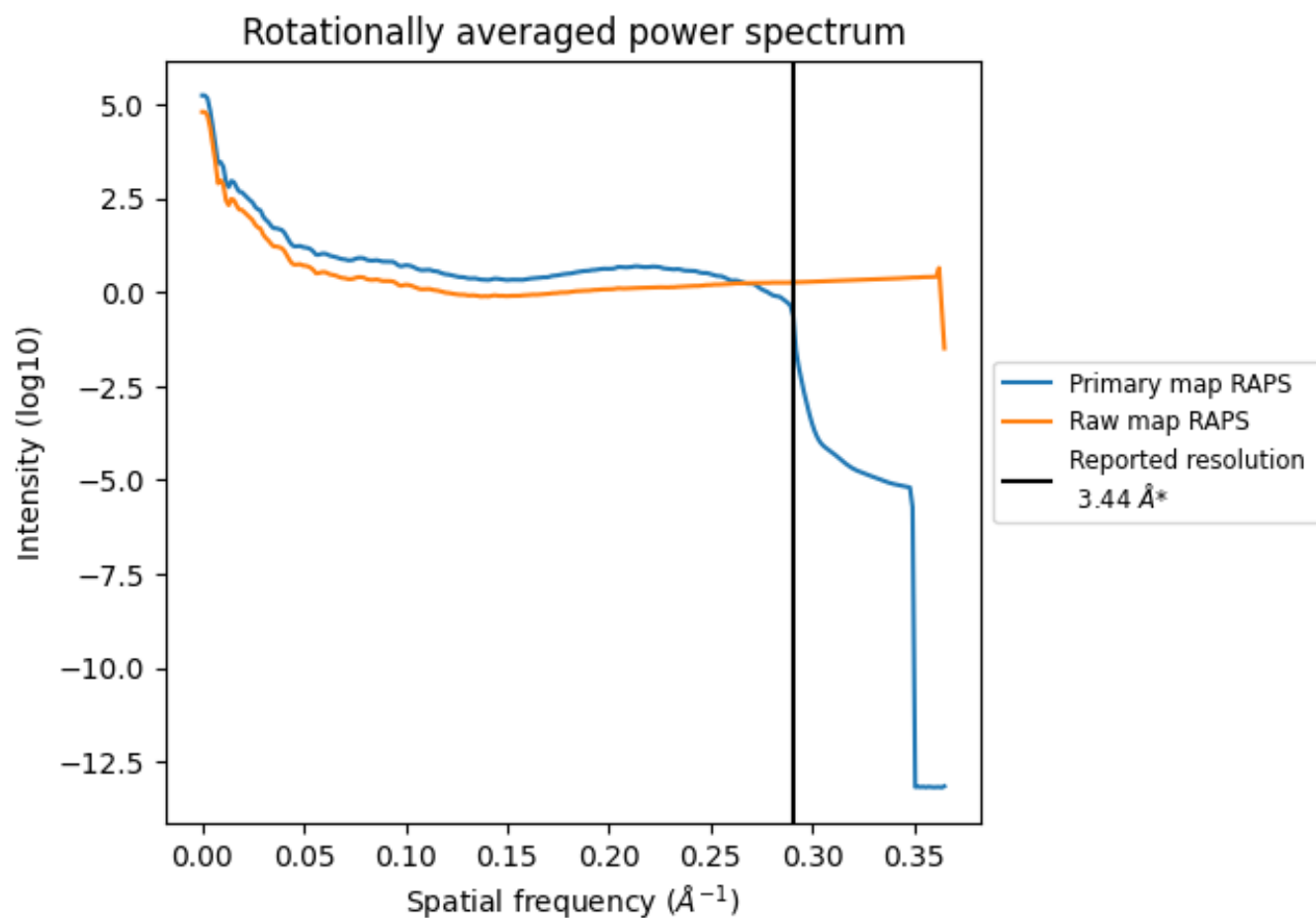
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3616 nm³; this corresponds to an approximate mass of 3266 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 ⓘ

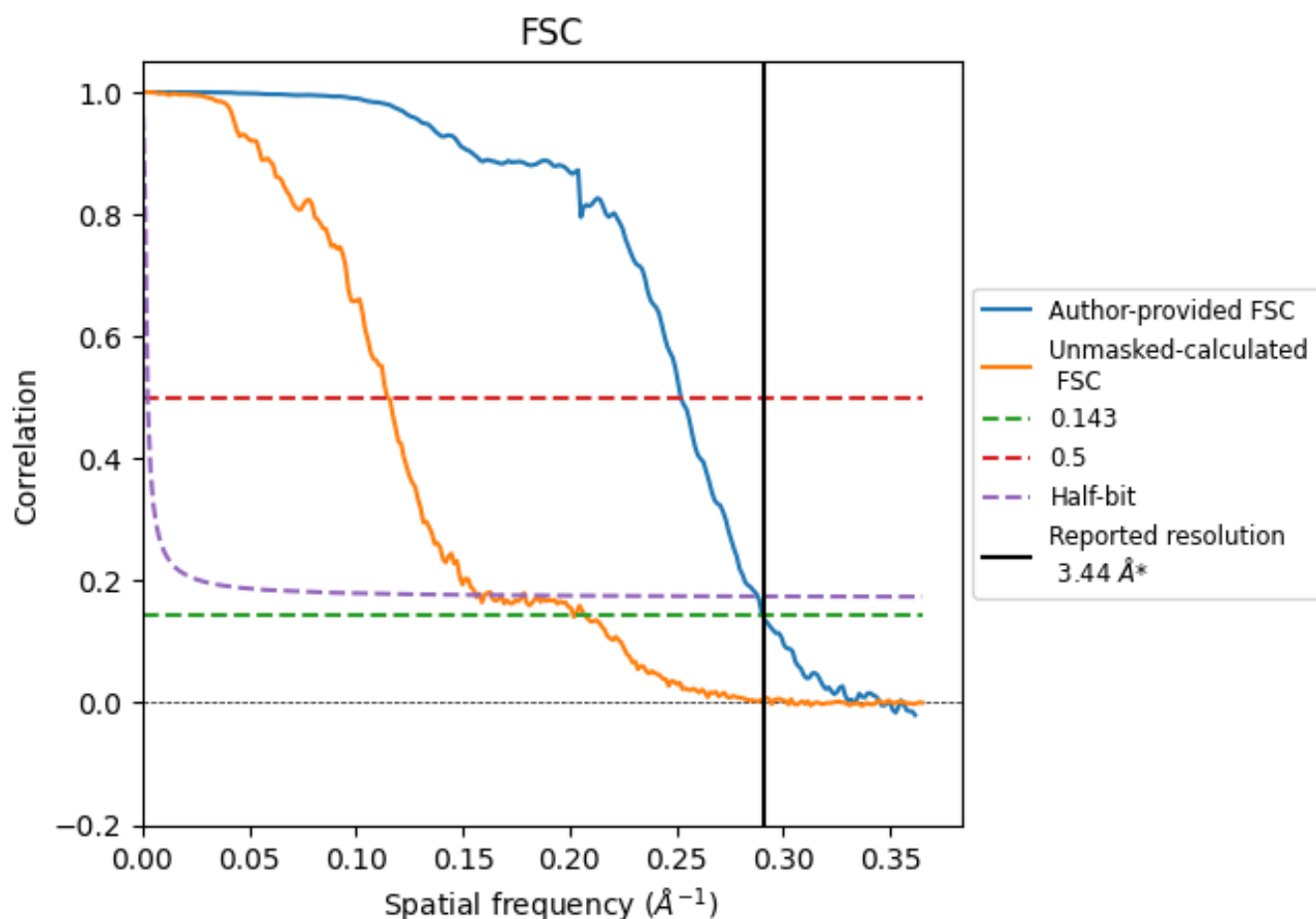


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.291 \AA^{-1}

8.2 Resolution estimates [i](#)

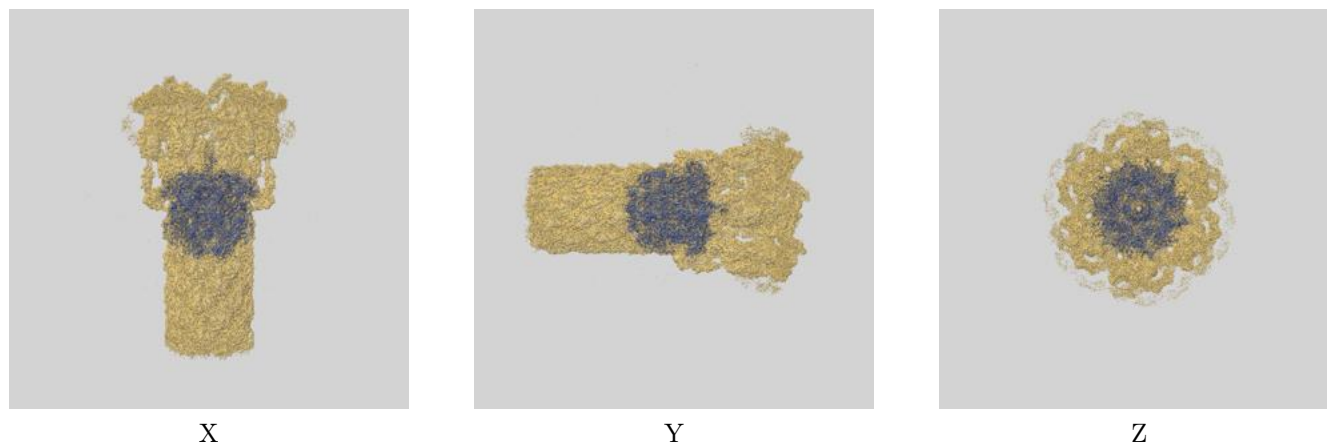
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	3.97	3.47
Unmasked-calculated*	4.96	8.71	6.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.96 differs from the reported value 3.44 by more than 10 %

9 Map-model fit [i](#)

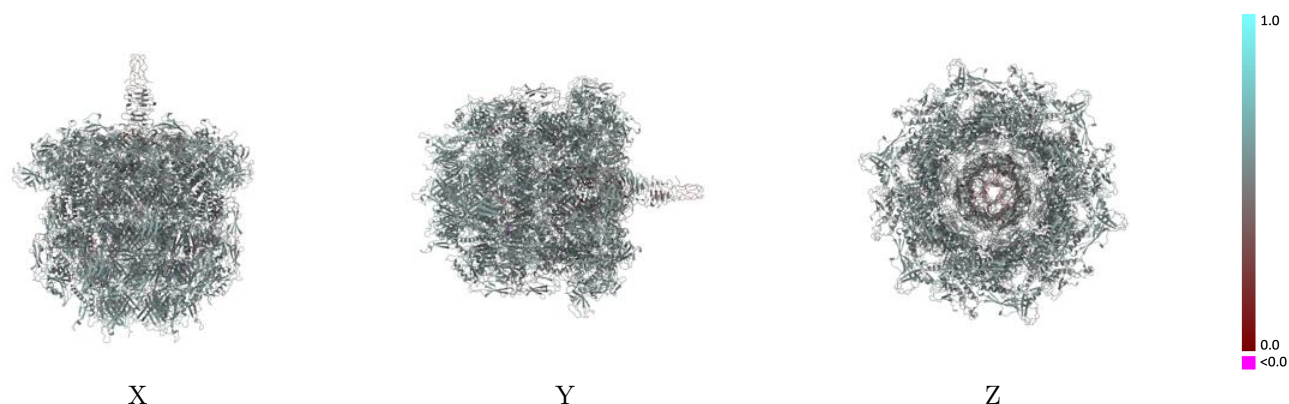
This section contains information regarding the fit between EMDB map EMD-54021 and PDB model 9RKU. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



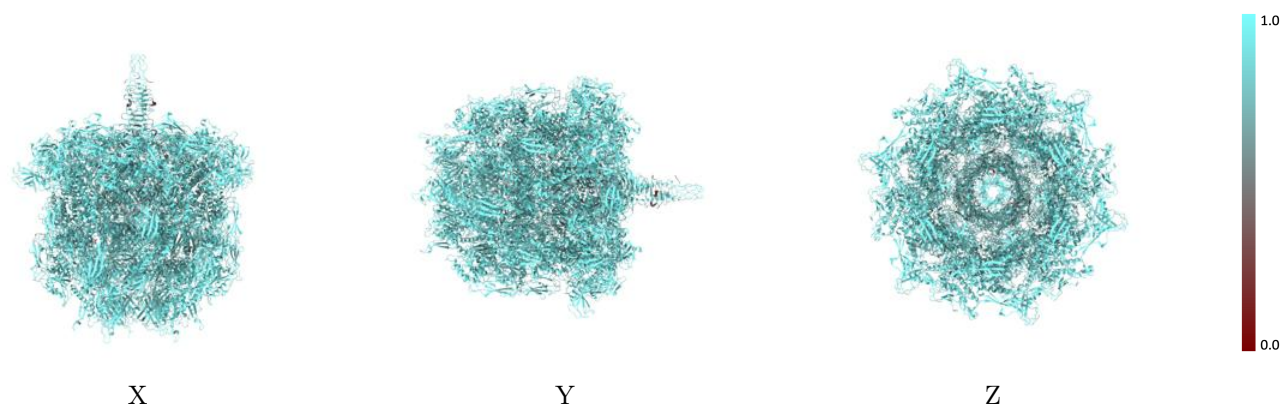
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



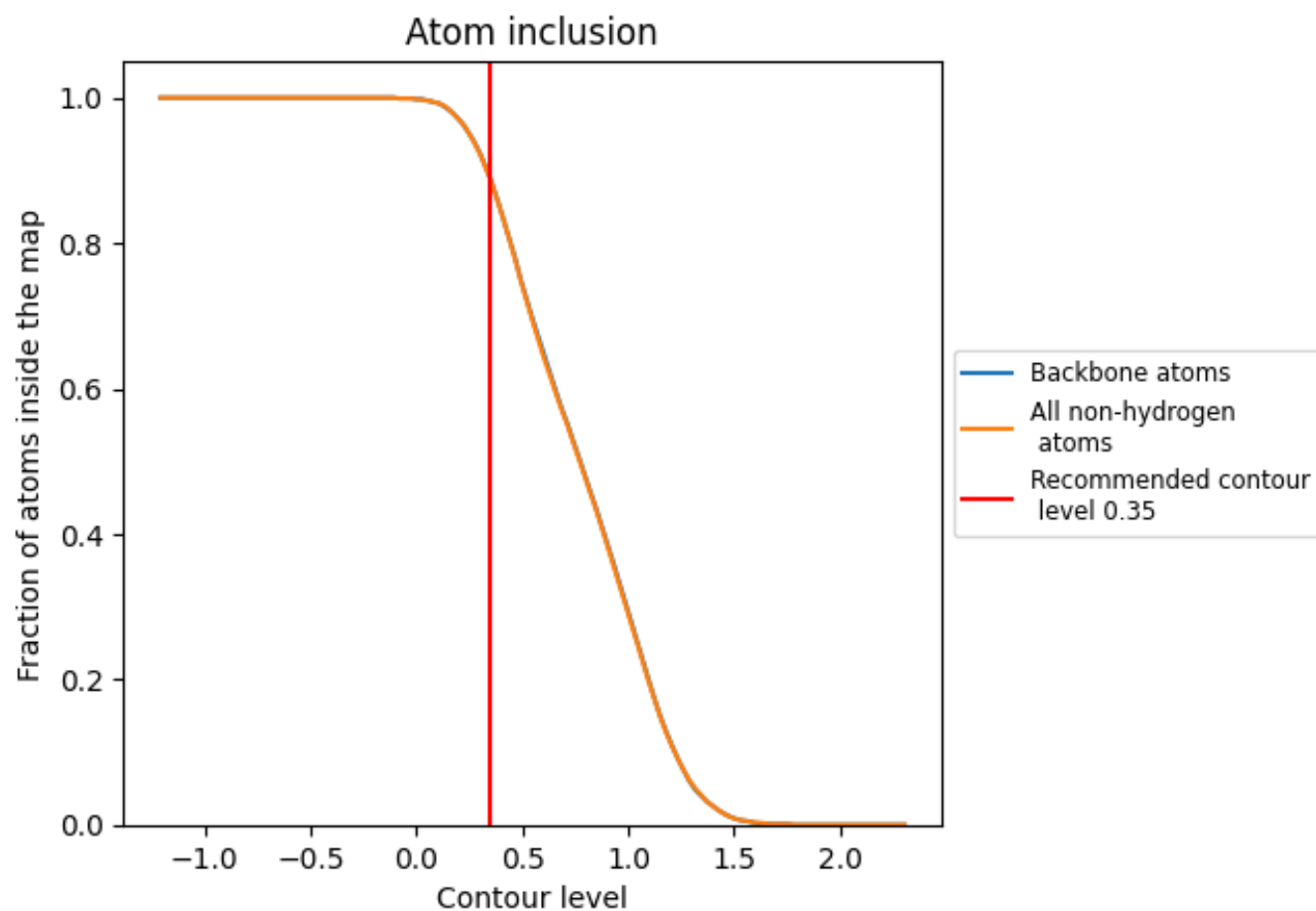
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.5210
A0	 0.8910	 0.5300
A1	 0.9010	 0.5340
A2	 0.8940	 0.5350
A3	 0.8980	 0.5340
A4	 0.9030	 0.5350
A5	 0.8940	 0.5330
A6	 0.8960	 0.5330
A7	 0.8890	 0.5290
A8	 0.8900	 0.5290
A9	 0.8850	 0.5290
Ac	 0.7980	 0.4390
Ad	 0.7960	 0.4350
Ae	 0.7970	 0.4280
Af	 0.7900	 0.4720
Ag	 0.7900	 0.4730
Ah	 0.7930	 0.4720
Ai	 0.9050	 0.5220
Aj	 0.9170	 0.5250
Ak	 0.9120	 0.5230
Al	 0.9130	 0.5280
Am	 0.9120	 0.5240
An	 0.9130	 0.5260
Ao	 0.9080	 0.5300
Ap	 0.9040	 0.5280
Aq	 0.9070	 0.5270
Ar	 0.9080	 0.5300
As	 0.9060	 0.5300
At	 0.9070	 0.5290
Au	 0.8880	 0.5200
Av	 0.8900	 0.5220
Aw	 0.8860	 0.5200
Ax	 0.8910	 0.5190
Ay	 0.8900	 0.5200
Az	 0.8880	 0.5210



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Chain	Atom inclusion	Q-score
BA	 0.8910	 0.5290
BB	 0.8840	 0.5270
BC	 0.8900	 0.5200
BD	 0.8950	 0.5200
BE	 0.8930	 0.5170
BF	 0.8990	 0.5200
BG	 0.8900	 0.5200
BH	 0.8970	 0.5200
BI	 0.8920	 0.5180
BJ	 0.8980	 0.5230
BK	 0.8900	 0.5180
BL	 0.8980	 0.5240
BM	 0.8840	 0.5170
BN	 0.9020	 0.5220
BO	 0.8950	 0.5530
BP	 0.8870	 0.5440
BQ	 0.8950	 0.5480
BR	 0.8870	 0.5480
BS	 0.9010	 0.5490
BT	 0.8960	 0.5470
BU	 0.9000	 0.5530
BV	 0.8930	 0.5490
BW	 0.8970	 0.5480
BX	 0.8880	 0.5480
BY	 0.9010	 0.5510
BZ	 0.8930	 0.5460