



Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 06:55 pm GMT

PDB ID : 8PHS
EMDB ID : EMD-17673
Title : Bottom cap of the Borrelia bacteriophage BB1 procapsid, fivefold-symmetrized outer shell
Authors : Rumnieks, J.; Fuzik, T.; Tars, K.
Deposited on : 2023-06-20
Resolution : 2.82 Å(reported)
Based on initial model : .

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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 Å.

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





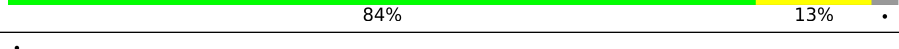
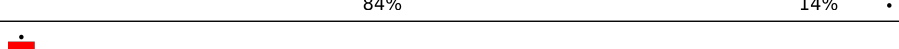
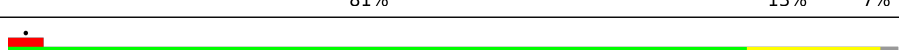

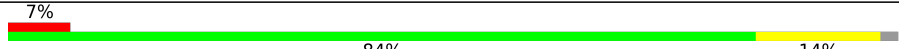



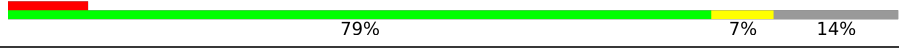

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	AB	319	
1	AC	319	
1	AJ	319	
1	AK	319	
1	AL	319	
1	AS	319	
1	AT	319	
1	AU	319	

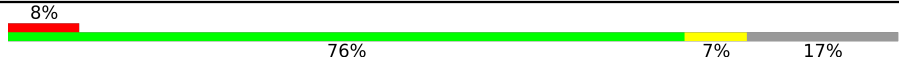

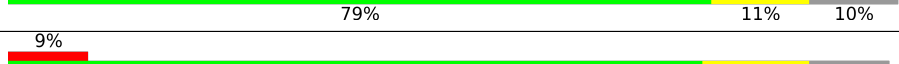
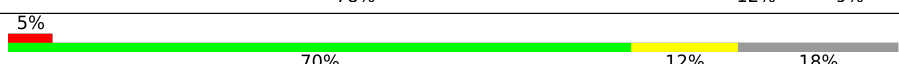


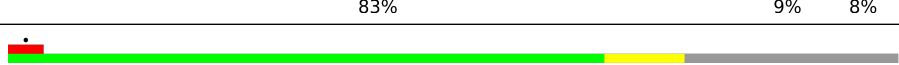
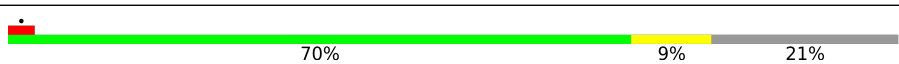


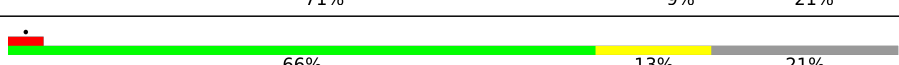



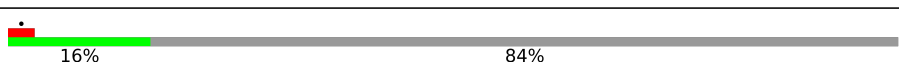








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Mol	Chain	Length	Quality of chain
1	BB	319	 84% 13%
1	BC	319	 82% 16%
1	BD	319	 86% 12%
1	BK	319	 82% 15%
1	BL	319	 89% 9%
1	BM	319	 87% 11%
1	BT	319	 84% 13%
1	BU	319	 87% 11%
1	BV	319	 86% 12%
1	CC	319	 84% 14%
1	CD	319	 81% 13% 7%
1	CE	319	 83% 15%
1	CL	319	 82% 16%
1	CM	319	 89% 9%
1	CN	319	 85% 8% 7%
1	CU	319	 84% 14%
1	CV	319	 84% 14%
1	CW	319	 82% 16%
2	AD	185	 60% 5% 21% 35%
2	AO	185	 74% 12% 15%
2	AW	185	 73% 10% 17%
2	AX	185	 79% 7% 14%
2	BF	185	 75% 10% 15%
2	BG	185	 70% 13% 17%
2	BN	185	 81% 14% 5%














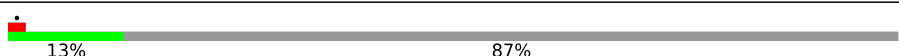
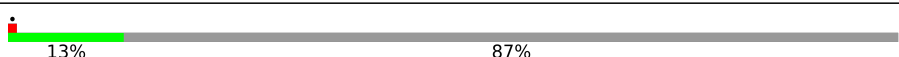
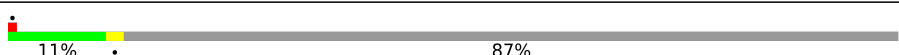
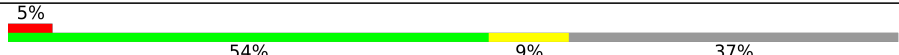
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Mol	Chain	Length	Quality of chain
2	BO	185	 8% 76% 7% 10%
2	BW	185	 5% 76% 9% 10%
2	BX	185	 5% 79% 11% 5%
2	CF	185	 9% 78% 12% 1%
2	CG	185	 5% 70% 12% 13%
2	CH	185	 9% 69% 14% 8%
2	CP	185	 8% 71% 11% 10%
2	CQ	185	 11% 83% 9% 1%
3	AF	190	 5% 67% 9% 19%
3	AN	190	 5% 70% 9% 16%
3	AV	190	 5% 73% 8% 14%
3	BE	190	 5% 66% 15% 14%
3	BP	190	 5% 71% 9% 15%
3	BY	190	 5% 66% 13% 16%
3	CO	190	 6% 64% 16% 14%
4	AH	230	 5% 15% 84%
4	AI	230	 12% 87%
4	AP	230	 16% 84%
4	AQ	230	 16% 84%
4	AR	230	 16% 84%
4	AY	230	 15% 84%
4	AZ	230	 16% 84%
4	BA	230	 16% 84%
4	BH	230	16% 84%
4	BI	230	16% 84%

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Mol	Chain	Length	Quality of chain
4	BJ	230	 15% 84%
4	BQ	230	 12% 88%
4	BR	230	 16% 84%
4	BS	230	 15% 84%
4	BZ	230	 14% 84%
4	CA	230	 15% 84%
4	CB	230	 11% 87%
4	CI	230	 15% 84%
4	CJ	230	 13% 87%
4	CK	230	 16% 84%
4	CR	230	 14% 84%
4	CS	230	 16% 84%
4	CT	230	 11% 87%
4	CX	230	 13% 87%
4	CY	230	 13% 87%
4	CZ	230	 11% 87%
5	AM	254	 5% 54% 9% 37%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 100011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AB	313	2510	1616	404	481	9	0	0
1	AC	300	2405	1549	390	457	9	0	0
1	AJ	309	2488	1604	400	475	9	0	0
1	AK	313	2510	1616	404	481	9	0	0
1	AL	313	2510	1616	404	481	9	0	0
1	AS	309	2488	1604	400	475	9	0	0
1	AT	313	2510	1616	404	481	9	0	0
1	AU	313	2510	1616	404	481	9	0	0
1	BB	309	2488	1604	400	475	9	0	0
1	BC	313	2510	1616	404	481	9	0	0
1	BD	313	2510	1616	404	481	9	0	0
1	BK	311	2505	1614	402	479	10	0	0
1	BL	313	2510	1616	404	481	9	0	0
1	BM	313	2510	1616	404	481	9	0	0
1	BT	309	2488	1604	400	475	9	0	0
1	BU	313	2510	1616	404	481	9	0	0
1	BV	311	2505	1614	402	479	10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CC	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CD	297	Total	C	N	O	S	0	0
			2383	1532	385	457	9		
1	CE	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CL	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CM	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CN	297	Total	C	N	O	S	0	0
			2383	1532	385	457	9		
1	CU	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CV	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CW	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		

- Molecule 2 is a protein called Decorator protein P03.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AD	120	Total	C	N	O	S	0	0
			917	584	151	180	2		
2	AO	158	Total	C	N	O	S	0	0
			1198	750	202	242	4		
2	AW	153	Total	C	N	O	S	0	0
			1164	733	194	233	4		
2	AX	160	Total	C	N	O	S	0	0
			1211	759	204	244	4		
2	BF	158	Total	C	N	O	S	0	0
			1194	747	201	242	4		
2	BG	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	BN	175	Total	C	N	O	S	0	0
			1337	840	225	268	4		
2	BO	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	BW	157	Total	C	N	O	S	0	0
			1189	744	200	241	4		
2	BX	166	Total	C	N	O	S	0	0
			1275	804	213	254	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CF	168	Total	C	N	O	S	0	0
			1288	813	215	256	4		
2	CG	152	Total	C	N	O	S	0	0
			1160	730	194	232	4		
2	CH	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	CP	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	CQ	170	Total	C	N	O	S	0	0
			1304	823	218	259	4		

- Molecule 3 is a protein called Decorator protein P05.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AF	144	Total	C	N	O	S	0	0
			1137	726	191	218	2		
3	AN	151	Total	C	N	O	S	0	0
			1187	755	201	229	2		
3	AV	154	Total	C	N	O	S	0	0
			1208	769	205	231	3		
3	BE	154	Total	C	N	O	S	0	0
			1208	769	205	231	3		
3	BP	151	Total	C	N	O	S	0	0
			1186	755	201	228	2		
3	BY	151	Total	C	N	O	S	0	0
			1186	755	201	228	2		
3	CO	152	Total	C	N	O	S	0	0
			1195	761	203	229	2		

- Molecule 4 is a protein called Scaffold protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AH	37	Total	C	N	O	0	0
			315	203	55	57		
4	AI	29	Total	C	N	O	0	0
			255	165	46	44		
4	AP	37	Total	C	N	O	0	0
			315	203	55	57		
4	AQ	37	Total	C	N	O	0	0
			315	203	55	57		
4	AR	37	Total	C	N	O	0	0
			315	203	55	57		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	AY	37	Total 315	C 203	N 55	O 57	0	0
4	AZ	37	Total 315	C 203	N 55	O 57	0	0
4	BA	37	Total 315	C 203	N 55	O 57	0	0
4	BH	37	Total 315	C 203	N 55	O 57	0	0
4	BI	37	Total 315	C 203	N 55	O 57	0	0
4	BJ	37	Total 315	C 203	N 55	O 57	0	0
4	BQ	28	Total 248	C 160	N 45	O 43	0	0
4	BR	37	Total 315	C 203	N 55	O 57	0	0
4	BS	37	Total 315	C 203	N 55	O 57	0	0
4	BZ	37	Total 315	C 203	N 55	O 57	0	0
4	CA	37	Total 315	C 203	N 55	O 57	0	0
4	CB	29	Total 255	C 165	N 46	O 44	0	0
4	CI	37	Total 315	C 203	N 55	O 57	0	0
4	CJ	29	Total 255	C 165	N 46	O 44	0	0
4	CK	37	Total 315	C 203	N 55	O 57	0	0
4	CR	37	Total 315	C 203	N 55	O 57	0	0
4	CS	37	Total 315	C 203	N 55	O 57	0	0
4	CT	29	Total 255	C 165	N 46	O 44	0	0
4	CX	30	Total 266	C 174	N 47	O 45	0	0
4	CY	30	Total 266	C 174	N 47	O 45	0	0
4	CZ	30	Total 266	C 174	N 47	O 45	0	0

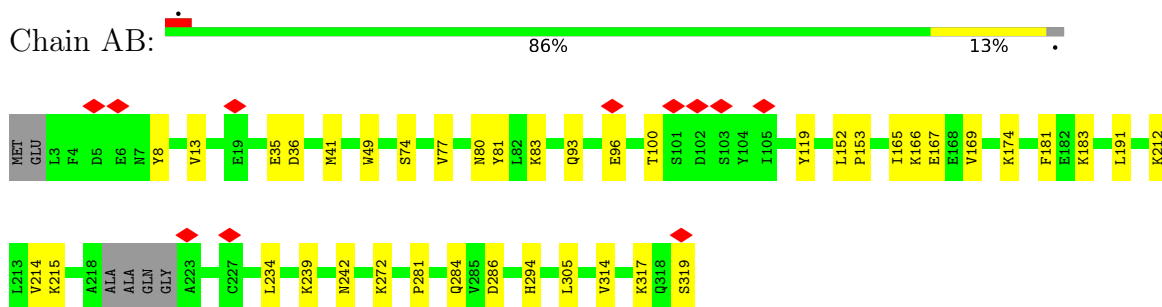
- Molecule 5 is a protein called Decorator protein P04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AM	161	1252	801	199	245	7	0	0

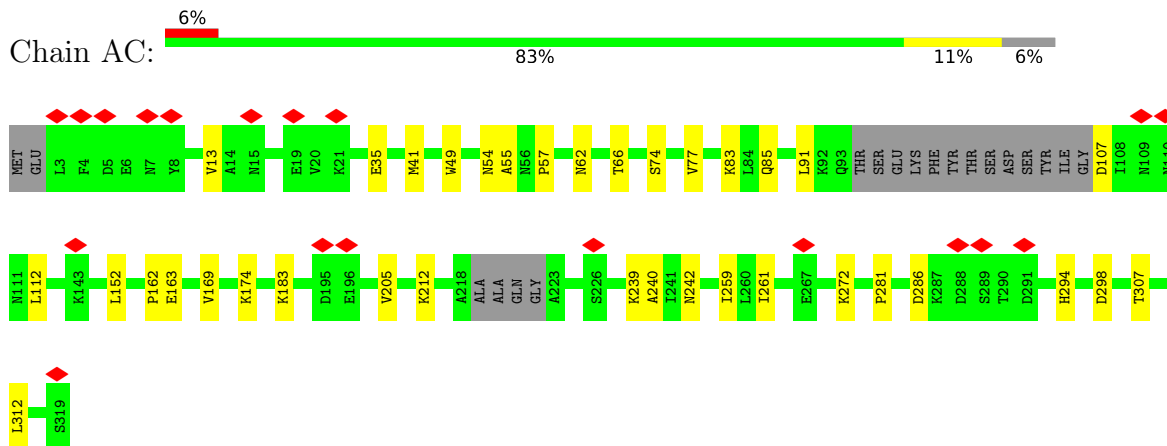
3 Residue-property plots [i](#)

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.

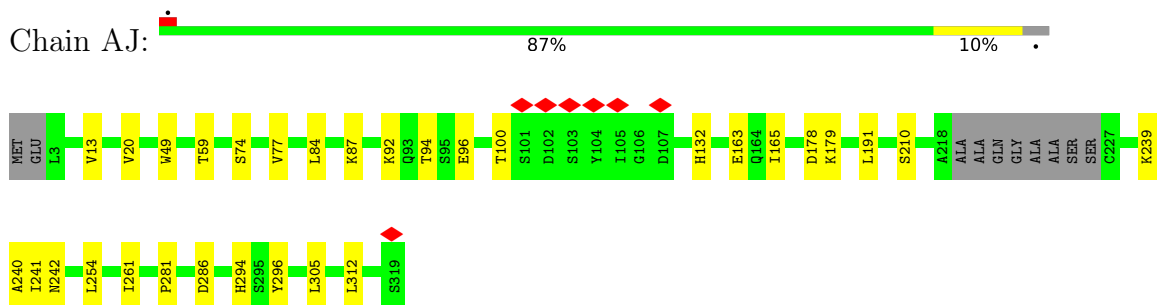
- Molecule 1: Major capsid protein



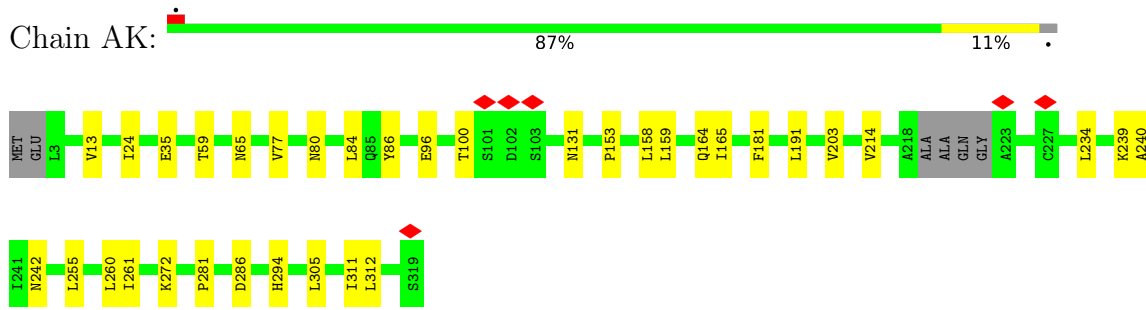
- Molecule 1: Major capsid protein



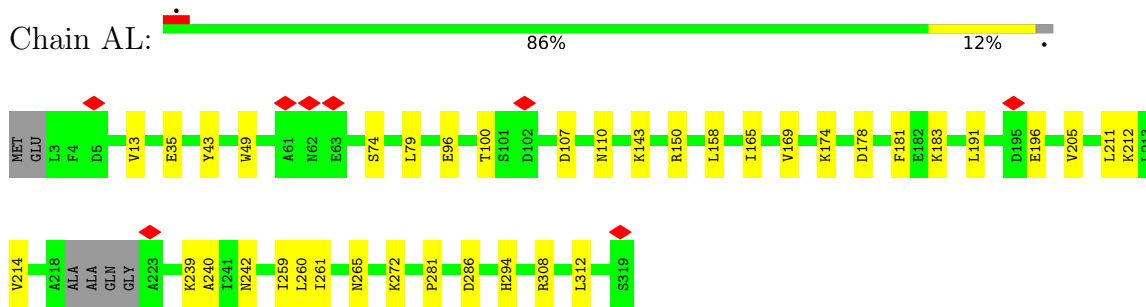
- Molecule 1: Major capsid protein



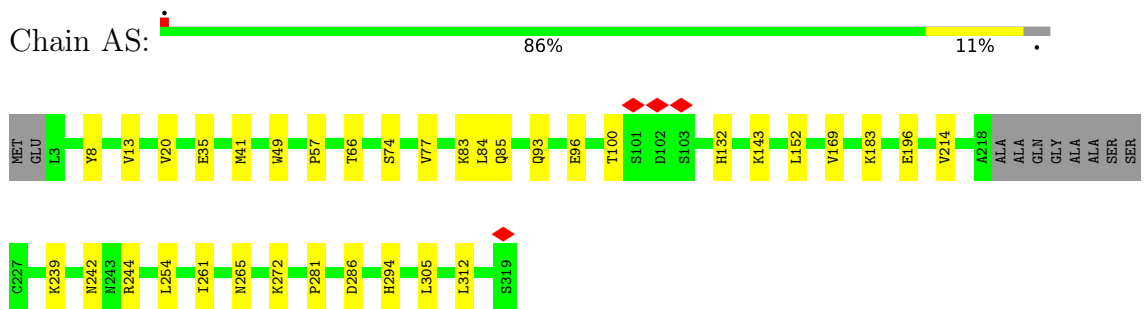
- Molecule 1: Major capsid protein



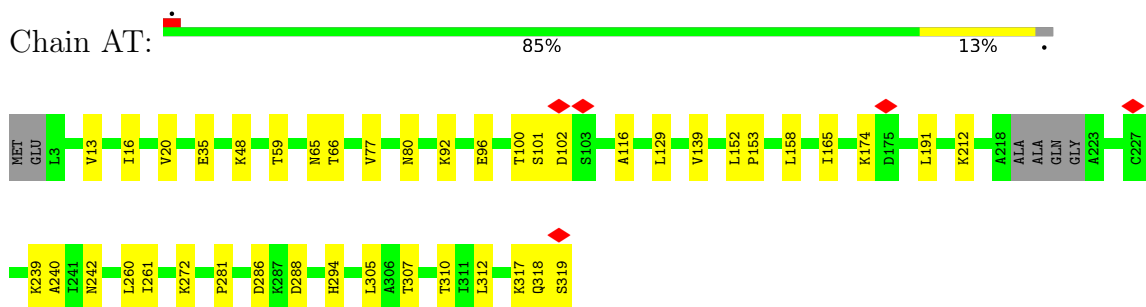
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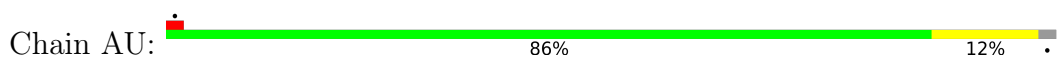
- Molecule 1: Major capsid protein

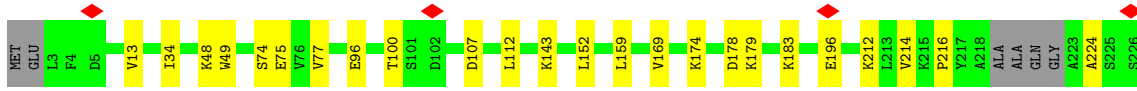


- Molecule 1: Major capsid protein

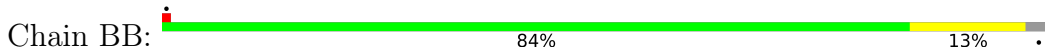


- Molecule 1: Major capsid protein

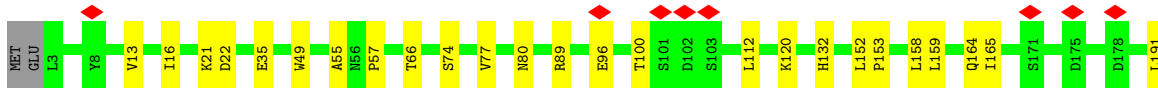
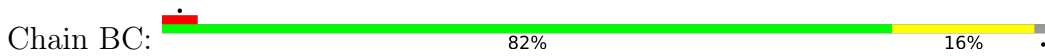




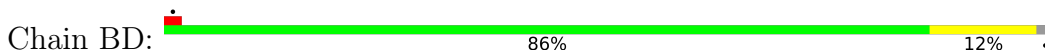
• Molecule 1: Major capsid protein



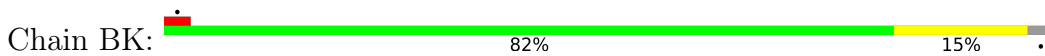
• Molecule 1: Major capsid protein



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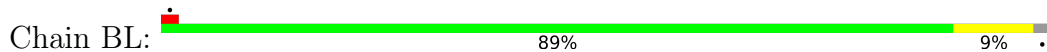


• Molecule 1: Major capsid protein

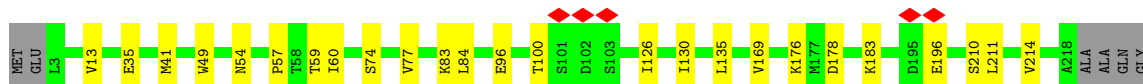
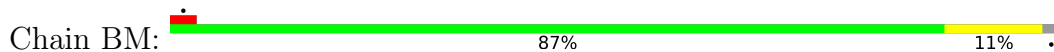




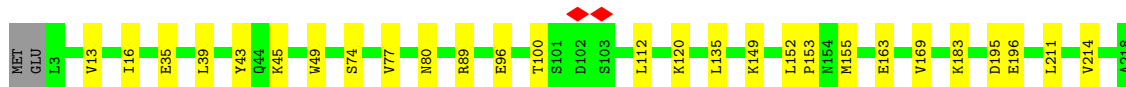
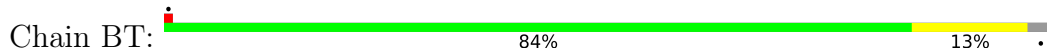
• Molecule 1: Major capsid protein



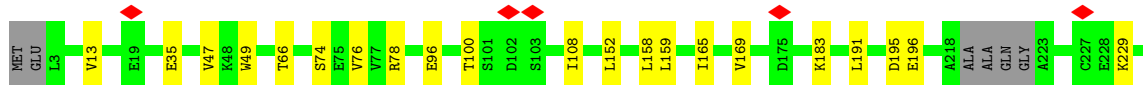
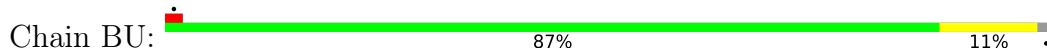
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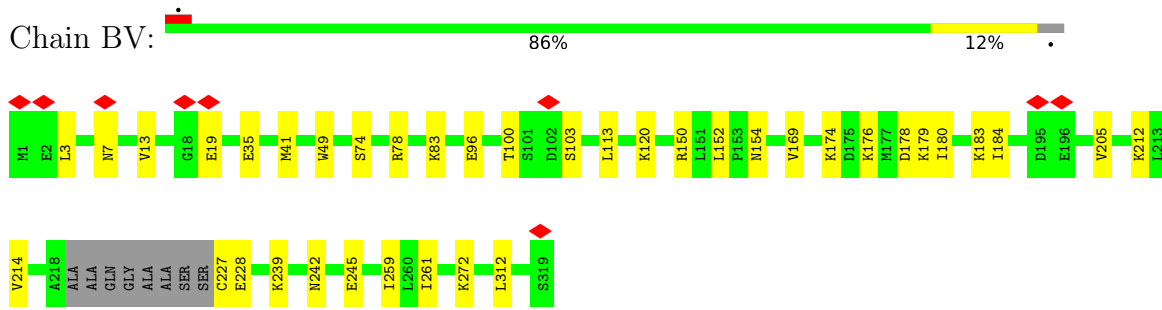
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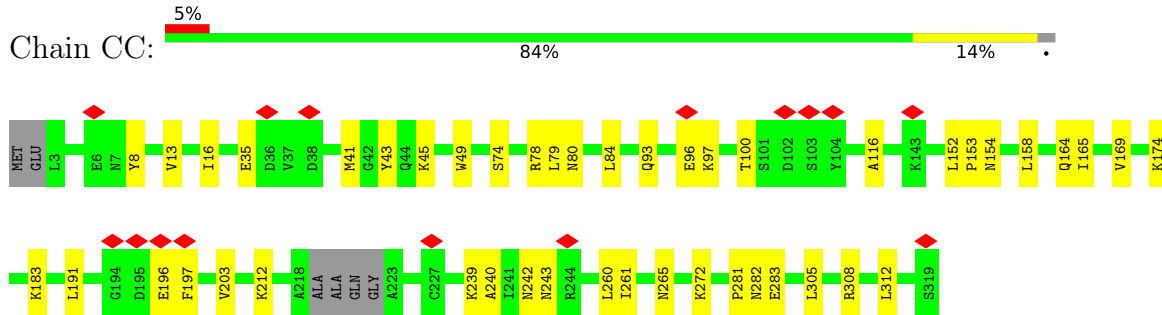
• Molecule 1: Major capsid protein



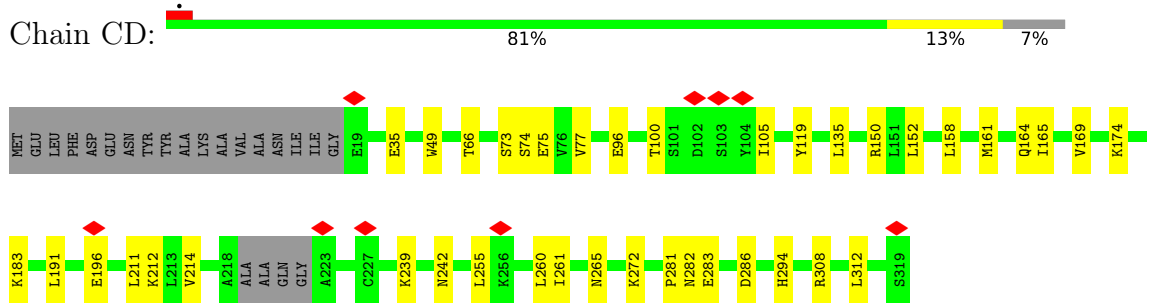
• Molecule 1: Major capsid protein



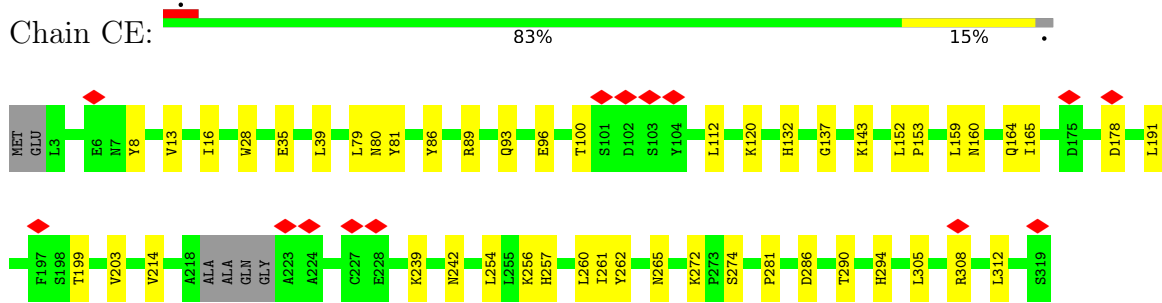
- Molecule 1: Major capsid protein



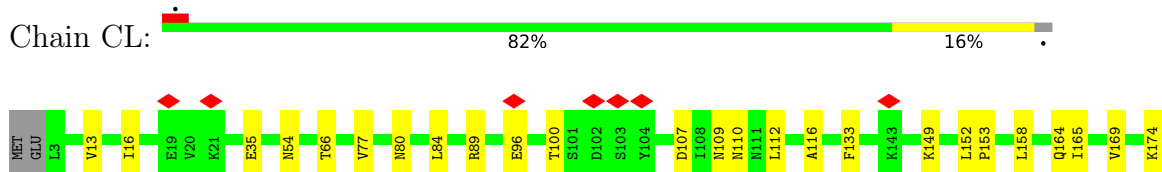
- Molecule 1: Major capsid protein

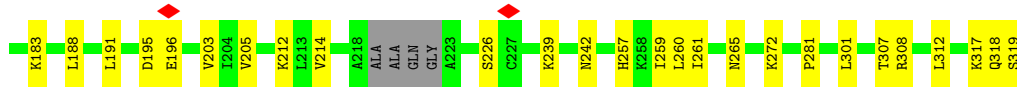


- Molecule 1: Major capsid protein

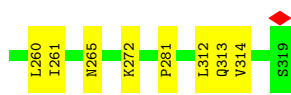


- Molecule 1: Major capsid protein

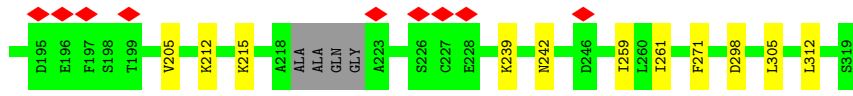
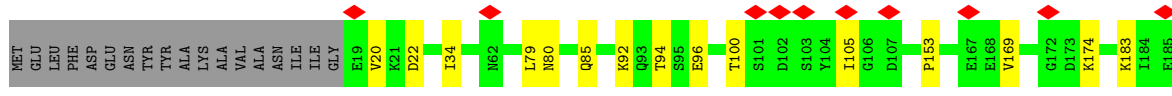
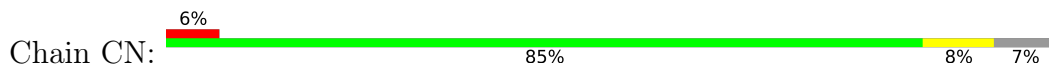




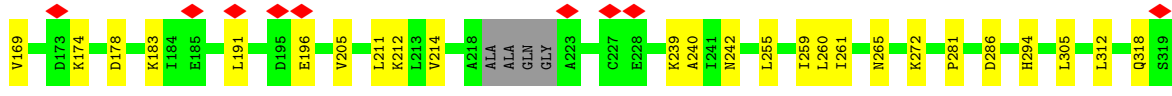
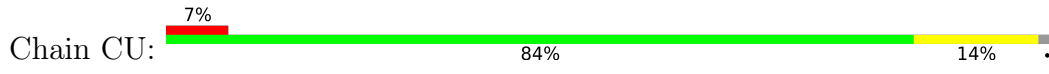
• Molecule 1: Major capsid protein



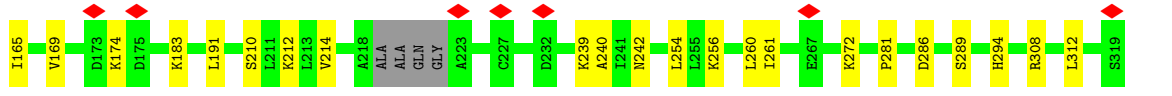
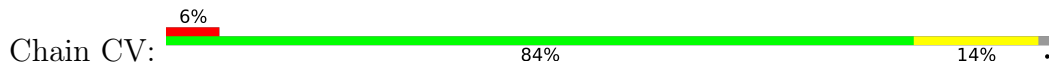
• Molecule 1: Major capsid protein



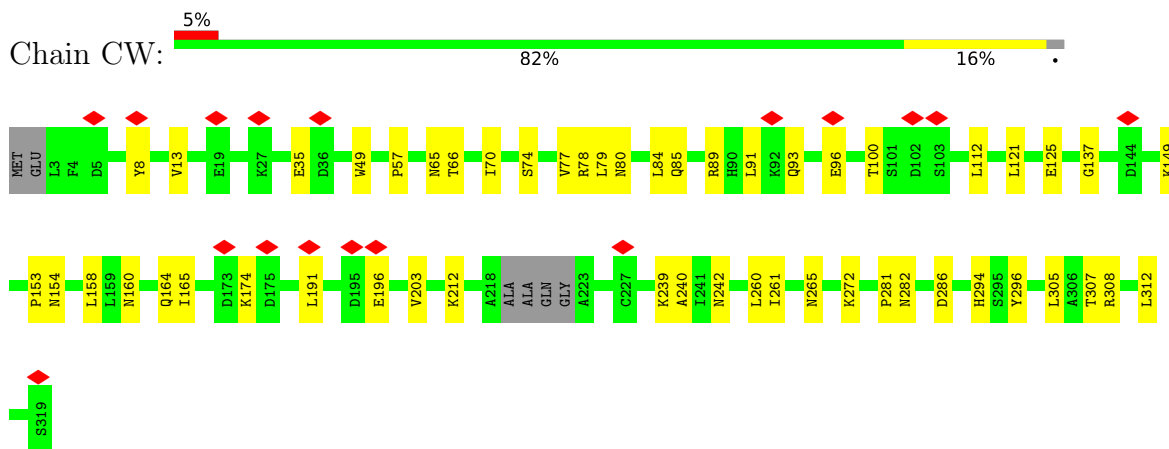
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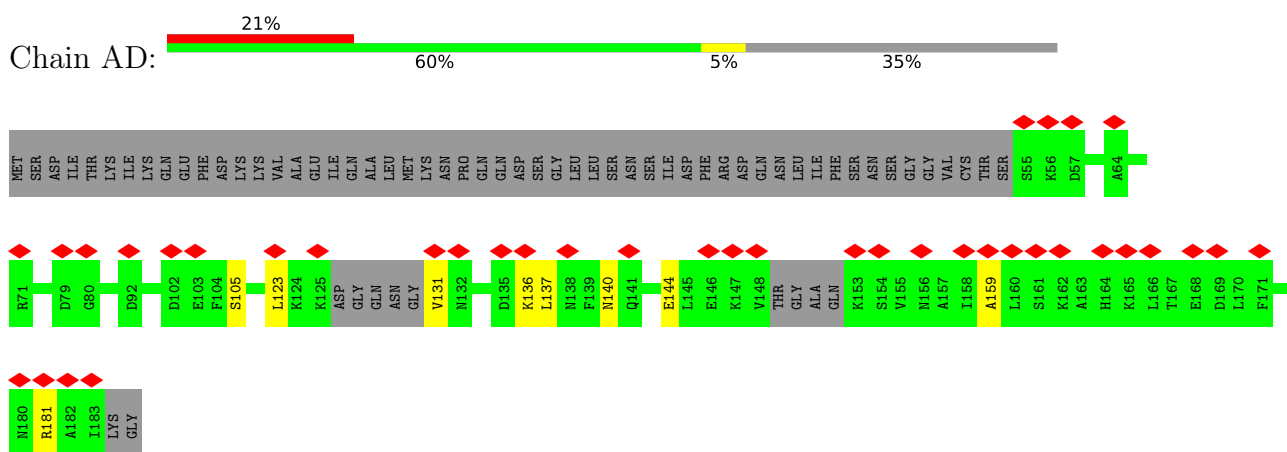
• Molecule 1: Major capsid protein



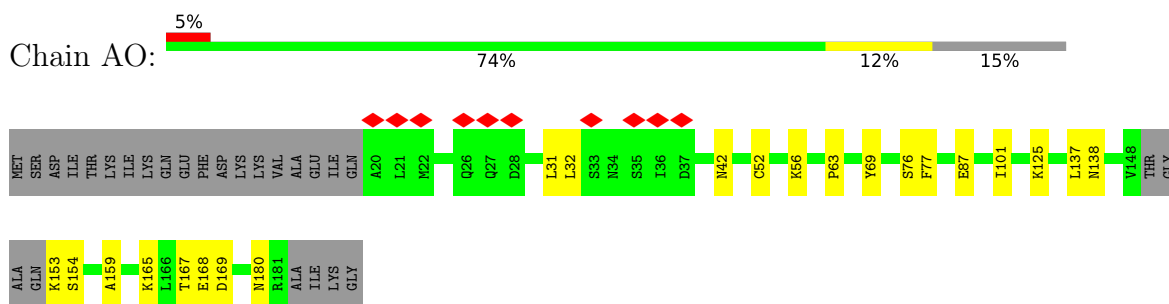
• Molecule 1: Major capsid protein



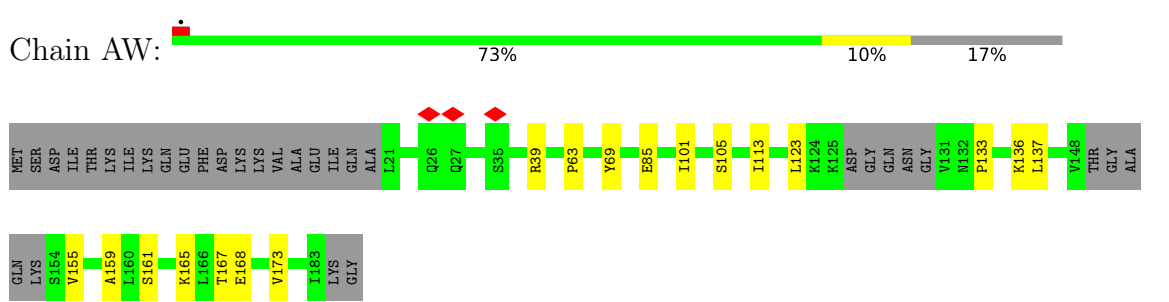
• Molecule 2: Decorator protein P03



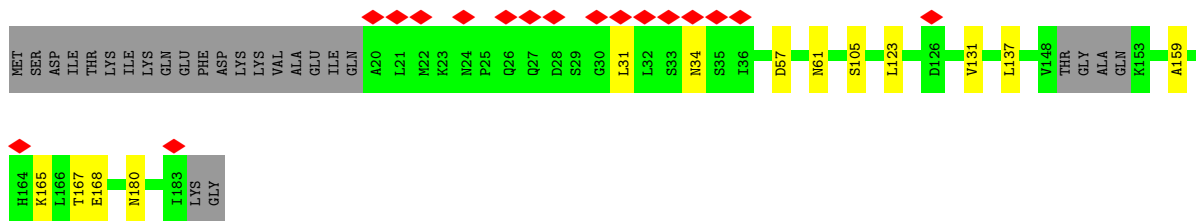
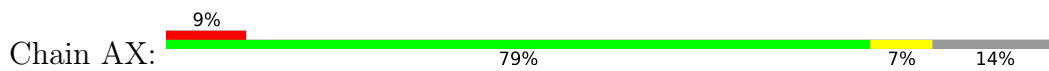
• Molecule 2: Decorator protein P03



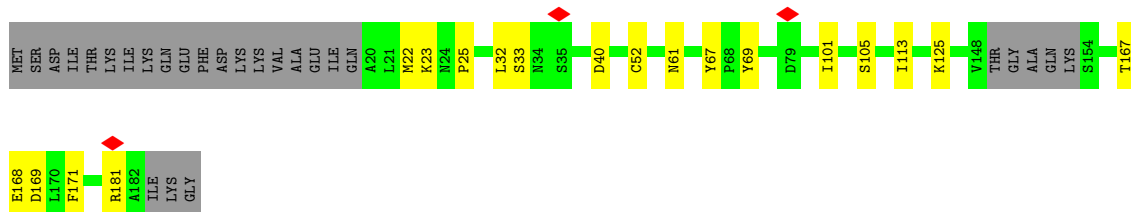
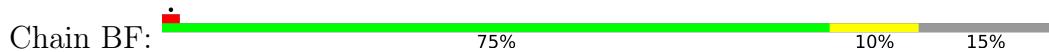
• Molecule 2: Decorator protein P03



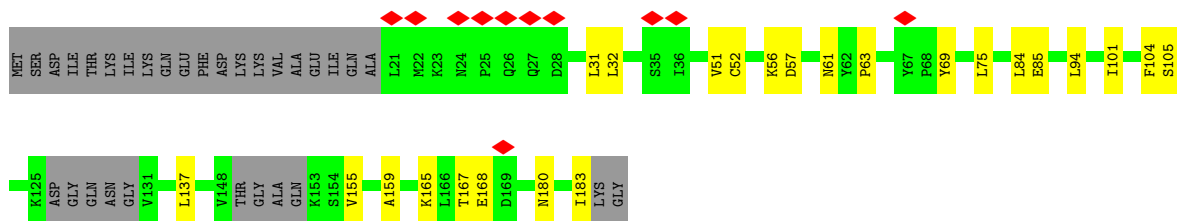
• Molecule 2: Decorator protein P03



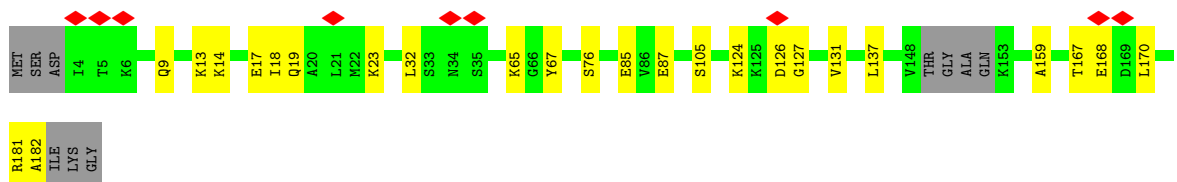
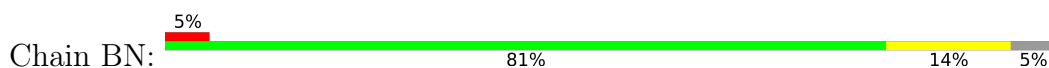
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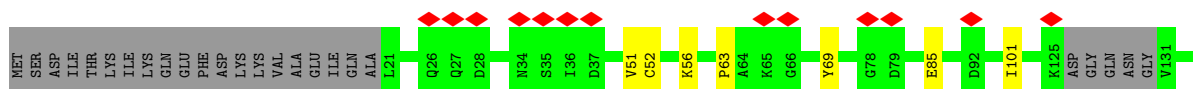
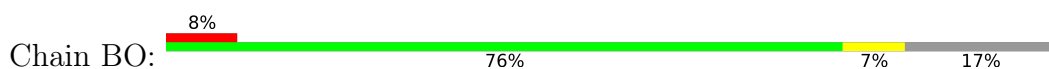
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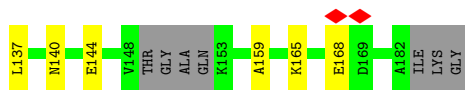


• Molecule 2: Decorator protein P03

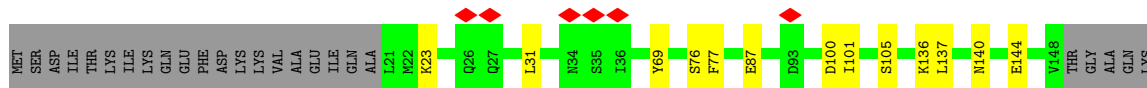
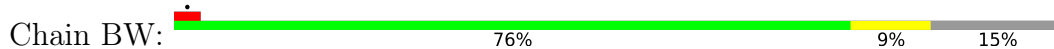


• Molecule 2: Decorator protein P03

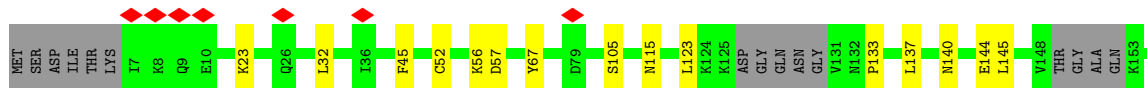
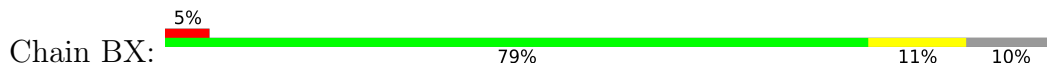




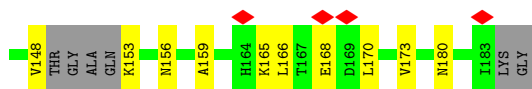
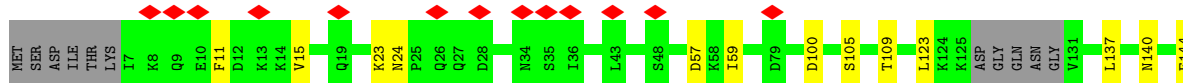
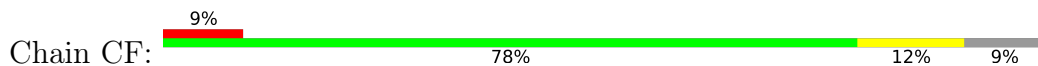
• Molecule 2: Decorator protein P03



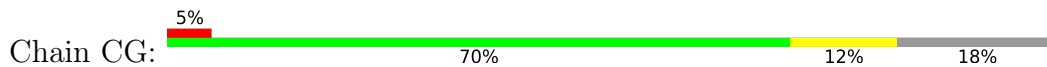
• Molecule 2: Decorator protein P03



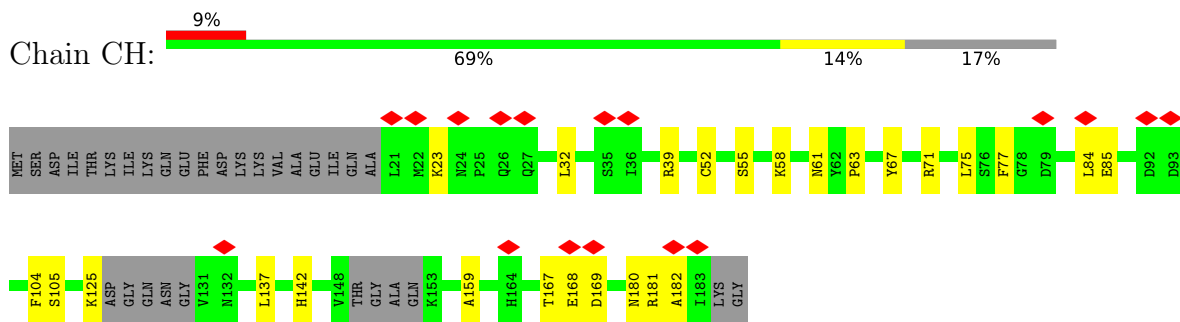
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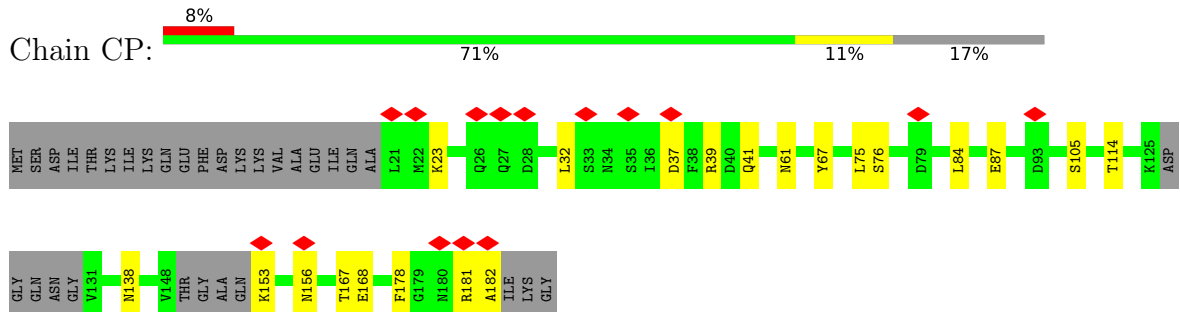
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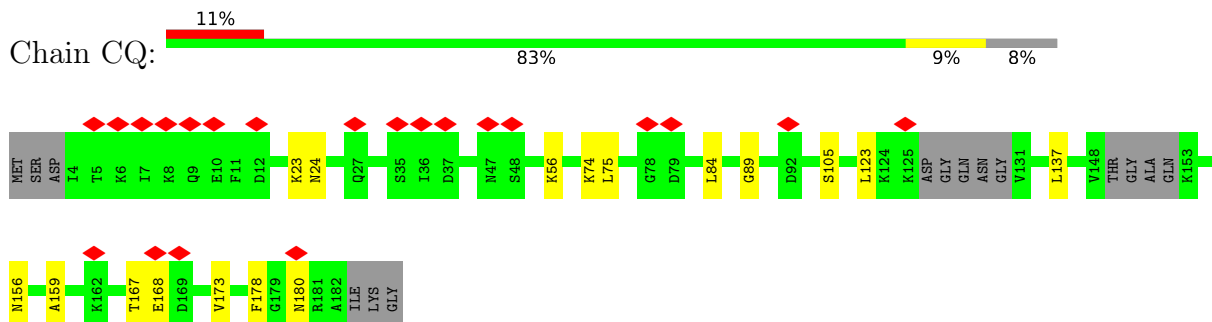
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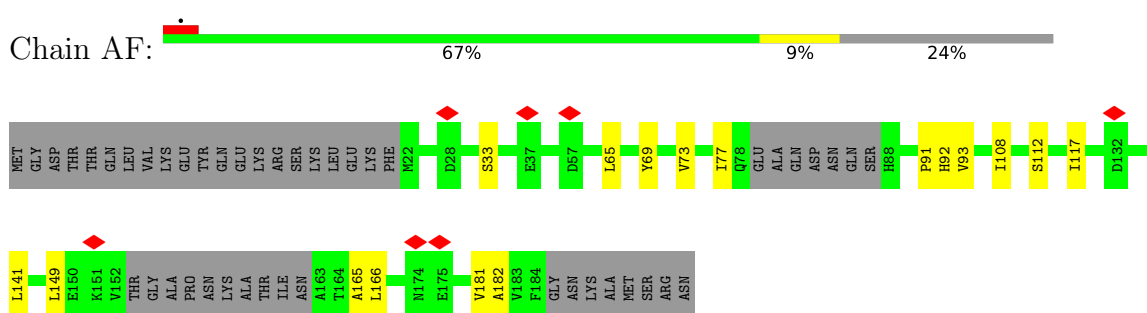
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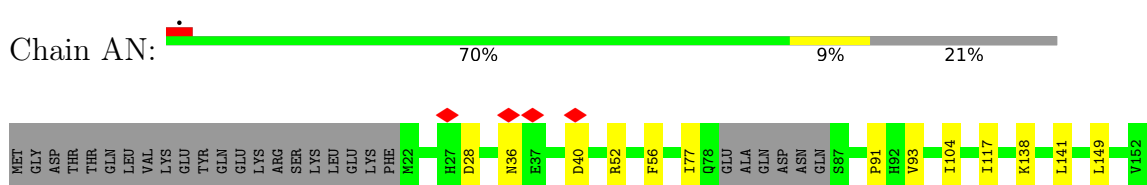
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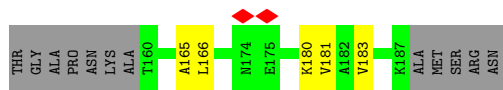


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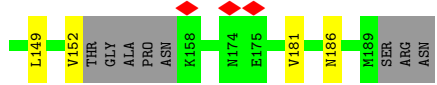
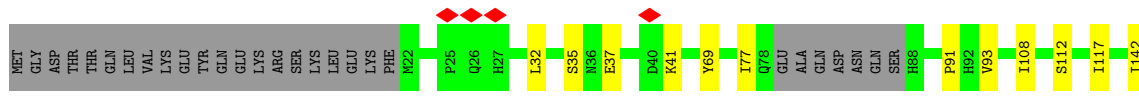
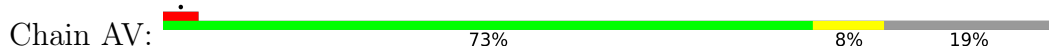


• Molecule 3: Decorator protein P05

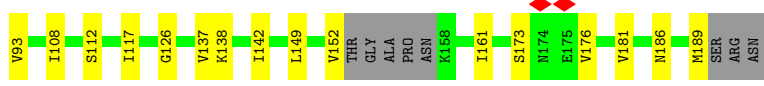




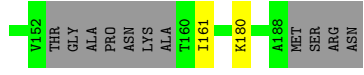
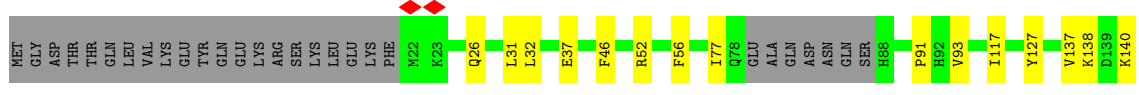
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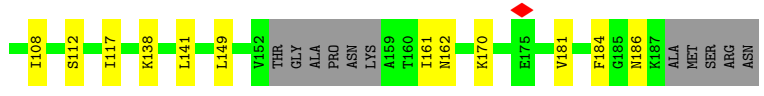
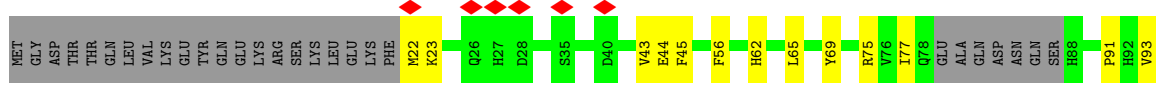
• Molecule 3: Decorator protein P05



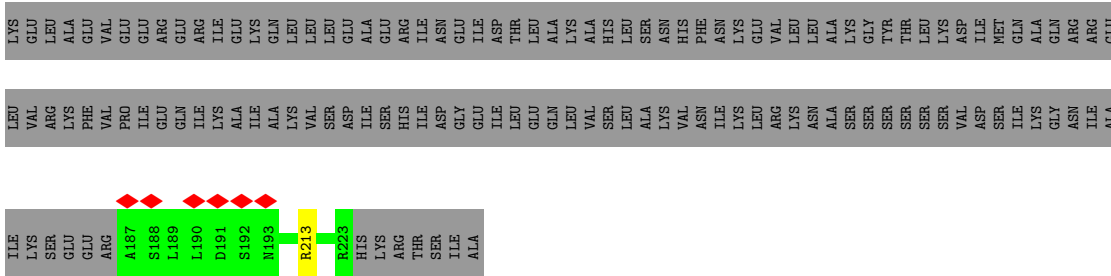
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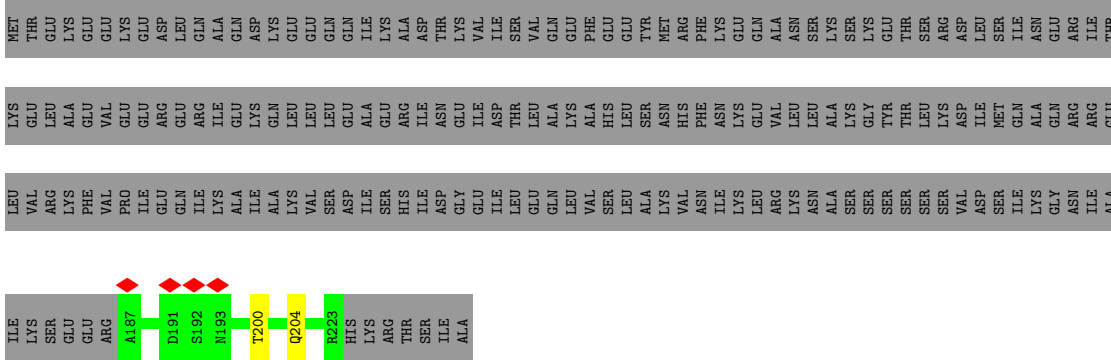
• Molecule 3: Decorator protein P05



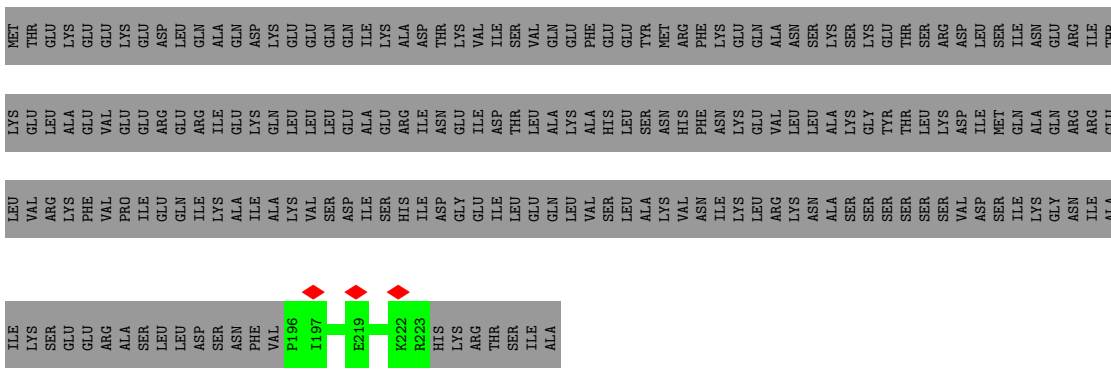
• Molecule 3: Decorator protein P05



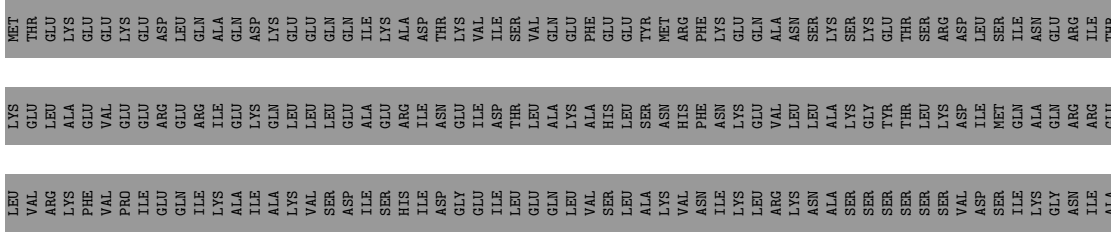
• Molecule 4: Scaffold protein

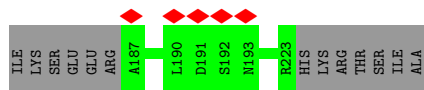


• Molecule 4: Scaffold protein

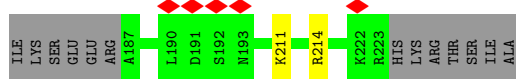
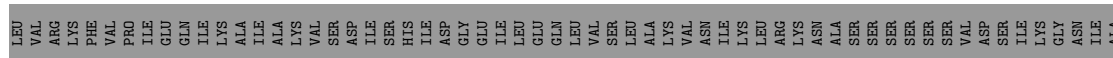
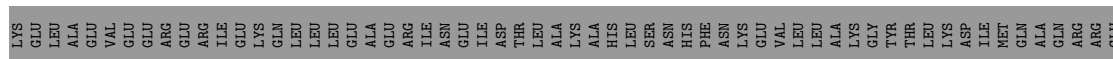
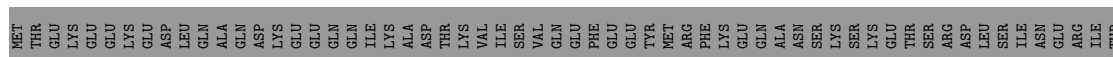


• Molecule 4: Scaffold protein

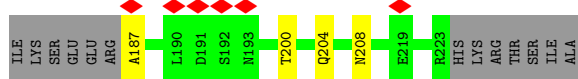
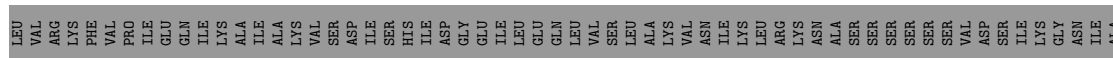
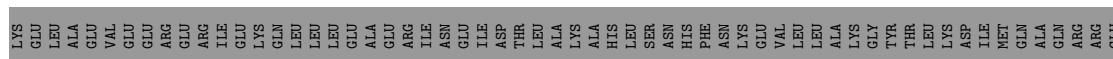
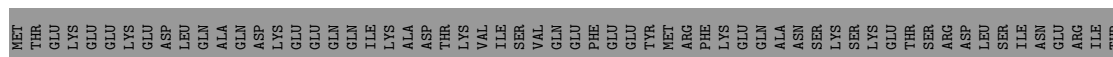




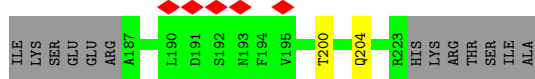
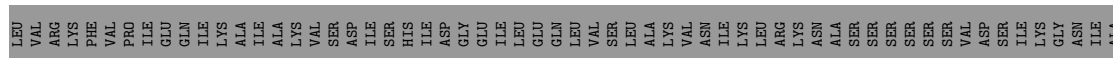
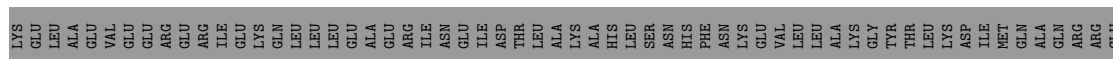
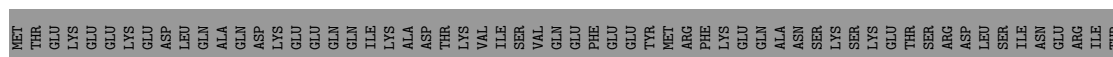
• Molecule 4: Scaffold protein



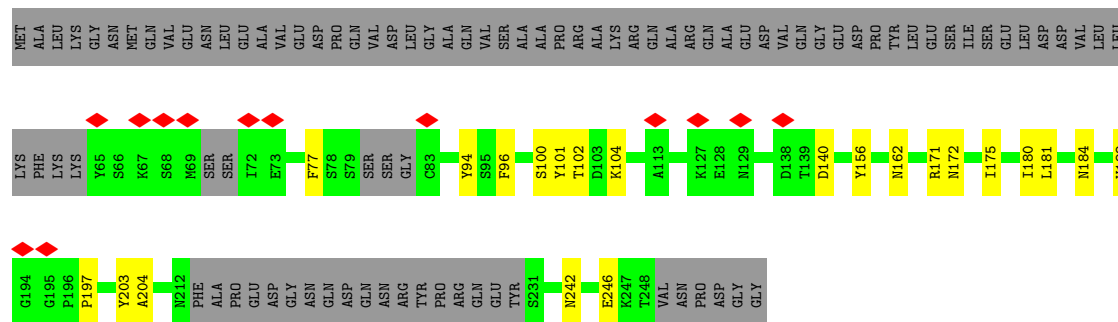
• Molecule 4: Scaffold protein



• Molecule 4: Scaffold protein



• Molecule 4: Scaffold protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	25958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	533.50397, 533.50397, 533.50397	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8335999, 0.8335999, 0.8335999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AB	0.25	0/2558	0.43	0/3458
1	AC	0.25	0/2449	0.43	0/3309
1	AJ	0.25	0/2536	0.43	0/3428
1	AK	0.24	0/2558	0.43	0/3458
1	AL	0.25	0/2558	0.43	0/3458
1	AS	0.25	0/2536	0.43	0/3428
1	AT	0.24	0/2558	0.43	0/3458
1	AU	0.25	0/2558	0.43	0/3458
1	BB	0.25	0/2536	0.43	0/3428
1	BC	0.24	0/2558	0.43	0/3458
1	BD	0.25	0/2558	0.43	0/3458
1	BK	0.25	0/2553	0.43	0/3450
1	BL	0.24	0/2558	0.44	0/3458
1	BM	0.24	0/2558	0.43	0/3458
1	BT	0.25	0/2536	0.43	0/3428
1	BU	0.24	0/2558	0.43	0/3458
1	BV	0.25	0/2553	0.44	0/3450
1	CC	0.24	0/2558	0.43	0/3458
1	CD	0.24	0/2428	0.44	0/3281
1	CE	0.24	0/2558	0.43	0/3458
1	CL	0.25	0/2558	0.43	0/3458
1	CM	0.25	0/2558	0.45	0/3458
1	CN	0.24	0/2428	0.43	0/3281
1	CU	0.24	0/2558	0.43	0/3458
1	CV	0.24	0/2558	0.43	0/3458
1	CW	0.24	0/2558	0.43	0/3458
2	AD	0.24	0/931	0.45	0/1252
2	AO	0.25	0/1216	0.45	0/1637
2	AW	0.25	0/1181	0.44	0/1590
2	AX	0.25	0/1229	0.45	0/1655
2	BF	0.25	0/1212	0.45	0/1633
2	BG	0.25	0/1190	0.44	0/1601
2	BN	0.25	0/1356	0.45	0/1823
2	BO	0.25	0/1182	0.45	0/1590

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BW	0.25	0/1207	0.44	0/1626
2	BX	0.25	0/1293	0.44	0/1737
2	CF	0.24	0/1306	0.44	0/1755
2	CG	0.24	0/1177	0.45	0/1583
2	CH	0.24	0/1190	0.44	0/1601
2	CP	0.25	0/1182	0.44	0/1590
2	CQ	0.25	0/1322	0.44	0/1776
3	AF	0.24	0/1158	0.44	0/1559
3	AN	0.25	0/1208	0.46	0/1626
3	AV	0.24	0/1229	0.45	0/1653
3	BE	0.25	0/1229	0.46	0/1653
3	BP	0.25	0/1207	0.46	0/1625
3	BY	0.25	0/1207	0.45	0/1625
3	CO	0.24	0/1216	0.46	0/1636
4	AH	0.26	0/321	0.44	0/432
4	AI	0.25	0/260	0.45	0/349
4	AP	0.26	0/321	0.43	0/432
4	AQ	0.26	0/321	0.43	0/432
4	AR	0.25	0/321	0.43	0/432
4	AY	0.26	0/321	0.44	0/432
4	AZ	0.26	0/321	0.43	0/432
4	BA	0.25	0/321	0.43	0/432
4	BH	0.26	0/321	0.43	0/432
4	BI	0.26	0/321	0.44	0/432
4	BJ	0.26	0/321	0.44	0/432
4	BQ	0.25	0/253	0.45	0/338
4	BR	0.26	0/321	0.44	0/432
4	BS	0.25	0/321	0.44	0/432
4	BZ	0.26	0/321	0.43	0/432
4	CA	0.25	0/321	0.43	0/432
4	CB	0.26	0/260	0.46	0/349
4	CI	0.26	0/321	0.44	0/432
4	CJ	0.25	0/260	0.45	0/349
4	CK	0.25	0/321	0.43	0/432
4	CR	0.25	0/321	0.44	0/432
4	CS	0.25	0/321	0.43	0/432
4	CT	0.26	0/260	0.46	0/349
4	CX	0.26	0/272	0.46	0/365
4	CY	0.25	0/272	0.46	0/365
4	CZ	0.25	0/272	0.44	0/365
5	AM	0.26	0/1274	0.46	0/1721
All	All	0.25	0/101830	0.44	0/137421

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	2510	0	2547	24	0
1	AC	2405	0	2453	24	0
1	AJ	2488	0	2527	19	0
1	AK	2510	0	2547	22	0
1	AL	2510	0	2547	23	0
1	AS	2488	0	2527	23	0
1	AT	2510	0	2547	26	0
1	AU	2510	0	2547	24	0
1	BB	2488	0	2527	27	0
1	BC	2510	0	2547	32	0
1	BD	2510	0	2547	25	0
1	BK	2505	0	2545	32	0
1	BL	2510	0	2547	19	0
1	BM	2510	0	2547	23	0
1	BT	2488	0	2527	28	0
1	BU	2510	0	2547	22	0
1	BV	2505	0	2545	23	0
1	CC	2510	0	2547	27	0
1	CD	2383	0	2425	27	0
1	CE	2510	0	2547	30	0
1	CL	2510	0	2547	34	0
1	CM	2510	0	2547	21	0
1	CN	2383	0	2425	15	0
1	CU	2510	0	2547	27	0
1	CV	2510	0	2547	25	0
1	CW	2510	0	2547	33	0
2	AD	917	0	912	5	0
2	AO	1198	0	1172	19	0
2	AW	1164	0	1145	11	0
2	AX	1211	0	1188	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BF	1194	0	1164	14	0
2	BG	1173	0	1158	20	0
2	BN	1337	0	1324	17	0
2	BO	1165	0	1147	8	0
2	BW	1189	0	1159	11	0
2	BX	1275	0	1263	14	0
2	CF	1288	0	1279	13	0
2	CG	1160	0	1142	17	0
2	CH	1173	0	1158	22	0
2	CP	1165	0	1147	15	0
2	CQ	1304	0	1299	11	0
3	AF	1137	0	1125	11	0
3	AN	1187	0	1176	13	0
3	AV	1208	0	1203	10	0
3	BE	1208	0	1203	20	0
3	BP	1186	0	1176	12	0
3	BY	1186	0	1176	17	0
3	CO	1195	0	1189	19	0
4	AH	315	0	312	2	0
4	AI	255	0	256	1	0
4	AP	315	0	312	1	0
4	AQ	315	0	312	0	0
4	AR	315	0	312	0	0
4	AY	315	0	312	2	0
4	AZ	315	0	312	1	0
4	BA	315	0	312	0	0
4	BH	315	0	312	1	0
4	BI	315	0	312	1	0
4	BJ	315	0	312	1	0
4	BQ	248	0	248	0	0
4	BR	315	0	312	0	0
4	BS	315	0	312	1	0
4	BZ	315	0	312	2	0
4	CA	315	0	312	1	0
4	CB	255	0	256	3	0
4	CI	315	0	312	1	0
4	CJ	255	0	256	0	0
4	CK	315	0	312	0	0
4	CR	315	0	312	2	0
4	CS	315	0	312	0	0
4	CT	255	0	256	3	0
4	CX	266	0	265	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CY	266	0	265	0	0
4	CZ	266	0	265	2	0
5	AM	1252	0	1235	18	0
All	All	100011	0	100623	848	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 (848) 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)
3:BP:77:ILE:HG13	3:BP:91:PRO:HB3	1.65	0.77
1:CU:165:ILE:HD13	1:CU:191:LEU:HD23	1.65	0.76
3:CO:77:ILE:HG13	3:CO:91:PRO:HB3	1.68	0.74
2:AW:63:PRO:HB2	2:AW:85:GLU:HG2	1.70	0.73
2:BX:180:ASN:O	3:BY:186:ASN:ND2	2.23	0.72
1:CM:165:ILE:HD13	1:CM:191:LEU:HD23	1.72	0.71
1:CC:152:LEU:HD21	2:CH:105:SER:HA	1.73	0.70
1:CE:199:THR:HG21	1:CE:265:ASN:HB2	1.73	0.70
3:BE:186:ASN:ND2	2:BG:180:ASN:O	2.24	0.69
1:BC:152:LEU:HD21	3:BE:112:SER:HA	1.73	0.69
1:CD:152:LEU:HD21	2:CG:105:SER:HA	1.75	0.69
3:AF:77:ILE:HG13	3:AF:91:PRO:HB3	1.74	0.69
1:CV:165:ILE:HD13	1:CV:191:LEU:HD23	1.73	0.69
1:AT:165:ILE:HD13	1:AT:191:LEU:HD23	1.74	0.69
3:BY:161:ILE:HA	3:BY:186:ASN:HA	1.75	0.67
1:AK:165:ILE:HD13	1:AK:191:LEU:HD23	1.74	0.67
1:CM:261:ILE:HD12	1:CM:312:LEU:HD23	1.77	0.67
1:AB:317:LYS:NZ	1:AB:319:SER:OXT	2.27	0.67
1:CE:261:ILE:HD12	1:CE:312:LEU:HD23	1.77	0.67
1:CL:261:ILE:HD12	1:CL:312:LEU:HD23	1.77	0.66
3:CO:161:ILE:HA	3:CO:186:ASN:HA	1.76	0.66
2:CF:148:VAL:HG11	2:CF:153:LYS:HD3	1.78	0.66
1:AK:261:ILE:HD12	1:AK:312:LEU:HD23	1.78	0.66
2:BW:140:ASN:HD21	2:BW:144:GLU:HB2	1.62	0.65
1:CW:165:ILE:HD13	1:CW:191:LEU:HD23	1.77	0.65
1:AT:317:LYS:NZ	1:AT:319:SER:OXT	2.29	0.65
1:CU:261:ILE:HD12	1:CU:312:LEU:HD23	1.78	0.65
1:AT:92:LYS:NZ	1:AT:288:ASP:O	2.30	0.65
1:BL:79:LEU:HD11	1:BL:305:LEU:HB2	1.79	0.65
1:CL:107:ASP:OD2	1:CL:110:ASN:ND2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:137:LEU:HD11	2:AD:159:ALA:HB2	1.79	0.64
1:CU:89:ARG:HH21	1:CU:112:LEU:HD21	1.60	0.64
1:BK:174:LYS:O	1:BK:212:LYS:NZ	2.30	0.64
2:BN:32:LEU:HG	1:BT:305:LEU:HD11	1.79	0.64
2:BO:63:PRO:HB2	2:BO:85:GLU:HG2	1.80	0.64
1:BU:152:LEU:HD21	2:BW:105:SER:HA	1.79	0.63
1:CD:261:ILE:HD12	1:CD:312:LEU:HD23	1.79	0.63
1:BT:152:LEU:HD21	2:BX:105:SER:HA	1.81	0.63
3:BY:69:TYR:HB2	3:BY:108:ILE:HD12	1.81	0.63
1:CW:164:GLN:HE22	1:CW:308:ARG:HA	1.64	0.63
1:BD:261:ILE:HD12	1:BD:312:LEU:HD23	1.81	0.63
1:CC:164:GLN:HE22	1:CC:308:ARG:HA	1.62	0.62
1:CU:80:ASN:ND2	1:CU:153:PRO:O	2.29	0.62
2:AD:136:LYS:HD3	2:AD:181:ARG:HH12	1.64	0.62
2:CH:32:LEU:HD23	1:CW:77:VAL:HG21	1.81	0.62
1:BD:77:VAL:HG21	2:CP:32:LEU:HD23	1.81	0.62
3:BE:161:ILE:HA	3:BE:186:ASN:HA	1.79	0.62
1:CV:261:ILE:HD12	1:CV:312:LEU:HD23	1.81	0.62
1:BB:261:ILE:HD12	1:BB:312:LEU:HD23	1.80	0.62
3:BP:26:GLN:HB3	1:CD:75:GLU:HG2	1.82	0.62
3:CO:93:VAL:HG21	3:CO:117:ILE:HD11	1.82	0.62
1:CC:261:ILE:HD12	1:CC:312:LEU:HD23	1.81	0.61
3:CO:161:ILE:O	3:CO:187:LYS:NZ	2.31	0.61
1:CV:174:LYS:O	1:CV:212:LYS:NZ	2.32	0.61
2:BG:31:LEU:HB2	1:CL:308:ARG:HH21	1.64	0.61
1:BB:152:LEU:HD21	2:BF:105:SER:HA	1.82	0.61
1:BB:77:VAL:HG11	1:BB:305:LEU:HD13	1.82	0.61
1:CN:261:ILE:HD12	1:CN:312:LEU:HD23	1.82	0.61
5:AM:197:PRO:HB2	5:AM:246:GLU:HB3	1.83	0.61
2:CG:116:ASN:HD21	2:CH:58:LYS:HE2	1.66	0.61
1:CM:143:LYS:HA	2:CP:39:ARG:HE	1.65	0.60
2:AO:69:TYR:HB2	2:AO:101:ILE:HD12	1.83	0.60
2:BG:165:LYS:HE3	2:BG:168:GLU:HA	1.83	0.60
1:CL:164:GLN:HE22	1:CL:308:ARG:HA	1.66	0.60
3:BE:32:LEU:HD23	1:BK:48:LYS:HD2	1.83	0.60
2:BG:32:LEU:HD23	1:CL:77:VAL:HG21	1.83	0.60
3:BY:149:LEU:HD13	3:BY:181:VAL:HG21	1.84	0.60
2:CG:65:LYS:HB2	2:CG:85:GLU:HG3	1.84	0.60
3:BE:69:TYR:HB2	3:BE:108:ILE:HD12	1.83	0.60
1:CL:317:LYS:NZ	1:CL:319:SER:OXT	2.32	0.60
1:AU:48:LYS:HE2	1:AU:75:GLU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:152:LEU:HD21	2:BG:105:SER:HA	1.83	0.60
1:AB:167:GLU:HB2	1:AB:314:VAL:HG22	1.84	0.60
1:AC:77:VAL:HG21	2:AO:32:LEU:HD23	1.83	0.60
1:AL:150:ARG:HE	2:AO:63:PRO:HB3	1.66	0.60
1:BV:227:CYS:SG	1:BV:228:GLU:N	2.71	0.60
1:AC:261:ILE:HD12	1:AC:312:LEU:HD23	1.82	0.60
1:AU:261:ILE:HD12	1:AU:312:LEU:HD23	1.84	0.60
1:BC:89:ARG:HH21	1:BC:112:LEU:HD21	1.66	0.60
2:CP:181:ARG:NH1	2:CP:182:ALA:O	2.35	0.59
1:CD:174:LYS:O	1:CD:212:LYS:NZ	2.34	0.59
1:BT:77:VAL:HG11	1:BT:305:LEU:HD13	1.85	0.59
1:AC:174:LYS:O	1:AC:212:LYS:NZ	2.35	0.59
1:AB:80:ASN:ND2	1:AB:153:PRO:O	2.35	0.59
1:BM:261:ILE:HD12	1:BM:312:LEU:HD23	1.85	0.59
3:BY:43:VAL:HG11	3:BY:170:LYS:HD3	1.84	0.59
2:AO:125:LYS:HD2	2:AO:169:ASP:HA	1.84	0.59
1:CL:109:ASN:O	3:CO:24:ASN:ND2	2.36	0.59
3:AN:77:ILE:HG12	3:AN:91:PRO:HB3	1.84	0.59
3:CO:149:LEU:HD13	3:CO:181:VAL:HG21	1.85	0.59
1:CV:80:ASN:ND2	1:CV:153:PRO:O	2.28	0.59
1:CE:89:ARG:HH21	1:CE:112:LEU:HD21	1.66	0.58
5:AM:242:ASN:ND2	2:AO:180:ASN:O	2.36	0.58
2:CF:100:ASP:HB3	2:CF:109:THR:HB	1.86	0.58
1:CN:205:VAL:HG12	1:CN:259:ILE:HG23	1.85	0.58
1:AL:165:ILE:HD13	1:AL:191:LEU:HD23	1.85	0.58
1:AB:13:VAL:HG11	1:AB:281:PRO:HG2	1.85	0.58
1:BK:92:LYS:NZ	1:BK:94:THR:OG1	2.37	0.58
2:AO:153:LYS:HG3	2:AO:154:SER:H	1.68	0.58
1:AT:261:ILE:HD12	1:AT:312:LEU:HD23	1.85	0.58
2:CG:69:TYR:HB2	2:CG:101:ILE:HD12	1.86	0.58
3:BE:189:MET:HA	2:BG:183:ILE:H	1.69	0.58
1:BK:11:LYS:HB2	1:BT:39:LEU:HD13	1.86	0.57
2:CH:23:LYS:N	2:CH:67:TYR:OH	2.37	0.57
1:BV:13:VAL:HG11	1:BV:103:SER:HA	1.85	0.57
1:BV:174:LYS:O	1:BV:212:LYS:NZ	2.37	0.57
1:AC:162:PRO:HG2	2:AO:31:LEU:HD11	1.87	0.57
1:BC:289:SER:HB2	1:BD:85:GLN:HE22	1.69	0.57
1:BC:22:ASP:OD1	4:BI:213:ARG:NE	2.38	0.57
1:AJ:92:LYS:NZ	1:AJ:94:THR:OG1	2.38	0.57
3:AV:77:ILE:HG13	3:AV:91:PRO:HB3	1.87	0.57
1:BC:21:LYS:NZ	1:CL:195:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:59:THR:O	2:BG:61:ASN:ND2	2.37	0.57
1:BV:78:ARG:O	1:BV:154:ASN:ND2	2.38	0.56
1:AB:152:LEU:HD21	2:AD:105:SER:HA	1.87	0.56
1:AT:152:LEU:HD21	3:AV:112:SER:HA	1.87	0.56
1:BL:261:ILE:HD12	1:BL:312:LEU:HD23	1.87	0.56
1:CL:152:LEU:HD21	2:CP:105:SER:HA	1.87	0.56
1:AC:54:ASN:HA	2:AO:42:ASN:HD22	1.69	0.56
1:CD:100:THR:HG22	1:CD:105:ILE:HG23	1.86	0.56
2:CH:63:PRO:HB2	2:CH:85:GLU:HG2	1.86	0.56
1:BD:70:ILE:HD11	1:CM:86:TYR:HD2	1.71	0.56
2:BF:167:THR:HG22	2:BF:168:GLU:H	1.71	0.56
1:AB:174:LYS:O	1:AB:212:LYS:NZ	2.38	0.56
1:AK:80:ASN:ND2	1:AK:153:PRO:O	2.38	0.56
3:BE:31:LEU:HD22	1:BK:163:GLU:HB2	1.88	0.56
2:BG:69:TYR:HB2	2:BG:101:ILE:HD12	1.86	0.56
2:BN:9:GLN:O	2:BN:13:LYS:HG2	2.05	0.56
1:AS:261:ILE:HD12	1:AS:312:LEU:HD23	1.87	0.56
1:CD:165:ILE:HD13	1:CD:191:LEU:HD23	1.88	0.56
2:CP:23:LYS:N	2:CP:67:TYR:OH	2.38	0.56
1:AJ:178:ASP:OD1	1:AJ:179:LYS:N	2.38	0.56
1:AL:261:ILE:HD12	1:AL:312:LEU:HD23	1.88	0.56
2:BN:124:LYS:HE2	2:BN:126:ASP:HB2	1.88	0.56
4:CB:211:LYS:HG3	4:CB:214:ARG:HH21	1.70	0.56
3:AF:69:TYR:HB2	3:AF:108:ILE:HD12	1.88	0.55
1:AT:20:VAL:O	4:AZ:213:ARG:NH2	2.28	0.55
3:CO:51:THR:HG21	3:CO:180:LYS:HE3	1.87	0.55
5:AM:94:TYR:CE2	5:AM:96:PHE:HB2	2.41	0.55
1:CM:181:PHE:HD1	1:CM:184:ILE:HD12	1.70	0.55
1:CU:286:ASP:HB2	1:CU:294:HIS:HB2	1.88	0.55
5:AM:181:LEU:HD11	5:AM:204:ALA:HB2	1.88	0.55
2:CG:56:LYS:NZ	2:CH:55:SER:O	2.38	0.55
1:CM:184:ILE:HG12	1:CM:314:VAL:HG21	1.87	0.55
1:BV:152:LEU:HD11	3:BY:112:SER:HA	1.89	0.55
2:CH:181:ARG:NH1	2:CH:182:ALA:O	2.40	0.55
1:BB:178:ASP:OD1	1:BB:179:LYS:N	2.39	0.55
1:CW:89:ARG:HH21	1:CW:112:LEU:HD21	1.71	0.55
2:BW:69:TYR:HB2	2:BW:101:ILE:HD12	1.89	0.55
1:BV:41:MET:HE2	1:BV:83:LYS:H	1.71	0.55
2:CH:75:LEU:HD22	2:CH:84:LEU:HD21	1.89	0.55
1:CD:286:ASP:HB2	1:CD:294:HIS:HB2	1.88	0.55
1:AB:284:GLN:NE2	1:AB:286:ASP:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:286:ASP:HB2	1:AJ:294:HIS:HB2	1.89	0.55
3:AF:149:LEU:HD13	3:AF:181:VAL:HG21	1.88	0.54
1:AS:152:LEU:HD21	2:AW:105:SER:HA	1.89	0.54
2:CH:137:LEU:HD11	2:CH:159:ALA:HB2	1.89	0.54
1:AT:77:VAL:HG11	1:AT:305:LEU:HD13	1.90	0.54
1:CU:174:LYS:O	1:CU:212:LYS:NZ	2.40	0.54
1:BK:49:TRP:CZ3	1:BK:74:SER:HB3	2.42	0.54
3:BP:137:VAL:HG12	3:BP:138:LYS:HG3	1.88	0.54
1:BT:43:TYR:HE1	1:BT:45:LYS:HG3	1.72	0.54
1:AT:286:ASP:HB2	1:AT:294:HIS:HB2	1.90	0.54
2:AO:165:LYS:HE3	2:AO:168:GLU:HA	1.90	0.54
1:BK:80:ASN:ND2	1:BK:153:PRO:O	2.41	0.54
1:BD:13:VAL:HG11	1:BD:281:PRO:HG2	1.90	0.54
1:AC:13:VAL:HG11	1:AC:281:PRO:HG2	1.89	0.54
3:BY:77:ILE:HG13	3:BY:91:PRO:HB3	1.89	0.54
2:AW:69:TYR:HB2	2:AW:101:ILE:HD12	1.89	0.54
2:BO:69:TYR:HB2	2:BO:101:ILE:HD12	1.90	0.54
1:CE:152:LEU:HD21	2:CF:105:SER:HA	1.90	0.54
2:BO:165:LYS:HE3	2:BO:168:GLU:HA	1.90	0.54
2:BW:77:PHE:CD1	3:BY:138:LYS:HG2	2.43	0.54
1:CL:80:ASN:ND2	1:CL:153:PRO:O	2.33	0.54
1:CV:158:LEU:HB3	1:CV:260:LEU:HD21	1.90	0.54
1:CW:79:LEU:HD11	1:CW:305:LEU:HB2	1.90	0.54
3:BE:93:VAL:HG21	3:BE:117:ILE:HD11	1.89	0.53
1:BU:13:VAL:HG11	1:BU:281:PRO:HG2	1.89	0.53
2:BG:63:PRO:HB2	2:BG:85:GLU:HG2	1.90	0.53
2:CP:37:ASP:O	2:CP:41:GLN:NE2	2.41	0.53
1:AC:107:ASP:HB3	1:AC:112:LEU:HB2	1.90	0.53
1:CC:240:ALA:HB2	1:CV:214:VAL:HG11	1.90	0.53
1:CE:8:TYR:CD2	1:CE:93:GLN:HG3	2.44	0.53
1:CW:158:LEU:HB3	1:CW:260:LEU:HD21	1.90	0.53
1:AB:77:VAL:HG11	1:AB:305:LEU:HD13	1.91	0.53
1:AJ:210:SER:HB3	1:AS:244:ARG:HH12	1.74	0.53
1:AS:20:VAL:O	4:AY:213:ARG:NH2	2.24	0.53
2:CH:167:THR:HG22	2:CH:168:GLU:H	1.72	0.53
1:CV:289:SER:HB2	1:CW:85:GLN:HE22	1.74	0.53
3:AV:93:VAL:HG21	3:AV:117:ILE:HD11	1.90	0.53
3:BE:73:VAL:HG21	3:BE:117:ILE:HD13	1.91	0.53
2:AX:137:LEU:HD11	2:AX:159:ALA:HB2	1.91	0.53
3:BP:140:LYS:HD3	3:BP:161:ILE:HD13	1.90	0.53
1:BT:261:ILE:HD12	1:BT:312:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:196:GLU:HB3	1:CC:265:ASN:HD22	1.73	0.53
2:CF:57:ASP:O	1:CW:65:ASN:ND2	2.41	0.53
1:AL:214:VAL:HG11	1:BU:240:ALA:HB2	1.91	0.53
1:BC:261:ILE:HD12	1:BC:312:LEU:HD23	1.90	0.53
1:BD:307:THR:HG22	2:CP:32:LEU:HB2	1.90	0.53
3:BE:149:LEU:HD13	3:BE:181:VAL:HG21	1.91	0.53
2:BG:137:LEU:HD11	2:BG:159:ALA:HB2	1.91	0.53
1:CE:164:GLN:HE22	1:CE:308:ARG:HA	1.74	0.53
3:BY:93:VAL:HG21	3:BY:117:ILE:HD11	1.91	0.52
1:CN:212:LYS:HA	1:CN:215:LYS:HE3	1.91	0.52
2:BW:136:LYS:HD3	2:BW:155:VAL:HG21	1.91	0.52
1:AK:158:LEU:HB3	1:AK:260:LEU:HD21	1.90	0.52
1:BC:256:LYS:HG2	1:BC:257:HIS:CD2	2.44	0.52
1:CL:89:ARG:HH21	1:CL:112:LEU:HD21	1.75	0.52
3:AF:165:ALA:HA	3:AF:181:VAL:HG22	1.91	0.52
1:AT:13:VAL:HG11	1:AT:281:PRO:HG2	1.91	0.52
1:BC:158:LEU:HB3	1:BC:260:LEU:HD21	1.91	0.52
1:BL:13:VAL:HG11	1:BL:281:PRO:HG2	1.91	0.52
1:BV:261:ILE:HD12	1:BV:312:LEU:HD23	1.92	0.52
1:CE:96:GLU:O	1:CE:100:THR:HG23	2.10	0.52
2:CF:166:LEU:HB2	2:CF:170:LEU:HD23	1.91	0.52
1:AL:107:ASP:OD2	1:AL:110:ASN:ND2	2.40	0.52
1:BU:257:HIS:CE1	1:BU:318:GLN:HG3	2.45	0.52
1:AL:49:TRP:CZ3	1:AL:74:SER:HB3	2.44	0.52
1:AC:57:PRO:HB2	1:AK:84:LEU:HB3	1.92	0.52
1:AK:65:ASN:ND2	2:AX:57:ASP:O	2.43	0.52
1:BB:214:VAL:HG11	1:BK:240:ALA:HB2	1.92	0.52
1:BC:66:THR:HG22	2:BO:52:CYS:HB3	1.91	0.52
1:BD:240:ALA:HB2	1:CM:214:VAL:HG11	1.92	0.52
1:BT:89:ARG:HH21	1:BT:112:LEU:HD13	1.75	0.52
1:CL:13:VAL:HG11	1:CL:281:PRO:HG2	1.91	0.52
1:BM:59:THR:O	2:CH:61:ASN:ND2	2.42	0.52
3:BP:52:ARG:HB3	1:CD:66:THR:HG22	1.92	0.52
1:BD:239:LYS:HA	1:BD:242:ASN:OD1	2.10	0.52
1:BK:261:ILE:HD12	1:BK:312:LEU:HD23	1.91	0.52
1:BL:152:LEU:HD21	2:BN:105:SER:HA	1.92	0.52
1:BV:96:GLU:O	1:BV:100:THR:HB	2.10	0.52
2:CH:75:LEU:HB3	2:CH:84:LEU:HD11	1.92	0.52
1:CN:20:VAL:O	4:CT:213:ARG:NH2	2.43	0.52
1:BM:169:VAL:HG22	1:BM:183:LYS:HG3	1.92	0.51
1:CM:196:GLU:OE1	1:CM:265:ASN:ND2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CW:174:LYS:O	1:CW:212:LYS:NZ	2.44	0.51
1:AS:286:ASP:HB2	1:AS:294:HIS:HB2	1.92	0.51
1:BC:13:VAL:HG11	1:BC:281:PRO:HG2	1.91	0.51
2:CF:140:ASN:OD1	2:CF:144:GLU:N	2.41	0.51
1:CE:165:ILE:HD13	1:CE:191:LEU:HD23	1.90	0.51
1:CN:100:THR:HG22	1:CN:105:ILE:HG23	1.91	0.51
1:AK:13:VAL:HG11	1:AK:281:PRO:HG2	1.92	0.51
1:AL:169:VAL:HG22	1:AL:183:LYS:HG3	1.92	0.51
1:AT:66:THR:HG22	2:BF:52:CYS:SG	2.51	0.51
1:BK:239:LYS:HA	1:BK:242:ASN:OD1	2.11	0.51
3:AV:149:LEU:HD13	3:AV:181:VAL:HG21	1.92	0.51
1:AC:286:ASP:HB2	1:AC:294:HIS:HB2	1.93	0.51
1:AL:143:LYS:HE3	3:AN:40:ASP:HB2	1.92	0.51
1:AS:77:VAL:HG11	1:AS:305:LEU:HD13	1.93	0.51
1:CE:143:LYS:HA	2:CH:39:ARG:HE	1.75	0.51
1:BB:239:LYS:HA	1:BB:242:ASN:OD1	2.11	0.51
2:BF:69:TYR:HB2	2:BF:101:ILE:HD12	1.91	0.51
1:CU:96:GLU:O	1:CU:100:THR:HG23	2.11	0.51
1:BM:54:ASN:HB3	2:CG:51:VAL:HG12	1.93	0.51
1:BT:239:LYS:HA	1:BT:242:ASN:OD1	2.10	0.51
1:CC:165:ILE:HD13	1:CC:191:LEU:HD23	1.93	0.51
1:CL:205:VAL:HG12	1:CL:259:ILE:HG23	1.92	0.51
1:BB:89:ARG:NH2	1:BB:112:LEU:HD21	2.26	0.50
1:AJ:261:ILE:HD12	1:AJ:312:LEU:HD23	1.93	0.50
3:AN:93:VAL:HG21	3:AN:117:ILE:HD11	1.91	0.50
1:BC:240:ALA:HB2	1:BM:214:VAL:HG11	1.93	0.50
1:CW:78:ARG:O	1:CW:154:ASN:ND2	2.34	0.50
1:CW:261:ILE:HD12	1:CW:312:LEU:HD23	1.93	0.50
1:AK:286:ASP:HB2	1:AK:294:HIS:HB2	1.94	0.50
1:AL:35:GLU:O	1:AL:272:LYS:HA	2.12	0.50
1:CL:257:HIS:CE1	1:CL:318:GLN:HG3	2.46	0.50
3:CO:127:TYR:HE1	3:CO:170:LYS:HZ3	1.58	0.50
1:CW:239:LYS:HA	1:CW:242:ASN:OD1	2.11	0.50
3:AF:73:VAL:HG21	3:AF:117:ILE:HD13	1.94	0.50
1:AJ:84:LEU:HB3	1:AS:57:PRO:HB2	1.93	0.50
1:CE:86:TYR:HD2	1:CW:70:ILE:HD11	1.75	0.50
2:CQ:137:LEU:HD11	2:CQ:159:ALA:HB2	1.94	0.50
1:CW:49:TRP:CZ3	1:CW:74:SER:HB3	2.46	0.50
1:AC:239:LYS:HA	1:AC:242:ASN:OD1	2.11	0.50
1:BD:169:VAL:HG22	1:BD:183:LYS:HG3	1.93	0.50
1:CC:13:VAL:HG11	1:CC:281:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CL:239:LYS:HA	1:CL:242:ASN:OD1	2.11	0.50
2:BW:158:ILE:HG13	2:BW:178:PHE:HE2	1.76	0.50
3:BY:44:GLU:CD	3:BY:45:PHE:H	2.15	0.50
1:BC:241:ILE:HG22	1:BM:211:LEU:HD21	1.93	0.50
1:BL:165:ILE:HD13	1:BL:191:LEU:HD23	1.94	0.50
1:BL:239:LYS:HA	1:BL:242:ASN:OD1	2.12	0.50
1:CC:239:LYS:HA	1:CC:242:ASN:OD1	2.11	0.50
1:CW:96:GLU:O	1:CW:100:THR:HG23	2.12	0.50
1:BC:159:LEU:HD12	1:BC:260:LEU:HD13	1.94	0.50
1:CU:158:LEU:HB3	1:CU:260:LEU:HD21	1.93	0.50
1:CV:41:MET:HE2	1:CV:83:LYS:H	1.75	0.50
1:BK:39:LEU:O	1:BK:274:SER:OG	2.22	0.50
1:BM:13:VAL:HG11	1:BM:281:PRO:HG2	1.92	0.50
1:CM:181:PHE:CD1	1:CM:184:ILE:HD12	2.46	0.50
1:CW:35:GLU:O	1:CW:272:LYS:HA	2.12	0.50
1:CU:13:VAL:HG11	1:CU:281:PRO:HG2	1.94	0.49
1:AL:96:GLU:O	1:AL:100:THR:HG23	2.12	0.49
5:AM:102:THR:HG22	3:AN:56:PHE:HD1	1.76	0.49
1:AS:41:MET:HE2	1:AS:83:LYS:H	1.77	0.49
1:AU:34:ILE:HG12	1:AU:271:PHE:HB3	1.94	0.49
3:AV:69:TYR:HB2	3:AV:108:ILE:HD12	1.93	0.49
1:BB:49:TRP:CZ3	1:BB:74:SER:HB3	2.47	0.49
1:CD:158:LEU:HB3	1:CD:260:LEU:HD21	1.93	0.49
1:CM:152:LEU:HD21	2:CQ:105:SER:HA	1.93	0.49
5:AM:101:TYR:CD2	5:AM:102:THR:HG23	2.47	0.49
5:AM:102:THR:HG21	3:AN:56:PHE:HA	1.93	0.49
1:BM:239:LYS:HA	1:BM:242:ASN:OD1	2.12	0.49
1:BU:158:LEU:HB3	1:BU:260:LEU:HD21	1.93	0.49
1:AJ:20:VAL:O	4:AP:213:ARG:NH2	2.29	0.49
1:AL:158:LEU:HB3	1:AL:260:LEU:HD21	1.95	0.49
1:AT:239:LYS:HA	1:AT:242:ASN:OD1	2.12	0.49
3:AV:32:LEU:HG	1:BB:305:LEU:HD11	1.95	0.49
2:BO:137:LEU:HD11	2:BO:159:ALA:HB2	1.92	0.49
1:BV:239:LYS:NZ	1:BV:245:GLU:O	2.44	0.49
2:BX:137:LEU:HD11	2:BX:159:ALA:HB2	1.93	0.49
2:CF:123:LEU:HD13	2:CF:173:VAL:HG11	1.94	0.49
1:CV:47:VAL:HG22	1:CV:76:VAL:HG22	1.95	0.49
1:CV:169:VAL:HG22	1:CV:183:LYS:HG3	1.95	0.49
1:BC:165:ILE:HD12	1:BC:191:LEU:HD23	1.93	0.49
2:CP:167:THR:HG22	2:CP:168:GLU:H	1.77	0.49
1:CU:79:LEU:HD11	1:CU:305:LEU:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:169:VAL:HG22	1:AU:183:LYS:HG3	1.94	0.49
1:AS:214:VAL:HG11	1:BB:240:ALA:HB2	1.95	0.49
2:CG:156:ASN:ND2	2:CG:180:ASN:O	2.45	0.49
1:AB:286:ASP:HB2	1:AB:294:HIS:HB2	1.95	0.49
1:AU:49:TRP:CZ3	1:AU:74:SER:HB3	2.47	0.49
1:CM:13:VAL:HG11	1:CM:281:PRO:HG2	1.95	0.49
1:CM:169:VAL:HG22	1:CM:183:LYS:HG3	1.95	0.49
1:CV:126:ILE:O	1:CV:130:ILE:HG13	2.13	0.49
1:AL:239:LYS:HA	1:AL:242:ASN:OD1	2.13	0.49
1:AT:48:LYS:NZ	2:BF:33:SER:O	2.41	0.49
1:BB:89:ARG:HH21	1:BB:112:LEU:HD21	1.77	0.49
1:CM:239:LYS:HA	1:CM:242:ASN:OD1	2.13	0.49
1:CV:286:ASP:HB2	1:CV:294:HIS:HB2	1.93	0.49
1:BC:196:GLU:HB3	1:BC:265:ASN:HD22	1.78	0.48
2:BN:76:SER:HB3	2:BN:87:GLU:HG2	1.94	0.48
1:CN:169:VAL:HG22	1:CN:183:LYS:HG3	1.94	0.48
1:AC:307:THR:HG22	2:AO:32:LEU:HB2	1.95	0.48
1:AS:239:LYS:HA	1:AS:242:ASN:OD1	2.13	0.48
1:CL:158:LEU:HB3	1:CL:260:LEU:HD21	1.95	0.48
1:AJ:165:ILE:HD13	1:AJ:191:LEU:HD23	1.95	0.48
1:AU:239:LYS:HA	1:AU:242:ASN:OD1	2.13	0.48
1:BU:159:LEU:HD12	1:BU:260:LEU:HD13	1.95	0.48
1:AJ:239:LYS:HA	1:AJ:242:ASN:OD1	2.14	0.48
1:AK:239:LYS:HA	1:AK:242:ASN:OD1	2.13	0.48
2:AW:137:LEU:HD11	2:AW:159:ALA:HB2	1.96	0.48
1:BL:240:ALA:HB2	1:BV:214:VAL:HG11	1.95	0.48
1:CM:35:GLU:O	1:CM:272:LYS:HA	2.14	0.48
1:CV:35:GLU:O	1:CV:272:LYS:HA	2.14	0.48
1:CW:286:ASP:HB2	1:CW:294:HIS:HB2	1.96	0.48
3:AN:104:ILE:HD11	3:AN:183:VAL:HG11	1.96	0.48
1:BC:16:ILE:HD11	1:BC:120:LYS:HE3	1.94	0.48
1:BV:239:LYS:HA	1:BV:242:ASN:OD1	2.13	0.48
1:CN:239:LYS:HA	1:CN:242:ASN:OD1	2.12	0.48
1:BK:112:LEU:HD21	1:BK:292:VAL:HG22	1.95	0.48
1:BU:165:ILE:HG13	1:BU:191:LEU:HD23	1.95	0.48
2:CF:165:LYS:HE3	2:CF:168:GLU:HA	1.96	0.48
3:CO:56:PHE:HD1	2:CQ:56:LYS:HD2	1.78	0.48
2:CQ:75:LEU:HD22	2:CQ:84:LEU:HD13	1.96	0.48
1:AK:77:VAL:HG11	1:AK:305:LEU:HD13	1.95	0.48
2:BG:52:CYS:HB3	1:CL:66:THR:HG22	1.94	0.48
3:BP:93:VAL:HG21	3:BP:117:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BN:19:GLN:HG3	1:BV:3:LEU:HD23	1.95	0.48
3:BE:28:ASP:OD1	3:BE:28:ASP:N	2.45	0.48
1:BK:13:VAL:HG21	1:BK:103:SER:HB2	1.95	0.48
1:BT:96:GLU:O	1:BT:100:THR:HG23	2.13	0.48
1:AJ:77:VAL:HG11	1:AJ:305:LEU:HD13	1.95	0.47
3:AN:149:LEU:HD13	3:AN:181:VAL:HG11	1.95	0.47
2:AW:165:LYS:HE3	2:AW:168:GLU:HA	1.96	0.47
1:BD:165:ILE:HG13	1:BD:191:LEU:HD23	1.96	0.47
1:CC:78:ARG:O	1:CC:154:ASN:ND2	2.35	0.47
1:AT:305:LEU:HD11	2:BF:32:LEU:HG	1.96	0.47
1:AU:13:VAL:HG11	1:AU:281:PRO:HG2	1.96	0.47
1:BD:49:TRP:CZ3	1:BD:74:SER:HB3	2.49	0.47
1:BM:196:GLU:HB3	1:BM:265:ASN:ND2	2.29	0.47
1:CW:203:VAL:HG13	1:CW:261:ILE:HG12	1.96	0.47
2:AD:140:ASN:OD1	2:AD:144:GLU:N	2.42	0.47
1:AU:152:LEU:HD21	2:AX:105:SER:HA	1.96	0.47
1:BC:55:ALA:HB2	2:BO:51:VAL:HB	1.96	0.47
1:BK:85:GLN:HE22	1:BM:289:SER:HB2	1.79	0.47
2:BW:23:LYS:NZ	2:BW:100:ASP:OD1	2.44	0.47
2:CH:125:LYS:NZ	2:CH:169:ASP:OD1	2.40	0.47
1:CN:22:ASP:OD1	4:CT:213:ARG:NE	2.41	0.47
1:CW:8:TYR:CD2	1:CW:93:GLN:HG3	2.50	0.47
1:CV:239:LYS:HA	1:CV:242:ASN:OD1	2.15	0.47
1:AB:239:LYS:HA	1:AB:242:ASN:OD1	2.14	0.47
1:BK:50:ASP:OD1	1:BK:51:ALA:N	2.47	0.47
1:BM:41:MET:HE2	1:BM:83:LYS:H	1.79	0.47
1:CE:286:ASP:HB2	1:CE:294:HIS:HB2	1.96	0.47
1:AS:132:HIS:HA	1:AS:254:LEU:HD13	1.97	0.47
1:AT:101:SER:OG	1:AT:102:ASP:N	2.48	0.47
1:BC:239:LYS:HA	1:BC:242:ASN:OD1	2.13	0.47
1:BM:49:TRP:CZ3	1:BM:74:SER:HB3	2.49	0.47
2:BN:167:THR:HB	2:BN:170:LEU:HB3	1.95	0.47
1:CL:133:PHE:CD2	1:CL:301:LEU:HD22	2.49	0.47
2:CP:138:ASN:HD22	2:CP:153:LYS:HG2	1.80	0.47
1:BU:239:LYS:HA	1:BU:242:ASN:OD1	2.15	0.47
2:CF:23:LYS:HG3	2:CF:24:ASN:H	1.80	0.47
2:CG:137:LEU:HD11	2:CG:159:ALA:HB2	1.97	0.47
1:CN:34:ILE:HA	1:CN:271:PHE:O	2.15	0.47
1:CV:96:GLU:O	1:CV:100:THR:HG23	2.15	0.47
1:CW:196:GLU:HB3	1:CW:265:ASN:HD22	1.79	0.47
1:AL:13:VAL:HG11	1:AL:281:PRO:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AO:138:ASN:HD22	2:AO:153:LYS:HE2	1.80	0.47
1:AT:174:LYS:O	1:AT:212:LYS:NZ	2.48	0.47
1:BB:16:ILE:HD11	1:BB:120:LYS:HE3	1.97	0.47
1:BC:49:TRP:CE3	1:BC:74:SER:HB3	2.49	0.47
1:BK:286:ASP:HB2	1:BK:294:HIS:HB2	1.96	0.47
2:BO:56:LYS:HD2	3:BP:56:PHE:HA	1.96	0.47
1:CD:239:LYS:HA	1:CD:242:ASN:OD1	2.15	0.47
1:CW:80:ASN:ND2	1:CW:153:PRO:O	2.32	0.47
1:AC:49:TRP:CZ3	1:AC:74:SER:HB3	2.49	0.47
1:AJ:13:VAL:HG11	1:AJ:281:PRO:HG2	1.97	0.47
5:AM:171:ARG:HG2	5:AM:190:ILE:HG22	1.96	0.47
2:CP:76:SER:HB3	2:CP:87:GLU:HG2	1.96	0.47
4:CT:200:THR:O	4:CT:204:GLN:HG2	2.16	0.46
1:AB:41:MET:HE2	1:AB:83:LYS:H	1.80	0.46
1:AK:159:LEU:HD12	1:AK:260:LEU:HD13	1.97	0.46
5:AM:102:THR:HA	2:AO:56:LYS:HB3	1.96	0.46
3:AV:142:ILE:HD11	3:AV:152:VAL:HG13	1.96	0.46
2:AX:123:LEU:HD21	2:AX:131:VAL:HG21	1.97	0.46
1:BC:226:SER:OG	1:CL:226:SER:O	2.29	0.46
1:BD:143:LYS:HE3	2:BF:40:ASP:HB2	1.98	0.46
3:BE:137:VAL:HG12	3:BE:138:LYS:HG3	1.96	0.46
1:CE:80:ASN:ND2	1:CE:153:PRO:O	2.35	0.46
1:CE:132:HIS:HA	1:CE:254:LEU:HD13	1.96	0.46
1:AB:169:VAL:HG22	1:AB:183:LYS:HG3	1.97	0.46
1:AC:85:GLN:NE2	1:AC:298:ASP:OD1	2.43	0.46
3:BP:127:TYR:CE1	3:BP:180:LYS:HB2	2.51	0.46
1:BT:80:ASN:ND2	1:BT:153:PRO:O	2.48	0.46
1:CC:174:LYS:O	1:CC:212:LYS:NZ	2.49	0.46
2:BG:75:LEU:HD22	2:BG:84:LEU:HD13	1.96	0.46
1:BM:57:PRO:HB2	1:CC:84:LEU:HB3	1.96	0.46
3:BY:22:MET:HB3	3:BY:23:LYS:H	1.55	0.46
1:CD:35:GLU:O	1:CD:272:LYS:HA	2.15	0.46
3:CO:64:PHE:CZ	3:CO:108:ILE:HD11	2.51	0.46
2:CP:75:LEU:HD22	2:CP:84:LEU:HD13	1.97	0.46
1:CV:89:ARG:HH21	1:CV:112:LEU:HD21	1.81	0.46
1:AC:55:ALA:O	1:AK:86:TYR:OH	2.26	0.46
1:BB:286:ASP:HB2	1:BB:294:HIS:HB2	1.97	0.46
2:BF:23:LYS:N	2:BF:67:TYR:OH	2.48	0.46
1:BL:178:ASP:OD1	1:BL:178:ASP:N	2.48	0.46
2:BW:23:LYS:HE3	2:BW:23:LYS:HB2	1.81	0.46
4:CA:200:THR:O	4:CA:204:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CG:23:LYS:N	2:CG:67:TYR:OH	2.49	0.46
3:CO:137:VAL:HG12	3:CO:138:LYS:HG3	1.98	0.46
1:AT:158:LEU:HB3	1:AT:260:LEU:HD21	1.97	0.46
1:BC:35:GLU:O	1:BC:272:LYS:HA	2.15	0.46
1:BC:96:GLU:O	1:BC:100:THR:HG23	2.16	0.46
3:BY:44:GLU:OE1	3:BY:45:PHE:N	2.48	0.46
1:CN:79:LEU:HD11	1:CN:305:LEU:HB2	1.97	0.46
3:AF:93:VAL:HG21	3:AF:117:ILE:HD11	1.96	0.46
1:BC:256:LYS:O	1:BC:258:LYS:HG2	2.16	0.46
1:BT:112:LEU:HD21	1:BT:292:VAL:HG22	1.97	0.46
1:BU:169:VAL:HG22	1:BU:183:LYS:HG3	1.96	0.46
1:CV:132:HIS:HA	1:CV:254:LEU:HD13	1.97	0.46
1:BC:218:ALA:HA	1:BC:224:ALA:HA	1.96	0.46
3:BE:35:SER:HB2	3:BE:41:LYS:HE3	1.97	0.46
1:BK:19:GLU:HA	1:BK:120:LYS:HD3	1.98	0.46
2:BW:137:LEU:HD11	2:BW:159:ALA:HB2	1.98	0.46
1:CC:158:LEU:HB3	1:CC:260:LEU:HD21	1.97	0.46
1:CE:81:TYR:OH	1:CE:272:LYS:O	2.28	0.46
1:AK:96:GLU:O	1:AK:100:THR:HG23	2.16	0.46
1:BB:96:GLU:O	1:BB:100:THR:HG23	2.16	0.46
1:BK:214:VAL:HG11	1:BT:240:ALA:HB2	1.97	0.46
1:BT:135:LEU:HD23	1:BT:254:LEU:HB2	1.97	0.46
1:BT:286:ASP:HB2	1:BT:294:HIS:HB2	1.97	0.46
4:BZ:187:ALA:O	4:BZ:208:ASN:ND2	2.43	0.46
1:CV:210:SER:O	1:CV:214:VAL:HG13	2.16	0.46
1:AL:205:VAL:HG12	1:AL:259:ILE:HG23	1.97	0.45
5:AM:171:ARG:HB3	5:AM:188:VAL:HG11	1.98	0.45
3:AN:166:LEU:HD12	3:AN:180:LYS:HG2	1.99	0.45
3:AV:186:ASN:HD21	2:AX:180:ASN:HB2	1.81	0.45
1:BB:84:LEU:HB3	1:BK:57:PRO:HB2	1.98	0.45
1:BC:164:GLN:OE1	1:BC:311:ILE:N	2.48	0.45
3:BE:77:ILE:HG12	3:BE:91:PRO:HB3	1.97	0.45
2:BF:22:MET:HB2	2:BF:25:PRO:HG3	1.97	0.45
2:BG:32:LEU:HB2	1:CL:307:THR:HG22	1.98	0.45
1:BL:305:LEU:HD11	2:BX:32:LEU:HG	1.97	0.45
1:CC:49:TRP:CZ3	1:CC:74:SER:HB3	2.51	0.45
1:CU:239:LYS:HA	1:CU:242:ASN:OD1	2.15	0.45
1:AU:257:HIS:CD2	1:AU:318:GLN:HG3	2.51	0.45
1:CE:79:LEU:HD11	1:CE:305:LEU:HB2	1.98	0.45
2:CP:167:THR:HG22	2:CP:168:GLU:N	2.30	0.45
1:BB:132:HIS:HA	1:BB:254:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:196:GLU:HB3	1:BK:265:ASN:ND2	2.31	0.45
1:CE:86:TYR:HE1	1:CW:57:PRO:HA	1.81	0.45
3:CO:37:GLU:HG3	3:CO:39:ARG:H	1.81	0.45
2:CQ:167:THR:HG22	2:CQ:168:GLU:N	2.31	0.45
1:CV:13:VAL:HG11	1:CV:281:PRO:HG2	1.97	0.45
1:AC:41:MET:HE2	1:AC:83:LYS:H	1.80	0.45
1:AU:174:LYS:O	1:AU:212:LYS:NZ	2.48	0.45
3:AV:35:SER:HB2	3:AV:41:LYS:HE3	1.99	0.45
4:CI:200:THR:O	4:CI:204:GLN:HG2	2.17	0.45
1:CV:164:GLN:HE22	1:CV:308:ARG:HA	1.81	0.45
1:AJ:49:TRP:CZ3	1:AJ:74:SER:HB3	2.51	0.45
1:AS:196:GLU:HB3	1:AS:265:ASN:ND2	2.31	0.45
2:BX:23:LYS:HA	2:BX:45:PHE:HD2	1.80	0.45
1:CC:16:ILE:HD12	1:CC:116:ALA:HB1	1.98	0.45
2:CH:77:PHE:CE1	2:CH:84:LEU:HD13	2.51	0.45
1:CM:260:LEU:HD23	1:CM:313:GLN:HG2	1.98	0.45
3:CO:159:ALA:HB3	3:CO:187:LYS:HD2	1.98	0.45
5:AM:180:ILE:HG12	5:AM:203:TYR:CE1	2.52	0.45
1:CM:203:VAL:HA	1:CM:260:LEU:O	2.17	0.45
1:AT:174:LYS:HE2	1:AT:318:GLN:HE21	1.81	0.45
1:BK:253:ASN:ND2	1:BT:195:ASP:OD1	2.41	0.45
3:BY:62:HIS:HE2	3:BY:75:ARG:HH21	1.63	0.45
1:CD:164:GLN:HE22	1:CD:308:ARG:HA	1.81	0.45
1:CD:169:VAL:HG22	1:CD:183:LYS:HG3	1.98	0.45
1:CE:203:VAL:HA	1:CE:260:LEU:O	2.16	0.45
1:CE:239:LYS:HA	1:CE:242:ASN:OD1	2.17	0.45
1:CW:13:VAL:HG11	1:CW:281:PRO:HG2	1.99	0.45
1:AC:205:VAL:HG12	1:AC:259:ILE:HG23	1.97	0.45
3:AF:141:LEU:HD11	3:AF:165:ALA:HB2	1.99	0.45
1:AT:307:THR:O	1:AT:310:THR:OG1	2.31	0.45
1:BD:257:HIS:CE1	1:BD:318:GLN:HG3	2.52	0.45
1:BM:196:GLU:HB3	1:BM:265:ASN:HD22	1.82	0.45
1:BT:163:GLU:HB3	1:BT:308:ARG:HG3	1.99	0.45
1:BV:169:VAL:HG22	1:BV:183:LYS:HG3	1.99	0.45
2:CF:11:PHE:O	2:CF:15:VAL:HG23	2.17	0.45
4:CR:200:THR:O	4:CR:204:GLN:HG2	2.17	0.45
1:BK:135:LEU:HD23	1:BK:254:LEU:HB2	1.98	0.45
1:BV:178:ASP:OD1	1:BV:179:LYS:N	2.50	0.45
3:CO:128:LEU:HD13	3:CO:143:PHE:HZ	1.81	0.45
1:AB:35:GLU:O	1:AB:272:LYS:HA	2.17	0.45
1:AJ:132:HIS:HA	1:AJ:254:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:49:TRP:CH2	1:AU:74:SER:HB3	2.51	0.45
1:BT:169:VAL:HG22	1:BT:183:LYS:HG3	1.99	0.45
2:CQ:156:ASN:ND2	2:CQ:180:ASN:O	2.50	0.45
1:AJ:240:ALA:HB2	1:BT:214:VAL:HG11	1.99	0.44
1:BC:164:GLN:HE22	1:BC:308:ARG:HA	1.81	0.44
1:BC:286:ASP:HB2	1:BC:294:HIS:HB2	1.98	0.44
1:BL:35:GLU:O	1:BL:272:LYS:HA	2.17	0.44
1:BU:47:VAL:HG22	1:BU:76:VAL:HG22	1.99	0.44
2:CF:59:ILE:H	1:CW:65:ASN:HB2	1.81	0.44
1:BM:35:GLU:O	1:BM:272:LYS:HA	2.17	0.44
2:BN:23:LYS:N	2:BN:67:TYR:OH	2.50	0.44
2:BX:140:ASN:OD1	2:BX:144:GLU:N	2.50	0.44
1:CC:8:TYR:CD2	1:CC:93:GLN:HG3	2.52	0.44
1:CD:196:GLU:HB3	1:CD:265:ASN:ND2	2.32	0.44
1:CE:35:GLU:O	1:CE:272:LYS:HA	2.17	0.44
1:CU:84:LEU:HD13	1:CV:57:PRO:HB2	1.99	0.44
1:AC:240:ALA:HB2	1:AK:214:VAL:HG11	2.00	0.44
4:AI:200:THR:O	4:AI:204:GLN:HG2	2.17	0.44
1:AU:96:GLU:O	1:AU:100:THR:HG23	2.17	0.44
1:BB:165:ILE:HD12	1:BB:165:ILE:H	1.82	0.44
3:BE:51:THR:HG23	3:BE:126:GLY:HA2	1.98	0.44
2:BG:155:VAL:HA	2:BG:180:ASN:HA	1.99	0.44
1:BT:35:GLU:O	1:BT:272:LYS:HA	2.18	0.44
2:BX:23:LYS:HB3	2:BX:67:TYR:OH	2.16	0.44
1:CC:35:GLU:O	1:CC:272:LYS:HA	2.17	0.44
1:CD:150:ARG:HH21	2:CG:63:PRO:HB3	1.82	0.44
2:CP:61:ASN:ND2	1:CU:59:THR:O	2.50	0.44
1:CV:49:TRP:CZ3	1:CV:74:SER:HB3	2.52	0.44
1:AK:164:GLN:HB3	1:AK:311:ILE:O	2.17	0.44
1:BT:80:ASN:HB2	1:BT:155:MET:HG3	2.00	0.44
1:BU:49:TRP:CE3	1:BU:74:SER:HB3	2.52	0.44
1:CL:196:GLU:HB3	1:CL:265:ASN:HD22	1.83	0.44
1:AB:165:ILE:HD13	1:AB:191:LEU:HD23	1.98	0.44
1:AU:143:LYS:HA	2:AW:39:ARG:HE	1.83	0.44
1:BD:174:LYS:O	1:BD:212:LYS:NZ	2.51	0.44
1:CD:135:LEU:HD21	1:CD:255:LEU:HG	1.99	0.44
1:CE:214:VAL:HG11	1:CW:240:ALA:HB2	2.00	0.44
5:AM:104:LYS:H	5:AM:162:ASN:ND2	2.15	0.44
1:AS:35:GLU:O	1:AS:272:LYS:HA	2.17	0.44
1:BB:20:VAL:O	4:BH:213:ARG:NH2	2.29	0.44
1:BU:229:LYS:O	1:BU:233:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CG:133:PRO:HG3	2:CG:161:SER:HA	1.99	0.44
1:CU:35:GLU:O	1:CU:272:LYS:HA	2.17	0.44
1:CU:81:TYR:OH	1:CU:272:LYS:O	2.27	0.44
1:AL:174:LYS:O	1:AL:212:LYS:NZ	2.51	0.44
3:AN:138:LYS:HG3	2:AO:77:PHE:HD2	1.82	0.44
2:AW:123:LEU:HD13	2:AW:173:VAL:HG11	2.00	0.44
2:AW:136:LYS:HD3	2:AW:155:VAL:HG21	1.99	0.44
1:BD:96:GLU:O	1:BD:100:THR:HG23	2.18	0.44
3:BE:173:SER:HB3	3:BE:176:VAL:HB	2.00	0.44
1:BK:35:GLU:O	1:BK:272:LYS:HA	2.17	0.44
2:BN:13:LYS:O	2:BN:17:GLU:HG3	2.16	0.44
1:BV:19:GLU:HA	1:BV:120:LYS:HD3	1.99	0.44
1:BV:35:GLU:O	1:BV:272:LYS:HA	2.18	0.44
1:CD:49:TRP:CZ3	1:CD:74:SER:HB3	2.53	0.44
1:CM:49:TRP:CZ3	1:CM:74:SER:HB3	2.52	0.44
2:AD:123:LEU:HD21	2:AD:131:VAL:HG21	2.00	0.44
4:AY:200:THR:O	4:AY:204:GLN:HG2	2.18	0.44
2:BN:167:THR:HG22	2:BN:168:GLU:N	2.33	0.44
1:CC:41:MET:HG2	2:CH:104:PHE:HE2	1.82	0.44
2:CH:71:ARG:NH1	2:CH:142:HIS:O	2.50	0.44
2:AW:167:THR:HG22	2:AW:168:GLU:H	1.82	0.44
1:CD:150:ARG:HE	2:CG:63:PRO:HB3	1.82	0.44
2:BF:125:LYS:HD2	2:BF:169:ASP:HA	2.00	0.43
1:BK:132:HIS:HA	1:BK:254:LEU:HD13	2.00	0.43
1:BV:49:TRP:CZ3	1:BV:74:SER:HB3	2.53	0.43
2:CQ:74:LYS:HE2	2:CQ:89:GLY:HA3	1.99	0.43
1:CU:29:PHE:O	4:CX:223:ARG:NH2	2.51	0.43
1:CU:205:VAL:HG12	1:CU:259:ILE:HG23	2.00	0.43
1:BD:70:ILE:HD11	1:CM:86:TYR:CD2	2.52	0.43
4:BJ:200:THR:O	4:BJ:204:GLN:HG2	2.18	0.43
1:BU:96:GLU:O	1:BU:100:THR:HG23	2.17	0.43
1:CD:196:GLU:HB3	1:CD:265:ASN:HD22	1.83	0.43
2:CH:32:LEU:HB2	1:CW:307:THR:HG22	2.00	0.43
1:CL:174:LYS:O	1:CL:212:LYS:NZ	2.50	0.43
1:CN:174:LYS:O	1:CN:212:LYS:NZ	2.51	0.43
1:BT:112:LEU:HD12	1:BT:112:LEU:HA	1.90	0.43
1:CC:96:GLU:O	1:CC:100:THR:HG23	2.19	0.43
1:CC:197:PHE:HD2	1:CC:243:ASN:HB2	1.83	0.43
1:CN:96:GLU:O	1:CN:100:THR:HG23	2.18	0.43
1:AT:240:ALA:HB2	1:BD:214:VAL:HG11	2.00	0.43
1:AU:107:ASP:HB3	1:AU:112:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:165:ILE:HD11	1:BK:191:LEU:HA	2.00	0.43
1:BL:164:GLN:HB3	1:BL:311:ILE:O	2.18	0.43
1:CU:126:ILE:O	1:CU:130:ILE:HG13	2.18	0.43
1:CU:214:VAL:HG11	1:CV:240:ALA:HB2	2.00	0.43
1:CW:91:LEU:HG	1:CW:112:LEU:HB3	2.00	0.43
1:BK:112:LEU:HD12	1:BK:112:LEU:HA	1.87	0.43
1:BM:96:GLU:O	1:BM:100:THR:HG23	2.18	0.43
2:BN:181:ARG:HG2	2:BN:182:ALA:H	1.82	0.43
2:CG:167:THR:HB	2:CG:170:LEU:HB3	1.99	0.43
2:CQ:123:LEU:HD13	2:CQ:173:VAL:HG11	2.00	0.43
4:CZ:200:THR:O	4:CZ:204:GLN:HG2	2.19	0.43
1:AS:49:TRP:CZ3	1:AS:74:SER:HB3	2.54	0.43
1:AS:84:LEU:HB3	1:BB:57:PRO:HB2	1.99	0.43
1:AT:16:ILE:HD12	1:AT:116:ALA:HB1	2.01	0.43
2:BF:125:LYS:HG3	2:BF:171:PHE:CE1	2.53	0.43
2:BN:65:LYS:HB2	2:BN:85:GLU:CD	2.39	0.43
1:BV:205:VAL:HG12	1:BV:259:ILE:HG23	2.01	0.43
1:CC:169:VAL:HG22	1:CC:183:LYS:HG3	2.01	0.43
1:CC:203:VAL:HG22	1:CC:261:ILE:HG23	2.00	0.43
1:CC:282:ASN:OD1	1:CC:283:GLU:N	2.52	0.43
1:CE:39:LEU:O	1:CE:274:SER:OG	2.23	0.43
3:CO:78:GLN:HB2	3:CO:88:HIS:CE1	2.53	0.43
1:AB:81:TYR:OH	1:AB:272:LYS:O	2.24	0.43
3:AN:141:LEU:HD11	3:AN:165:ALA:HB2	2.00	0.43
1:AS:8:TYR:CG	1:AS:93:GLN:HG3	2.54	0.43
1:CM:96:GLU:O	1:CM:100:THR:HG23	2.19	0.43
1:BB:13:VAL:HG11	1:BB:281:PRO:HG2	1.99	0.43
1:BB:35:GLU:O	1:BB:272:LYS:HA	2.18	0.43
4:BS:211:LYS:O	4:BS:214:ARG:HG2	2.18	0.43
1:CW:282:ASN:HB3	1:CW:296:TYR:HB2	2.01	0.43
3:AN:36:ASN:HB3	1:BU:195:ASP:HB2	2.00	0.43
1:BB:196:GLU:HB3	1:BB:265:ASN:ND2	2.33	0.43
3:BE:142:ILE:HG13	3:BE:152:VAL:HG22	2.01	0.43
1:BL:49:TRP:CZ3	1:BV:113:LEU:HD11	2.53	0.43
1:CU:178:ASP:N	1:CU:178:ASP:OD1	2.52	0.43
1:BB:101:SER:OG	1:BB:102:ASP:N	2.52	0.43
1:BC:77:VAL:HG11	1:BC:305:LEU:HD13	2.00	0.43
3:BE:32:LEU:HB2	1:BK:307:THR:HG22	2.00	0.43
1:BM:60:ILE:HG23	1:CE:290:THR:HG22	2.00	0.43
1:BT:16:ILE:HD11	1:BT:120:LYS:HE3	2.01	0.43
1:CE:159:LEU:HD12	1:CE:260:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CU:196:GLU:HB3	1:CU:265:ASN:HD22	1.84	0.43
5:AM:172:ASN:HB3	5:AM:175:ILE:HD11	2.01	0.42
1:AS:85:GLN:HE22	1:AU:289:SER:HB2	1.83	0.42
1:AT:96:GLU:O	1:AT:100:THR:HG23	2.19	0.42
2:AW:133:PRO:HG3	2:AW:161:SER:HA	2.01	0.42
1:CC:80:ASN:ND2	1:CC:153:PRO:O	2.52	0.42
1:AJ:163:GLU:HB2	2:BW:31:LEU:HD22	2.00	0.42
1:AL:196:GLU:HB3	1:AL:265:ASN:ND2	2.34	0.42
5:AM:77:PHE:CE2	1:AS:305:LEU:HD21	2.54	0.42
1:AU:278:LEU:HD23	1:AU:278:LEU:HA	1.87	0.42
1:BL:143:LYS:HE3	3:BP:37:GLU:HG2	2.01	0.42
1:CC:43:TYR:HE2	1:CC:45:LYS:HE2	1.84	0.42
2:CF:156:ASN:ND2	2:CF:180:ASN:O	2.52	0.42
2:CH:125:LYS:HD2	2:CH:169:ASP:HA	2.01	0.42
1:AB:8:TYR:CD2	1:AB:93:GLN:HG3	2.55	0.42
3:AF:33:SER:HA	1:AL:308:ARG:HG3	2.02	0.42
3:AF:166:LEU:HD11	3:AF:182:ALA:HB2	2.01	0.42
1:BB:186:ALA:O	1:BB:190:LYS:HG3	2.20	0.42
1:BC:57:PRO:HB2	1:BM:84:LEU:HB3	2.01	0.42
3:BE:56:PHE:HD1	2:BG:56:LYS:HD2	1.84	0.42
1:BL:49:TRP:CZ3	1:BL:74:SER:HB3	2.54	0.42
1:BU:35:GLU:O	1:BU:272:LYS:HA	2.19	0.42
1:CE:28:TRP:O	1:CE:262:TYR:OH	2.28	0.42
1:CL:169:VAL:HG22	1:CL:183:LYS:HG3	2.00	0.42
3:BY:141:LEU:HB3	3:BY:149:LEU:HD22	2.01	0.42
1:AB:214:VAL:HG11	1:AL:240:ALA:HB2	2.02	0.42
1:AC:163:GLU:HB2	2:AO:31:LEU:HD13	2.01	0.42
1:AK:59:THR:O	2:AX:61:ASN:ND2	2.52	0.42
1:BL:96:GLU:O	1:BL:100:THR:HG23	2.18	0.42
3:BP:32:LEU:HD23	1:CD:77:VAL:HG21	2.01	0.42
1:BT:196:GLU:HB3	1:BT:265:ASN:ND2	2.34	0.42
2:BX:23:LYS:HA	2:BX:45:PHE:CD2	2.54	0.42
1:CL:16:ILE:HD12	1:CL:116:ALA:HB1	2.01	0.42
1:CL:214:VAL:HG11	1:CU:240:ALA:HB2	2.00	0.42
2:CQ:156:ASN:HB3	2:CQ:178:PHE:CE2	2.54	0.42
1:AL:211:LEU:HD23	1:AL:211:LEU:HA	1.89	0.42
1:BD:217:TYR:O	1:BD:225:SER:N	2.38	0.42
2:BO:140:ASN:OD1	2:BO:144:GLU:N	2.47	0.42
1:CM:231:GLU:O	1:CM:235:ILE:HG13	2.20	0.42
3:CO:186:ASN:ND2	2:CQ:180:ASN:O	2.39	0.42
1:AC:152:LEU:HD21	3:AF:112:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AM:184:ASN:HB3	5:AM:190:ILE:HD13	2.02	0.42
1:BD:78:ARG:HH21	2:BG:104:PHE:HE1	1.67	0.42
1:BD:87:LYS:HG3	1:BD:296:TYR:CE2	2.54	0.42
2:BF:181:ARG:HH22	2:BG:94:LEU:HB3	1.83	0.42
1:BK:214:VAL:HG21	1:BT:240:ALA:HB2	2.02	0.42
1:BM:77:VAL:HG21	2:CG:32:LEU:HD23	2.01	0.42
1:BM:176:LYS:HB3	1:BM:178:ASP:OD1	2.19	0.42
1:BV:180:ILE:O	1:BV:184:ILE:HG13	2.19	0.42
1:CC:79:LEU:HD11	1:CC:305:LEU:HB2	2.01	0.42
2:CH:52:CYS:HB3	1:CW:66:THR:HG22	2.00	0.42
1:CU:211:LEU:HD23	1:CU:211:LEU:HA	1.91	0.42
1:AC:66:THR:HG22	2:AO:52:CYS:SG	2.59	0.42
1:AK:181:PHE:CZ	1:AK:234:LEU:HB2	2.55	0.42
1:BD:196:GLU:HB3	1:BD:265:ASN:ND2	2.35	0.42
1:BK:77:VAL:HG11	1:BK:305:LEU:HD11	2.02	0.42
1:BL:107:ASP:OD2	1:BL:110:ASN:ND2	2.52	0.42
1:CE:16:ILE:HD11	1:CE:120:LYS:HE3	2.02	0.42
1:CL:96:GLU:O	1:CL:100:THR:HG23	2.19	0.42
3:CO:121:THR:O	2:CP:114:THR:HB	2.19	0.42
3:AN:52:ARG:HB3	1:BU:66:THR:HG22	2.02	0.42
2:AX:167:THR:HG22	2:AX:168:GLU:H	1.85	0.42
1:BL:66:THR:HG22	2:BX:52:CYS:HB3	2.02	0.42
2:BN:127:GLY:O	2:BN:131:VAL:HG23	2.20	0.42
2:CF:137:LEU:HD11	2:CF:159:ALA:HB2	2.02	0.42
1:CL:35:GLU:O	1:CL:272:LYS:HA	2.19	0.42
1:CM:49:TRP:CE3	1:CM:74:SER:HB3	2.55	0.42
3:CO:133:SER:HB3	3:CO:177:TYR:CE1	2.55	0.42
1:AB:49:TRP:CZ3	1:AB:74:SER:HB3	2.55	0.42
1:BC:132:HIS:HA	1:BC:254:LEU:HD13	2.01	0.42
1:CU:174:LYS:HE2	1:CU:318:GLN:HE21	1.85	0.42
1:CV:7:ASN:HB3	1:CV:10:ALA:HB3	2.02	0.42
1:AB:96:GLU:O	1:AB:100:THR:HG23	2.19	0.41
1:AJ:241:ILE:HG22	1:BT:211:LEU:HD21	2.02	0.41
2:BF:113:ILE:HD12	2:BF:113:ILE:HA	1.91	0.41
1:BU:49:TRP:CZ3	1:BU:74:SER:HB3	2.55	0.41
1:CL:203:VAL:HG13	1:CL:261:ILE:HG12	2.02	0.41
1:AJ:59:THR:HG1	1:BT:149:LYS:HZ1	1.59	0.41
1:AK:240:ALA:HB2	1:AU:214:VAL:HG11	2.02	0.41
1:AK:255:LEU:HD23	1:AK:255:LEU:HA	1.94	0.41
1:AS:143:LYS:HE2	3:AV:37:GLU:HG2	2.01	0.41
1:AT:65:ASN:ND2	2:BG:57:ASP:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:80:ASN:ND2	1:AT:153:PRO:O	2.53	0.41
1:BC:244:ARG:NH1	1:BM:210:SER:OG	2.52	0.41
1:BM:126:ILE:O	1:BM:130:ILE:HG13	2.20	0.41
1:CD:96:GLU:O	1:CD:100:THR:HG23	2.21	0.41
1:CD:282:ASN:OD1	1:CD:283:GLU:N	2.53	0.41
1:AB:181:PHE:CZ	1:AB:234:LEU:HB2	2.55	0.41
4:AH:200:THR:O	4:AH:204:GLN:HG2	2.20	0.41
1:AL:178:ASP:OD1	1:AL:178:ASP:N	2.53	0.41
2:AX:31:LEU:HB3	2:AX:34:ASN:HD21	1.86	0.41
1:BD:286:ASP:HB2	1:BD:294:HIS:HB2	2.02	0.41
1:BK:7:ASN:ND2	1:BV:7:ASN:HB2	2.35	0.41
1:BK:15:ASN:HD22	1:BK:105:ILE:HG13	1.86	0.41
1:BL:158:LEU:HB3	1:BL:260:LEU:HD21	2.01	0.41
2:BX:133:PRO:HG3	2:BX:161:SER:HA	2.01	0.41
1:CE:13:VAL:HG11	1:CE:281:PRO:HG2	2.01	0.41
1:CL:188:LEU:HD23	1:CL:191:LEU:HD12	2.01	0.41
1:CN:92:LYS:NZ	1:CN:94:THR:OG1	2.49	0.41
5:AM:100:SER:HB2	1:AS:66:THR:HA	2.01	0.41
5:AM:140:ASP:OD1	5:AM:140:ASP:N	2.53	0.41
1:AT:129:LEU:HD11	1:AT:139:VAL:HG13	2.02	0.41
1:BM:135:LEU:HD21	1:BM:255:LEU:HG	2.01	0.41
1:CC:97:LYS:HB3	1:CC:97:LYS:HE2	1.86	0.41
1:AC:169:VAL:HG22	1:AC:183:LYS:HG3	2.02	0.41
1:AK:35:GLU:O	1:AK:272:LYS:HA	2.20	0.41
1:AL:43:TYR:HA	1:AL:79:LEU:O	2.21	0.41
1:AC:62:ASN:HB2	5:AM:156:TYR:CZ	2.56	0.41
1:AJ:87:LYS:HD3	1:AJ:296:TYR:CE2	2.55	0.41
2:AO:167:THR:HG22	2:AO:168:GLU:N	2.35	0.41
1:AT:35:GLU:O	1:AT:272:LYS:HA	2.19	0.41
1:BB:92:LYS:NZ	1:BB:95:SER:OG	2.43	0.41
3:BE:37:GLU:O	3:BE:41:LYS:HD2	2.21	0.41
1:BU:108:ILE:H	1:BU:108:ILE:HD12	1.86	0.41
2:BW:76:SER:HB3	2:BW:87:GLU:HG2	2.03	0.41
1:CD:211:LEU:HD23	1:CD:211:LEU:HA	1.90	0.41
1:CN:80:ASN:ND2	1:CN:153:PRO:O	2.53	0.41
1:AC:91:LEU:HD21	1:AC:112:LEU:HD13	2.03	0.41
1:AL:286:ASP:HB2	1:AL:294:HIS:HB2	2.03	0.41
1:AU:159:LEU:HD11	1:AU:258:LYS:HD3	2.02	0.41
1:AU:253:ASN:N	1:AU:253:ASN:OD1	2.54	0.41
2:BN:181:ARG:HG2	2:BN:182:ALA:N	2.35	0.41
3:BP:46:PHE:CE1	1:CD:73:SER:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BU:286:ASP:HB2	1:BU:294:HIS:HB2	2.01	0.41
1:CD:211:LEU:O	1:CD:214:VAL:HG22	2.21	0.41
1:AJ:96:GLU:O	1:AJ:100:THR:HG23	2.20	0.41
1:AS:96:GLU:O	1:AS:100:THR:HG23	2.21	0.41
2:BG:167:THR:HG22	2:BG:168:GLU:H	1.86	0.41
2:BN:137:LEU:HD11	2:BN:159:ALA:HB2	2.03	0.41
2:CG:180:ASN:O	2:CH:180:ASN:ND2	2.53	0.41
1:CN:85:GLN:NE2	1:CN:298:ASP:OD1	2.52	0.41
1:CU:49:TRP:CZ3	1:CU:74:SER:HB3	2.55	0.41
1:CW:137:GLY:HA3	1:CW:160:ASN:OD1	2.20	0.41
1:AB:36:ASP:CG	4:AH:214:ARG:HH22	2.24	0.41
1:AB:166:LYS:HB3	1:AB:166:LYS:HE2	1.88	0.41
3:AN:28:ASP:OD2	1:BU:78:ARG:HB3	2.21	0.41
2:AO:76:SER:HB3	2:AO:87:GLU:HG2	2.03	0.41
2:BN:14:LYS:O	2:BN:18:ILE:HG13	2.21	0.41
2:BN:23:LYS:HE3	2:BN:23:LYS:HB2	1.87	0.41
1:BV:150:ARG:HH12	3:BY:65:LEU:HG	1.86	0.41
1:BV:176:LYS:HB3	1:BV:178:ASP:OD1	2.21	0.41
3:BY:162:ASN:HB3	3:BY:184:PHE:CZ	2.55	0.41
4:BZ:200:THR:O	4:BZ:204:GLN:HG2	2.20	0.41
1:CE:178:ASP:N	1:CE:178:ASP:OD1	2.53	0.41
1:CU:135:LEU:HD21	1:CU:255:LEU:HG	2.02	0.41
1:CV:256:LYS:HE3	1:CV:256:LYS:HB2	1.81	0.41
1:AB:119:TYR:CE1	1:AB:281:PRO:HG3	2.56	0.41
1:AC:35:GLU:O	1:AC:272:LYS:HA	2.21	0.41
1:AS:13:VAL:HG11	1:AS:281:PRO:HG2	2.03	0.41
1:AU:178:ASP:OD1	1:AU:179:LYS:N	2.54	0.41
1:BT:13:VAL:HG11	1:BT:281:PRO:HG2	2.03	0.41
2:BX:57:ASP:HA	2:BX:115:ASN:HD21	1.85	0.41
2:CP:156:ASN:HB3	2:CP:178:PHE:CE2	2.56	0.41
2:CQ:23:LYS:HG3	2:CQ:24:ASN:N	2.36	0.41
1:CU:169:VAL:HG22	1:CU:183:LYS:HG3	2.01	0.41
4:CZ:198:ASN:OD1	4:CZ:201:GLU:HG3	2.21	0.41
2:AO:167:THR:HG22	2:AO:168:GLU:H	1.86	0.40
1:AU:196:GLU:HB3	1:AU:265:ASN:HD22	1.85	0.40
1:AU:255:LEU:HD23	1:AU:255:LEU:HA	1.94	0.40
2:AX:165:LYS:HE3	2:AX:168:GLU:HA	2.03	0.40
1:BB:28:TRP:CZ3	1:BB:135:LEU:HB2	2.56	0.40
2:BG:51:VAL:HG12	1:CL:54:ASN:HB3	2.03	0.40
1:CC:41:MET:HE2	1:CC:41:MET:HB2	1.94	0.40
1:CL:84:LEU:HD22	1:CL:149:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CL:308:ARG:H	1:CL:308:ARG:HG2	1.75	0.40
1:CW:84:LEU:HD22	1:CW:149:LYS:HE3	2.03	0.40
1:AK:24:ILE:HG12	1:AK:131:ASN:ND2	2.36	0.40
1:AS:169:VAL:HG22	1:AS:183:LYS:HG3	2.03	0.40
2:BX:123:LEU:HD12	2:BX:145:LEU:O	2.22	0.40
2:BX:165:LYS:HE3	2:BX:168:GLU:HA	2.03	0.40
4:CB:215:ILE:O	4:CB:219:GLU:HG3	2.22	0.40
2:CH:167:THR:HG22	2:CH:168:GLU:N	2.36	0.40
1:CL:196:GLU:OE1	1:CL:265:ASN:ND2	2.53	0.40
1:AU:216:PRO:HB2	1:AU:224:ALA:HB1	2.03	0.40
2:AX:31:LEU:HB3	2:AX:34:ASN:ND2	2.37	0.40
1:BL:9:TYR:CE1	1:BL:90:HIS:HE1	2.39	0.40
3:BP:31:LEU:HD21	1:CD:161:MET:HG3	2.02	0.40
1:BT:49:TRP:CZ3	1:BT:74:SER:HB3	2.57	0.40
1:BU:261:ILE:HD12	1:BU:312:LEU:HD23	2.03	0.40
1:CD:119:TYR:CZ	1:CD:281:PRO:HG3	2.57	0.40
1:CE:86:TYR:CD2	1:CW:70:ILE:HD11	2.56	0.40
1:CE:256:LYS:HG2	1:CE:257:HIS:CD2	2.56	0.40
3:AF:65:LEU:HD12	3:AF:92:HIS:CE1	2.56	0.40
2:AO:137:LEU:HD11	2:AO:159:ALA:HB2	2.03	0.40
1:AU:77:VAL:HG11	1:AU:305:LEU:HD11	2.03	0.40
2:AW:113:ILE:HD12	2:AW:113:ILE:HA	1.92	0.40
1:BC:80:ASN:ND2	1:BC:153:PRO:O	2.52	0.40
2:BX:56:LYS:HD2	3:BY:56:PHE:HA	2.03	0.40
1:CE:137:GLY:HA3	1:CE:160:ASN:OD1	2.21	0.40
2:CG:28:ASP:N	2:CG:28:ASP:OD1	2.55	0.40
2:CG:156:ASN:HB3	2:CG:178:PHE:CE2	2.57	0.40
1:CL:165:ILE:HD13	1:CL:191:LEU:HD23	2.02	0.40
1:AB:215:LYS:HE2	1:AL:181:PHE:HE2	1.85	0.40
1:AK:203:VAL:HG22	1:AK:261:ILE:HG12	2.03	0.40
1:BB:165:ILE:HD13	1:BB:191:LEU:HD23	2.03	0.40
1:BD:28:TRP:O	1:BD:262:TYR:OH	2.28	0.40
1:BD:178:ASP:N	1:BD:178:ASP:OD1	2.54	0.40
2:BF:61:ASN:ND2	1:BK:59:THR:O	2.55	0.40
1:BU:196:GLU:HB3	1:BU:265:ASN:ND2	2.37	0.40
4:CB:211:LYS:O	4:CB:215:ILE:HG13	2.21	0.40
3:CO:78:GLN:NE2	3:CO:89:TYR:HB2	2.37	0.40
4:CR:190:LEU:HG	4:CR:209:THR:HG23	2.04	0.40
1:CW:121:LEU:O	1:CW:125:GLU:HG2	2.21	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	AB	309/319 (97%)	302 (98%)	7 (2%)	0	100	100
1	AC	294/319 (92%)	286 (97%)	8 (3%)	0	100	100
1	AJ	305/319 (96%)	300 (98%)	5 (2%)	0	100	100
1	AK	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	AL	309/319 (97%)	303 (98%)	6 (2%)	0	100	100
1	AS	305/319 (96%)	300 (98%)	5 (2%)	0	100	100
1	AT	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	AU	309/319 (97%)	303 (98%)	6 (2%)	0	100	100
1	BB	305/319 (96%)	300 (98%)	5 (2%)	0	100	100
1	BC	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	BD	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	BK	307/319 (96%)	302 (98%)	5 (2%)	0	100	100
1	BL	309/319 (97%)	302 (98%)	7 (2%)	0	100	100
1	BM	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	BT	305/319 (96%)	302 (99%)	3 (1%)	0	100	100
1	BU	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	BV	307/319 (96%)	302 (98%)	5 (2%)	0	100	100
1	CC	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	CD	293/319 (92%)	289 (99%)	4 (1%)	0	100	100
1	CE	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CL	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	CM	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CN	293/319 (92%)	284 (97%)	9 (3%)	0	100	100
1	CU	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CV	309/319 (97%)	306 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CW	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
2	AD	114/185 (62%)	112 (98%)	2 (2%)	0	100	100
2	AO	154/185 (83%)	152 (99%)	2 (1%)	0	100	100
2	AW	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	AX	156/185 (84%)	154 (99%)	2 (1%)	0	100	100
2	BF	154/185 (83%)	152 (99%)	2 (1%)	0	100	100
2	BG	148/185 (80%)	145 (98%)	3 (2%)	0	100	100
2	BN	171/185 (92%)	168 (98%)	3 (2%)	0	100	100
2	BO	147/185 (80%)	145 (99%)	2 (1%)	0	100	100
2	BW	153/185 (83%)	150 (98%)	3 (2%)	0	100	100
2	BX	160/185 (86%)	159 (99%)	1 (1%)	0	100	100
2	CF	162/185 (88%)	161 (99%)	1 (1%)	0	100	100
2	CG	146/185 (79%)	144 (99%)	2 (1%)	0	100	100
2	CH	148/185 (80%)	145 (98%)	3 (2%)	0	100	100
2	CP	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	CQ	164/185 (89%)	163 (99%)	1 (1%)	0	100	100
3	AF	138/190 (73%)	136 (99%)	2 (1%)	0	100	100
3	AN	145/190 (76%)	143 (99%)	2 (1%)	0	100	100
3	AV	148/190 (78%)	147 (99%)	1 (1%)	0	100	100
3	BE	148/190 (78%)	145 (98%)	3 (2%)	0	100	100
3	BP	145/190 (76%)	143 (99%)	2 (1%)	0	100	100
3	BY	145/190 (76%)	141 (97%)	4 (3%)	0	100	100
3	CO	146/190 (77%)	144 (99%)	2 (1%)	0	100	100
4	AH	35/230 (15%)	35 (100%)	0	0	100	100
4	AI	27/230 (12%)	27 (100%)	0	0	100	100
4	AP	35/230 (15%)	35 (100%)	0	0	100	100
4	AQ	35/230 (15%)	35 (100%)	0	0	100	100
4	AR	35/230 (15%)	35 (100%)	0	0	100	100
4	AY	35/230 (15%)	35 (100%)	0	0	100	100
4	AZ	35/230 (15%)	35 (100%)	0	0	100	100
4	BA	35/230 (15%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BH	35/230 (15%)	35 (100%)	0	0	100	100
4	BI	35/230 (15%)	35 (100%)	0	0	100	100
4	BJ	35/230 (15%)	35 (100%)	0	0	100	100
4	BQ	26/230 (11%)	26 (100%)	0	0	100	100
4	BR	35/230 (15%)	35 (100%)	0	0	100	100
4	BS	35/230 (15%)	35 (100%)	0	0	100	100
4	BZ	35/230 (15%)	35 (100%)	0	0	100	100
4	CA	35/230 (15%)	35 (100%)	0	0	100	100
4	CB	27/230 (12%)	27 (100%)	0	0	100	100
4	CI	35/230 (15%)	35 (100%)	0	0	100	100
4	CJ	27/230 (12%)	27 (100%)	0	0	100	100
4	CK	35/230 (15%)	35 (100%)	0	0	100	100
4	CR	35/230 (15%)	35 (100%)	0	0	100	100
4	CS	35/230 (15%)	35 (100%)	0	0	100	100
4	CT	27/230 (12%)	27 (100%)	0	0	100	100
4	CX	28/230 (12%)	28 (100%)	0	0	100	100
4	CY	28/230 (12%)	28 (100%)	0	0	100	100
4	CZ	28/230 (12%)	28 (100%)	0	0	100	100
5	AM	153/254 (60%)	152 (99%)	1 (1%)	0	100	100
All	All	12254/18633 (66%)	12083 (99%)	171 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	283/286 (99%)	283 (100%)	0	100	100
1	AC	271/286 (95%)	271 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AJ	281/286 (98%)	281 (100%)	0	100	100
1	AK	283/286 (99%)	283 (100%)	0	100	100
1	AL	283/286 (99%)	283 (100%)	0	100	100
1	AS	281/286 (98%)	281 (100%)	0	100	100
1	AT	283/286 (99%)	283 (100%)	0	100	100
1	AU	283/286 (99%)	283 (100%)	0	100	100
1	BB	281/286 (98%)	281 (100%)	0	100	100
1	BC	283/286 (99%)	283 (100%)	0	100	100
1	BD	283/286 (99%)	283 (100%)	0	100	100
1	BK	283/286 (99%)	283 (100%)	0	100	100
1	BL	283/286 (99%)	283 (100%)	0	100	100
1	BM	283/286 (99%)	283 (100%)	0	100	100
1	BT	281/286 (98%)	281 (100%)	0	100	100
1	BU	283/286 (99%)	283 (100%)	0	100	100
1	BV	283/286 (99%)	283 (100%)	0	100	100
1	CC	283/286 (99%)	283 (100%)	0	100	100
1	CD	271/286 (95%)	271 (100%)	0	100	100
1	CE	283/286 (99%)	283 (100%)	0	100	100
1	CL	283/286 (99%)	283 (100%)	0	100	100
1	CM	283/286 (99%)	283 (100%)	0	100	100
1	CN	271/286 (95%)	271 (100%)	0	100	100
1	CU	283/286 (99%)	283 (100%)	0	100	100
1	CV	283/286 (99%)	283 (100%)	0	100	100
1	CW	283/286 (99%)	283 (100%)	0	100	100
2	AD	99/154 (64%)	99 (100%)	0	100	100
2	AO	132/154 (86%)	132 (100%)	0	100	100
2	AW	129/154 (84%)	129 (100%)	0	100	100
2	AX	133/154 (86%)	133 (100%)	0	100	100
2	BF	131/154 (85%)	131 (100%)	0	100	100
2	BG	130/154 (84%)	130 (100%)	0	100	100
2	BN	147/154 (96%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BO	129/154 (84%)	129 (100%)	0	100	100
2	BW	131/154 (85%)	131 (100%)	0	100	100
2	BX	141/154 (92%)	141 (100%)	0	100	100
2	CF	142/154 (92%)	142 (100%)	0	100	100
2	CG	129/154 (84%)	129 (100%)	0	100	100
2	CH	130/154 (84%)	130 (100%)	0	100	100
2	CP	129/154 (84%)	129 (100%)	0	100	100
2	CQ	144/154 (94%)	144 (100%)	0	100	100
3	AF	124/163 (76%)	124 (100%)	0	100	100
3	AN	130/163 (80%)	130 (100%)	0	100	100
3	AV	131/163 (80%)	131 (100%)	0	100	100
3	BE	131/163 (80%)	131 (100%)	0	100	100
3	BP	129/163 (79%)	129 (100%)	0	100	100
3	BY	129/163 (79%)	129 (100%)	0	100	100
3	CO	130/163 (80%)	130 (100%)	0	100	100
4	AH	35/210 (17%)	35 (100%)	0	100	100
4	AI	28/210 (13%)	28 (100%)	0	100	100
4	AP	35/210 (17%)	35 (100%)	0	100	100
4	AQ	35/210 (17%)	35 (100%)	0	100	100
4	AR	35/210 (17%)	35 (100%)	0	100	100
4	AY	35/210 (17%)	35 (100%)	0	100	100
4	AZ	35/210 (17%)	35 (100%)	0	100	100
4	BA	35/210 (17%)	35 (100%)	0	100	100
4	BH	35/210 (17%)	35 (100%)	0	100	100
4	BI	35/210 (17%)	35 (100%)	0	100	100
4	BJ	35/210 (17%)	35 (100%)	0	100	100
4	BQ	27/210 (13%)	27 (100%)	0	100	100
4	BR	35/210 (17%)	35 (100%)	0	100	100
4	BS	35/210 (17%)	35 (100%)	0	100	100
4	BZ	35/210 (17%)	35 (100%)	0	100	100
4	CA	35/210 (17%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CB	28/210 (13%)	28 (100%)	0	100	100
4	CI	35/210 (17%)	35 (100%)	0	100	100
4	CJ	28/210 (13%)	28 (100%)	0	100	100
4	CK	35/210 (17%)	35 (100%)	0	100	100
4	CR	35/210 (17%)	35 (100%)	0	100	100
4	CS	35/210 (17%)	35 (100%)	0	100	100
4	CT	28/210 (13%)	28 (100%)	0	100	100
4	CX	29/210 (14%)	29 (100%)	0	100	100
4	CY	29/210 (14%)	29 (100%)	0	100	100
4	CZ	29/210 (14%)	29 (100%)	0	100	100
5	AM	141/218 (65%)	141 (100%)	0	100	100
All	All	11191/16565 (68%)	11191 (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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	AF	24	ASN
5	AM	162	ASN
2	AW	41	GLN
1	BL	90	HIS
2	BN	24	ASN
2	BN	47	ASN
2	BO	41	GLN
1	CC	257	HIS
1	CC	318	GLN
1	CD	318	GLN
2	CP	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

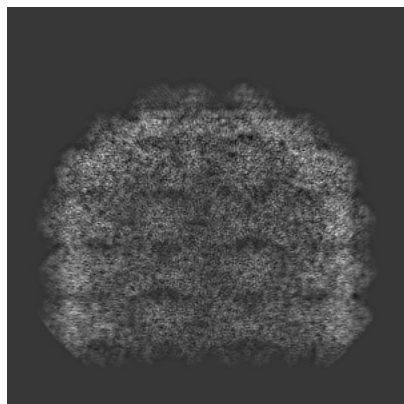
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17673. These allow visual inspection of the internal detail of the map and identification of artifacts.

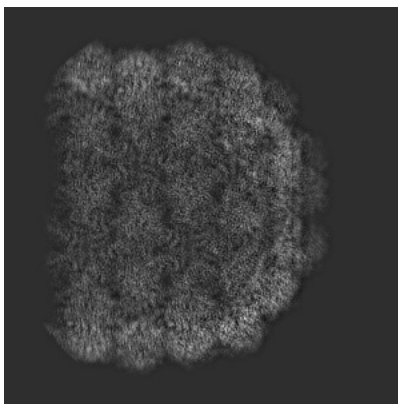
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

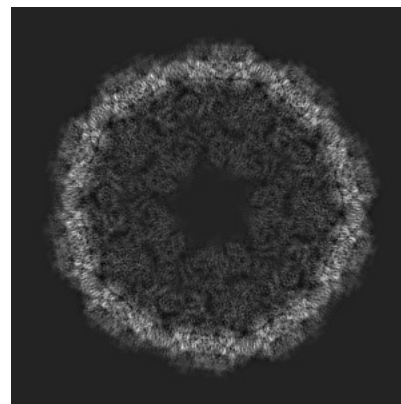
6.1.1 Primary map



X

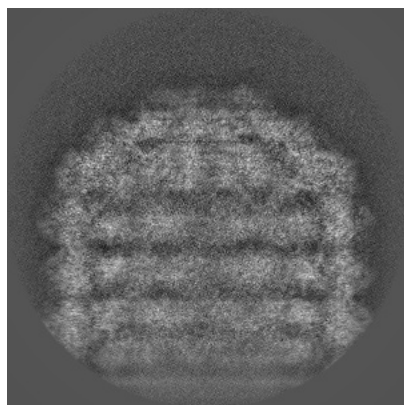


Y

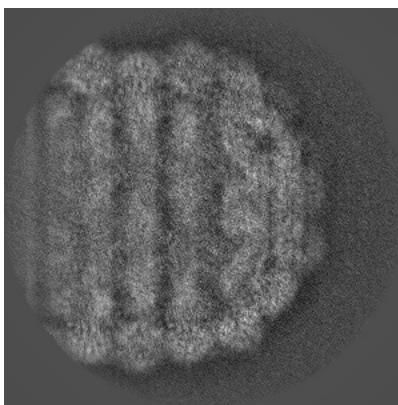


Z

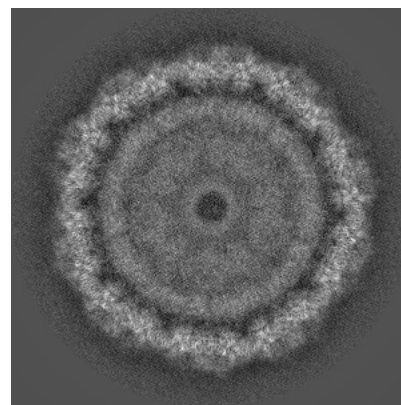
6.1.2 Raw map



X



Y



Z

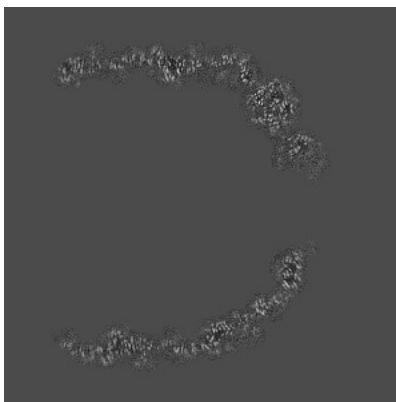
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

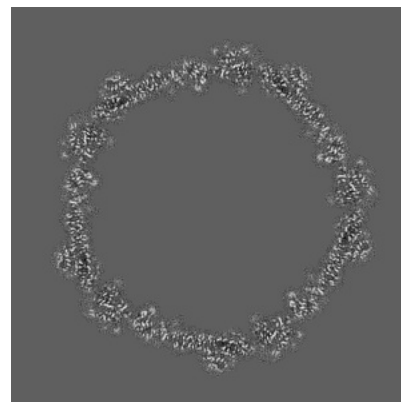
6.2.1 Primary map



X Index: 320

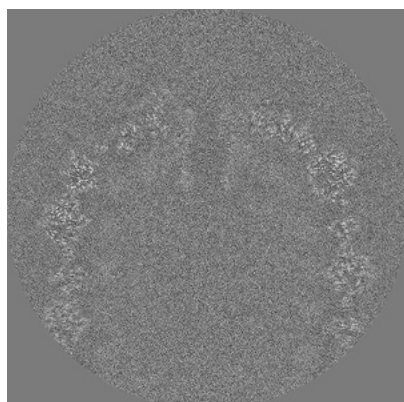


Y Index: 320

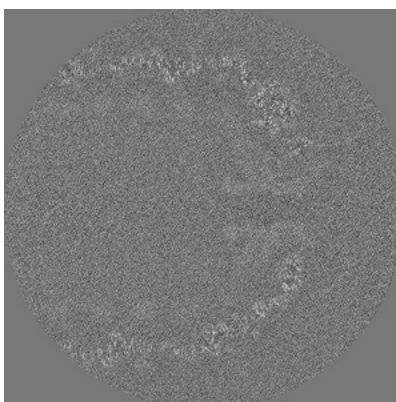


Z Index: 320

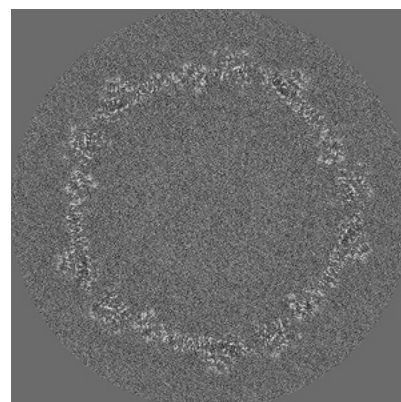
6.2.2 Raw map



X Index: 320



Y Index: 320

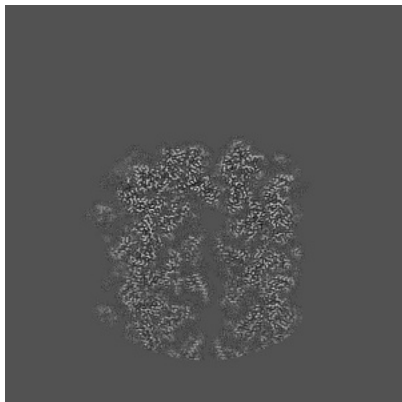


Z Index: 320

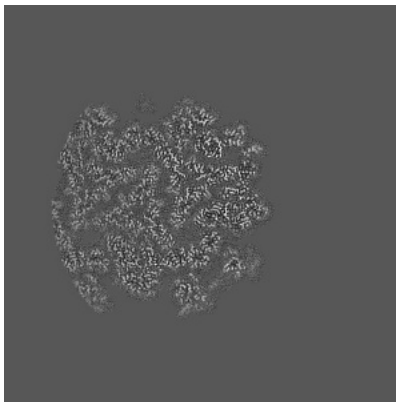
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

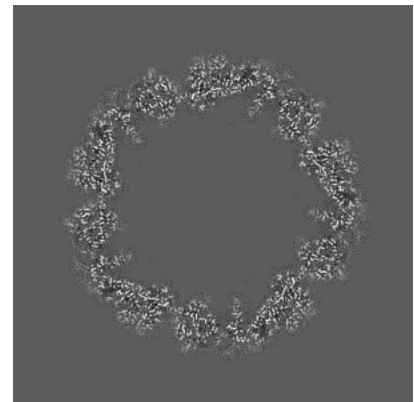
6.3.1 Primary map



X Index: 117

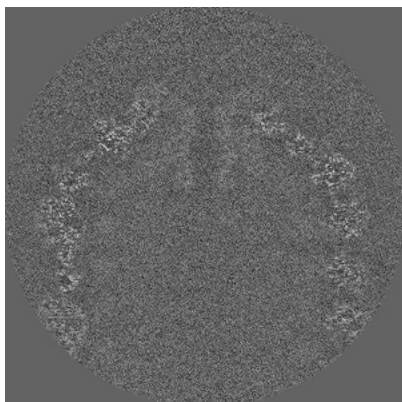


Y Index: 529

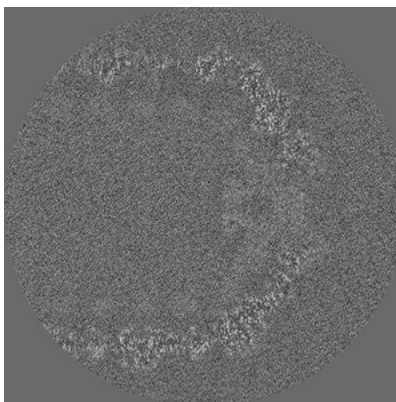


Z Index: 385

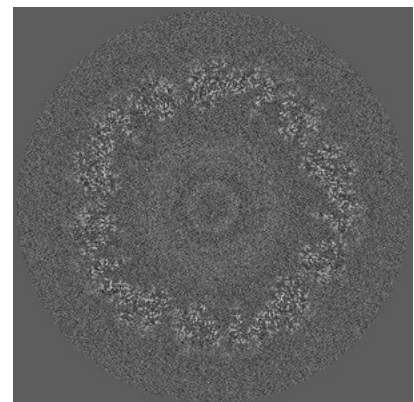
6.3.2 Raw map



X Index: 336



Y Index: 295

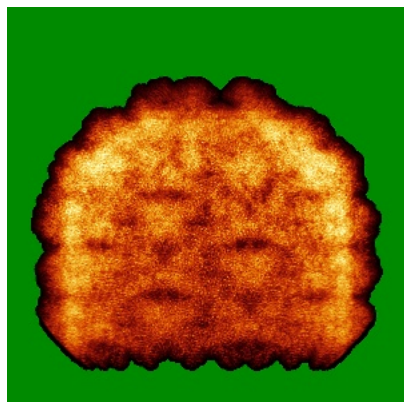


Z Index: 384

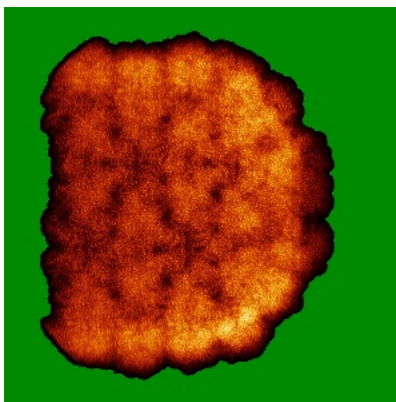
The images above show the largest variance slices of the map in three orthogonal directions.

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

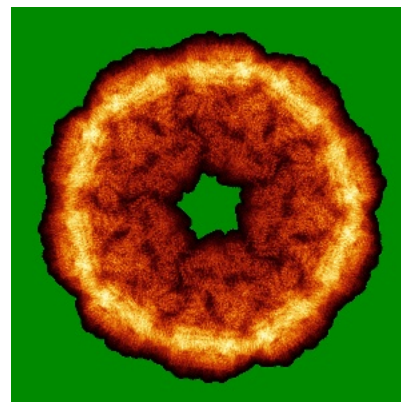
6.4.1 Primary map



X

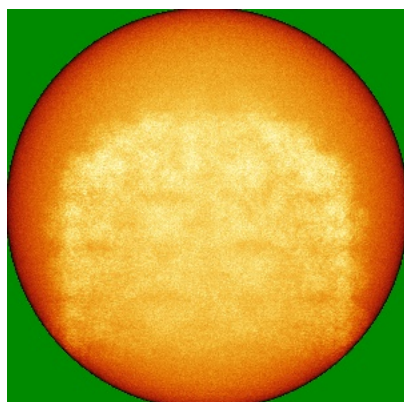


Y

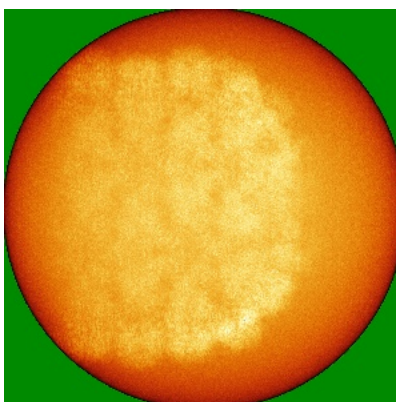


Z

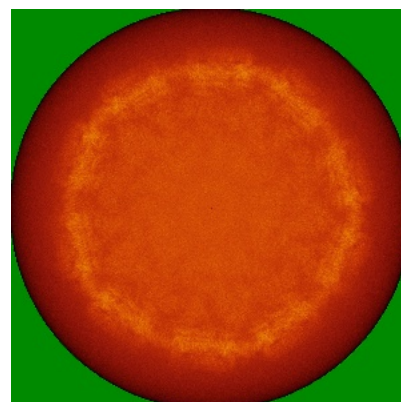
6.4.2 Raw map



X



Y

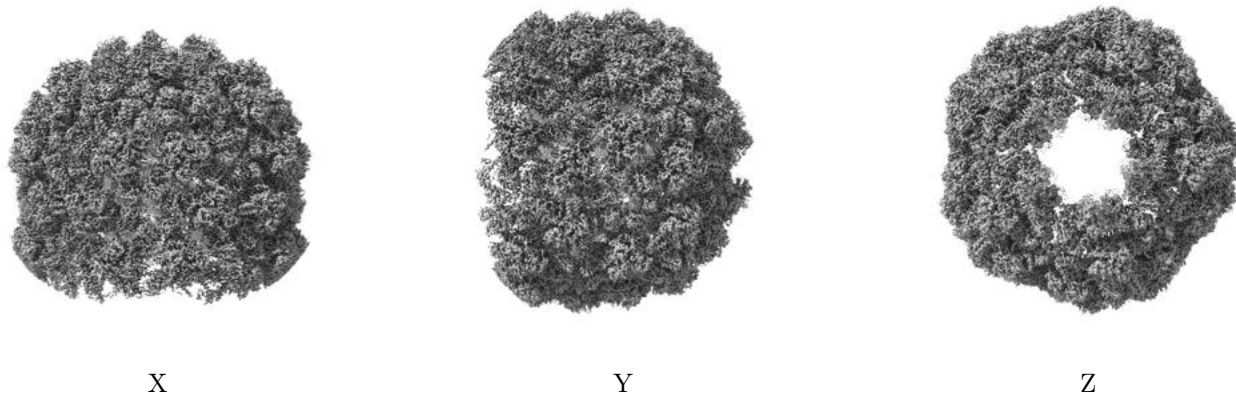


Z

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.

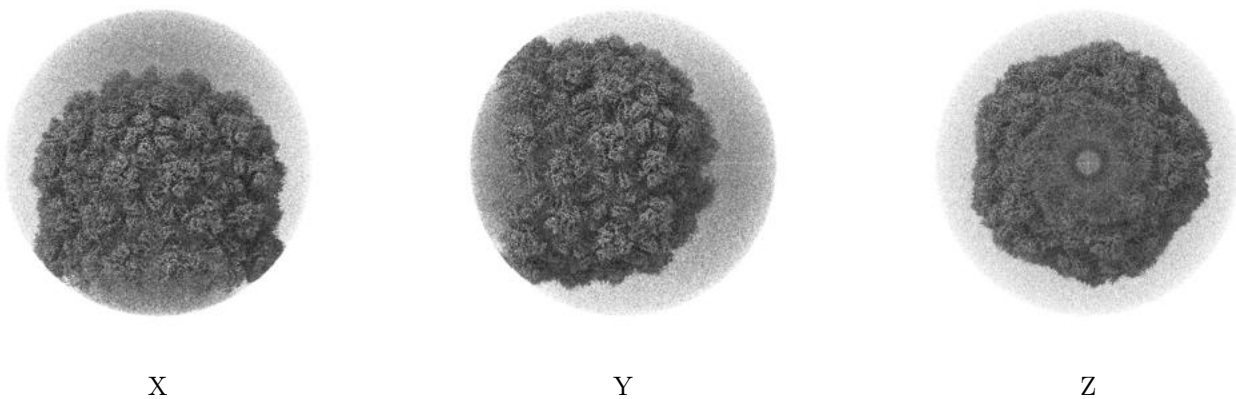
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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



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

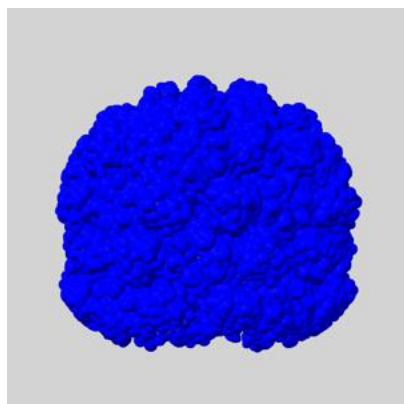
6.6 Mask visualisation [i](#)

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

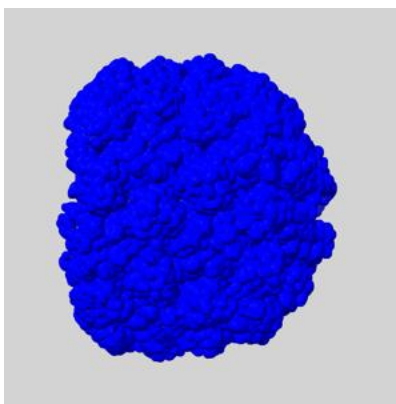
A mask typically either:

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

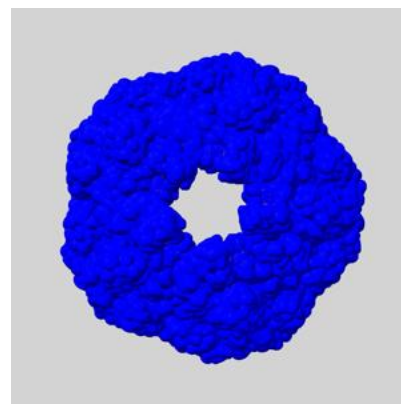
6.6.1 emd_17673_msk_1.map [i](#)



X



Y

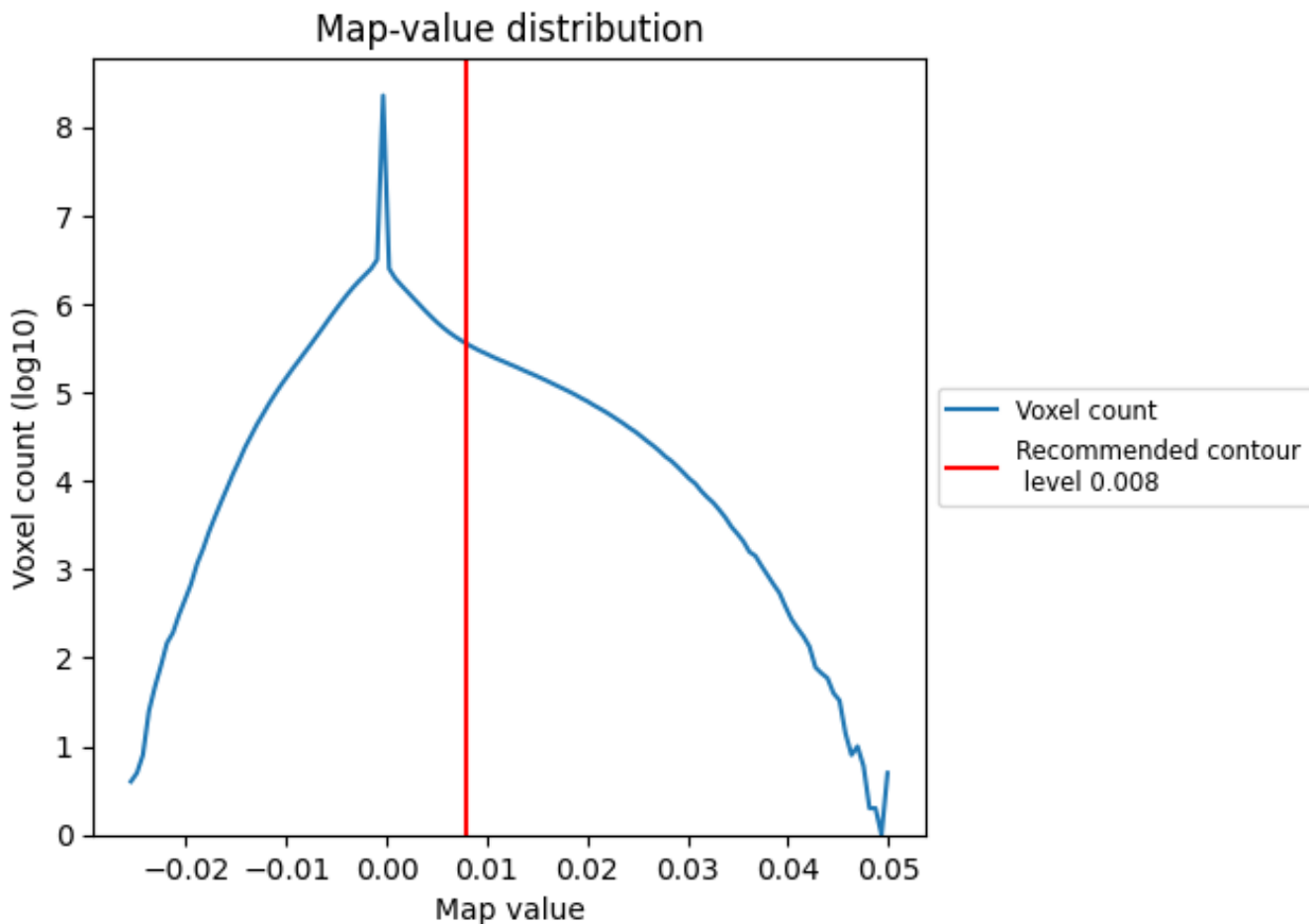


Z

7 Map analysis [i](#)

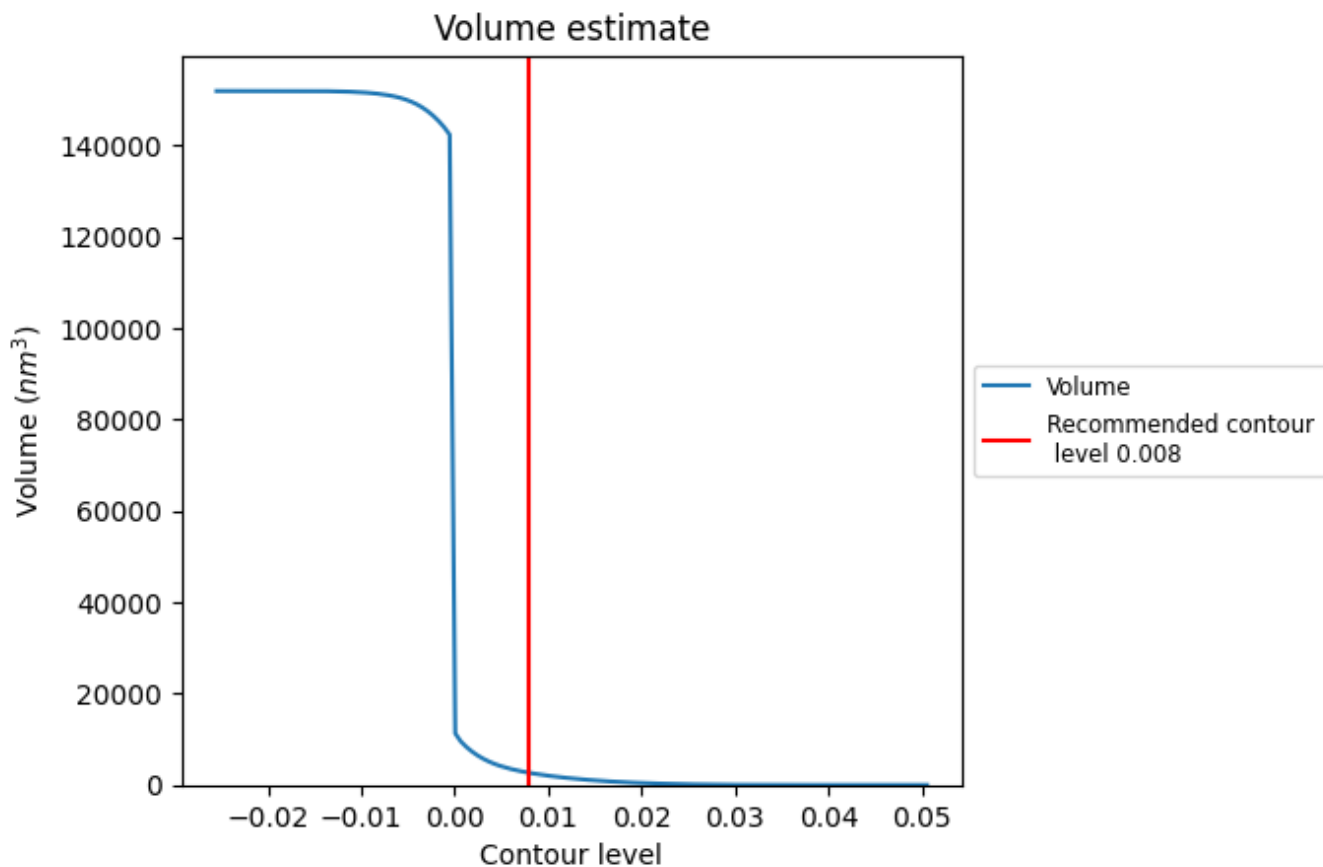
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

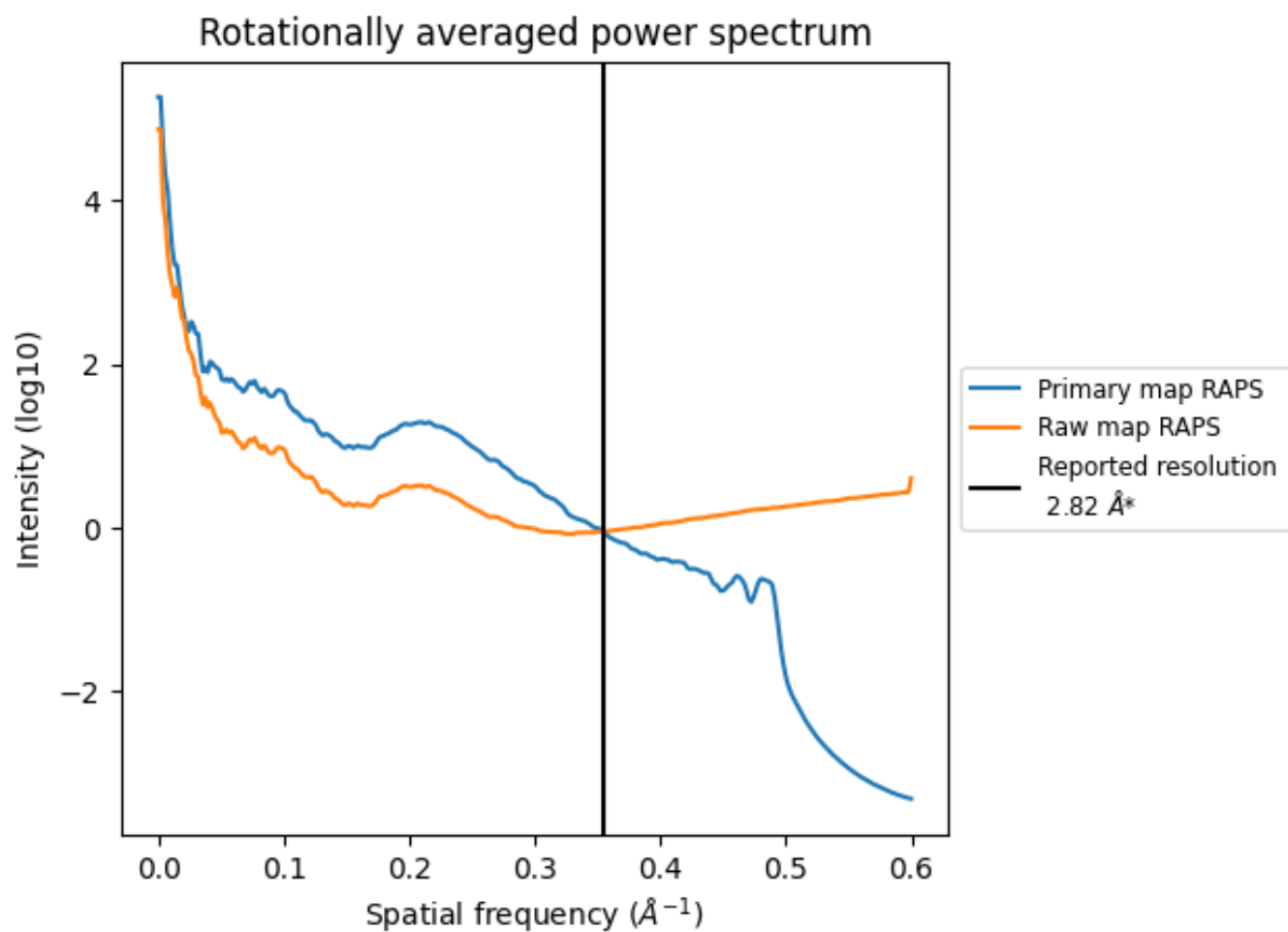
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2649 nm^3 ; this corresponds to an approximate mass of 2393 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

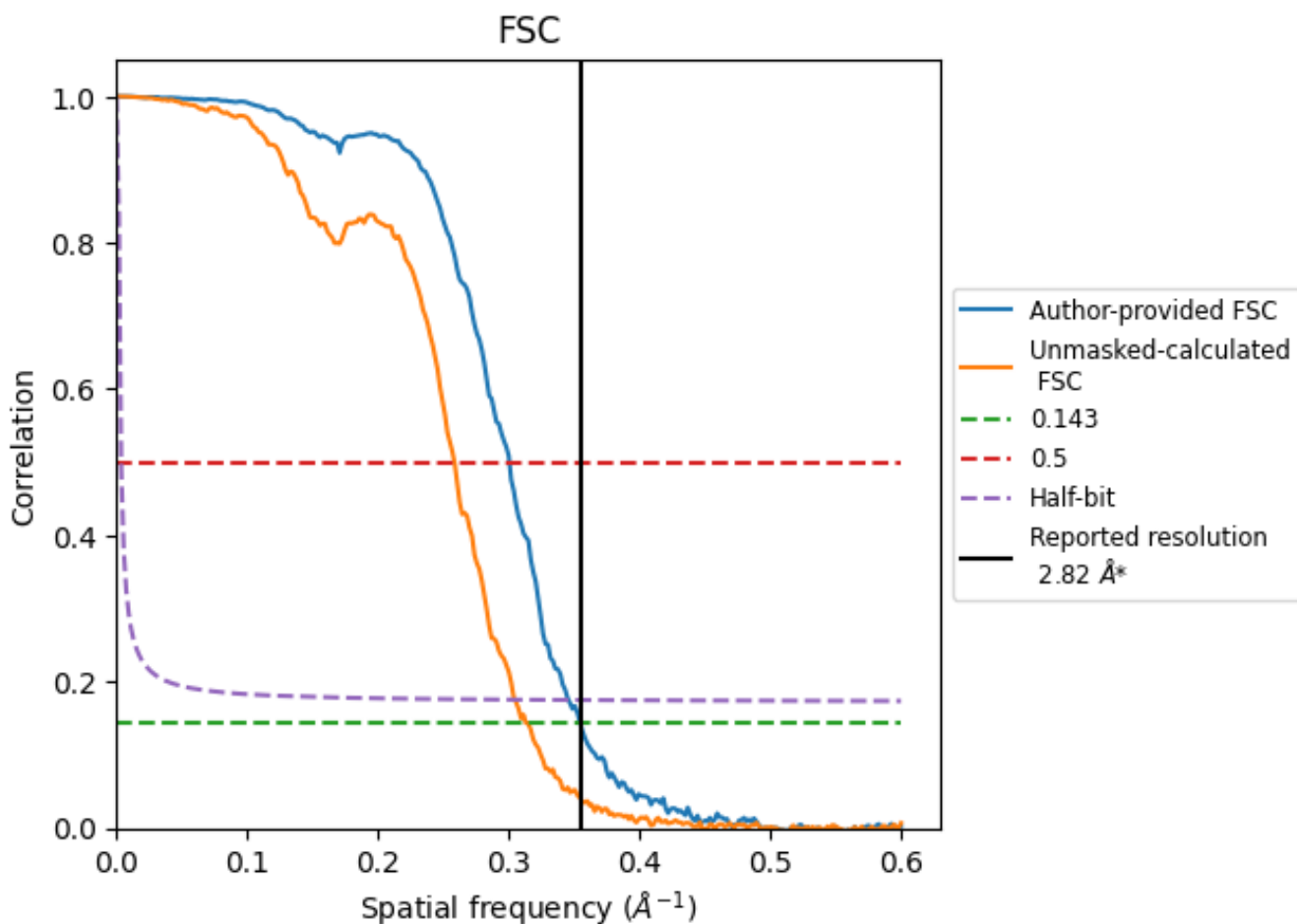


*Reported resolution corresponds to spatial frequency of 0.355 Å⁻¹

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 0.355\AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.33	2.89
Unmasked-calculated*	3.18	3.87	3.28

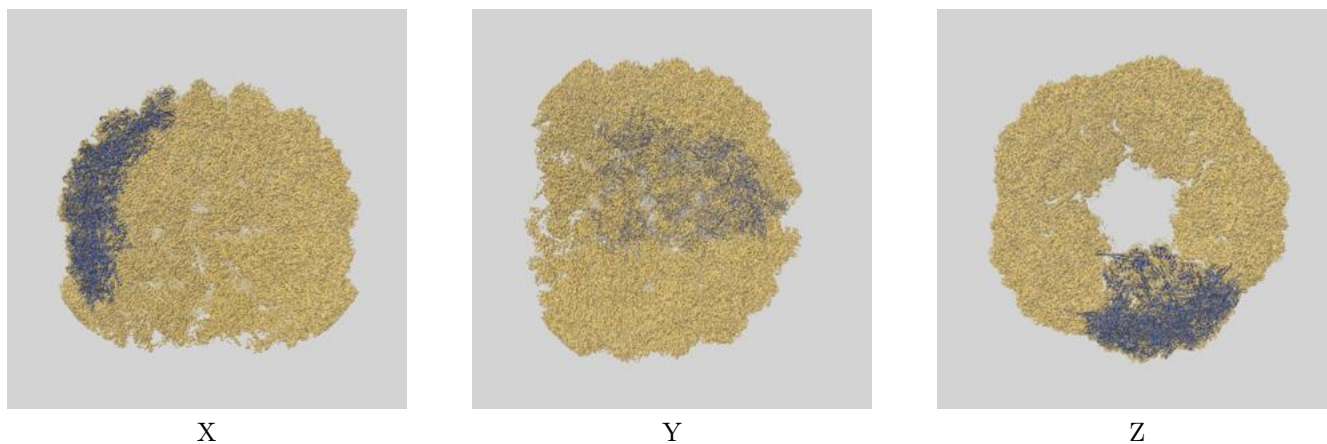
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.82 by more than 10 %

9 Map-model fit [i](#)

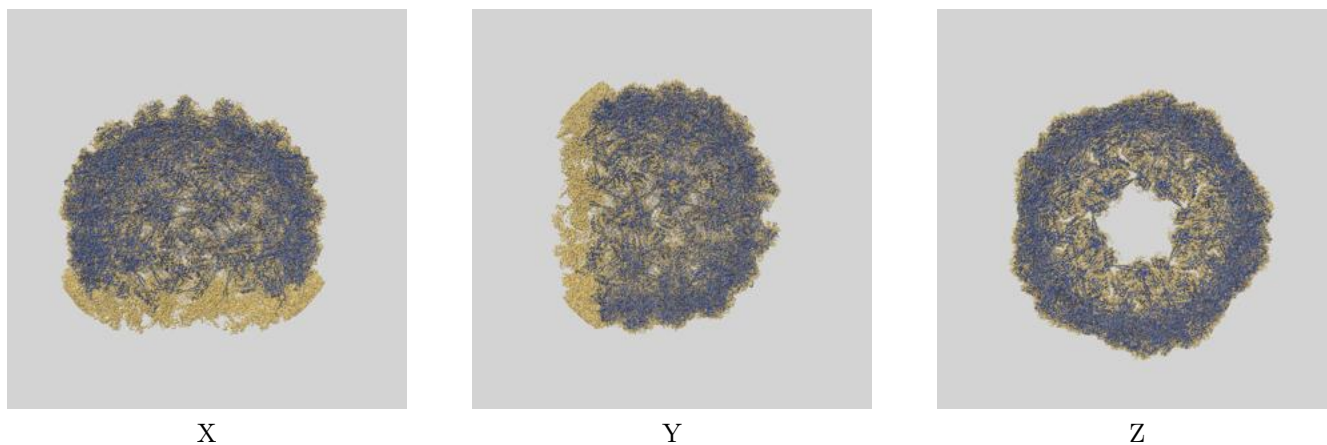
This section contains information regarding the fit between EMDB map EMD-17673 and PDB model 8PHS. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

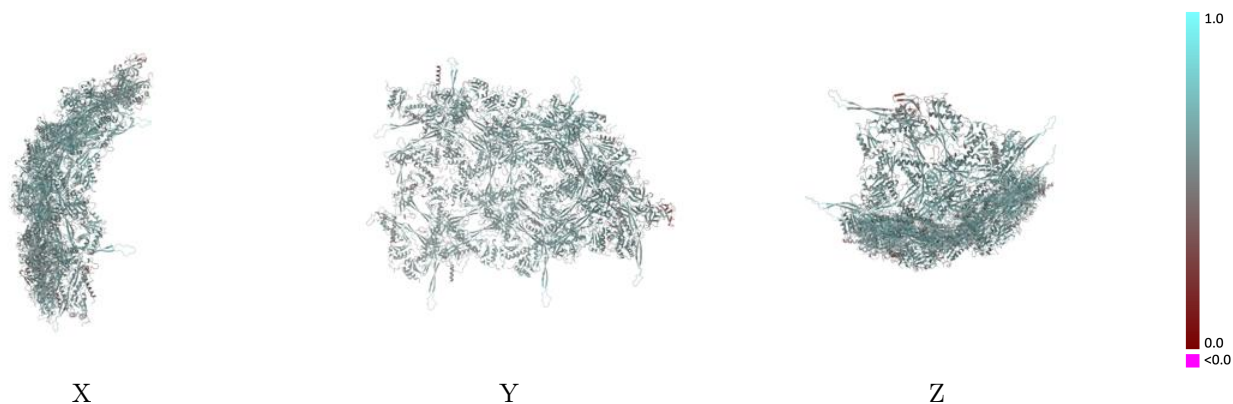


9.1.2 Map-model assembly overlay [i](#)



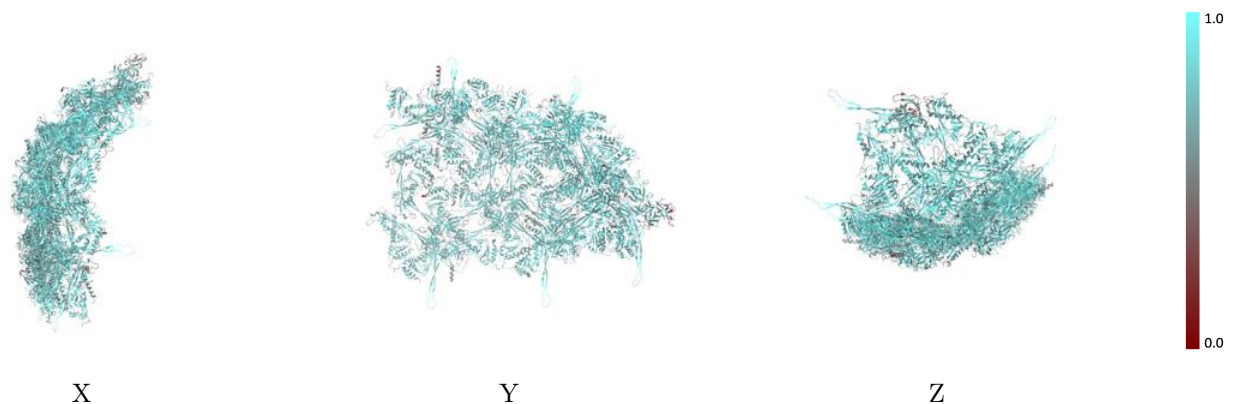
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



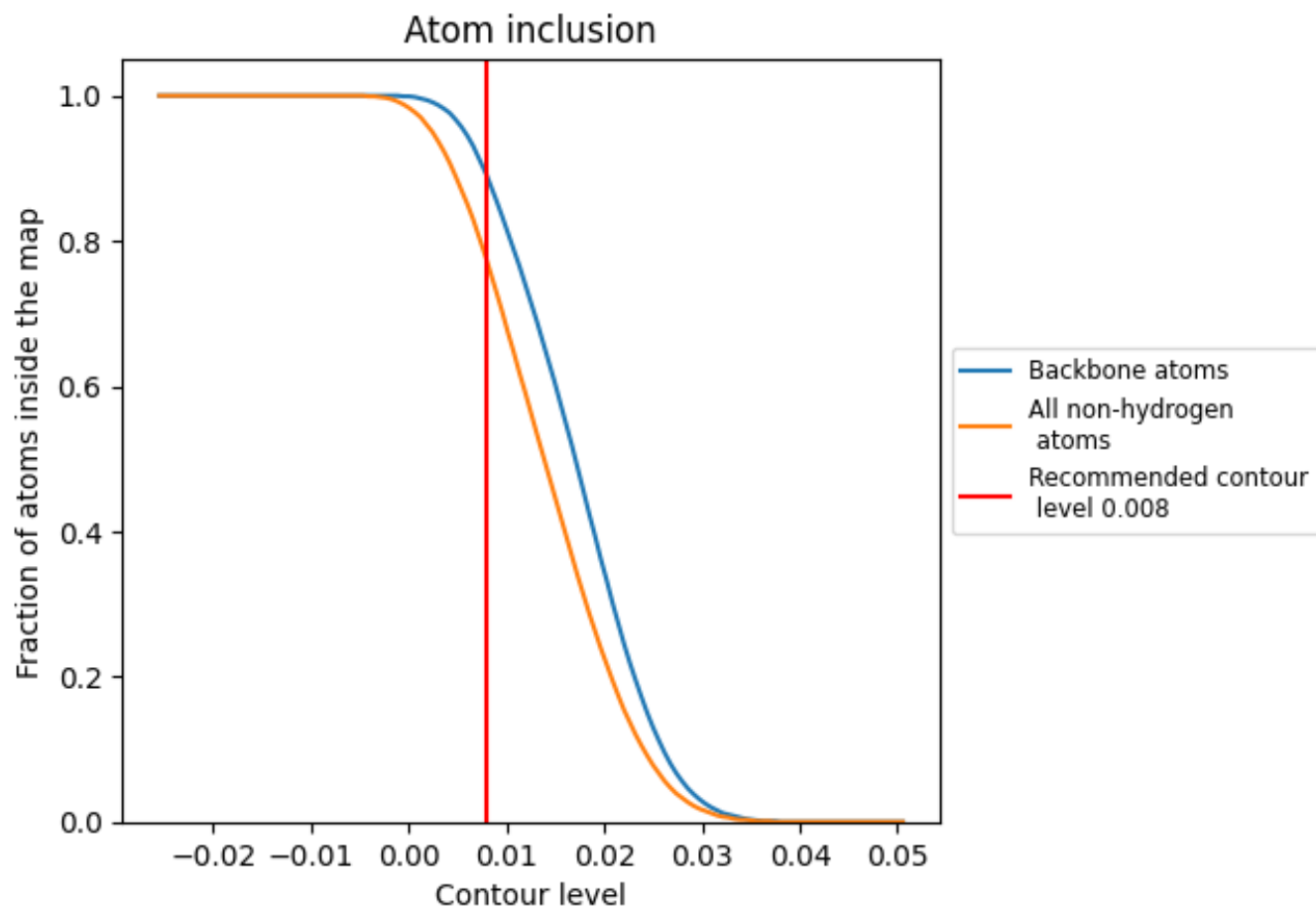
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 77% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5680
AB	 0.7450	 0.5450
AC	 0.7510	 0.5550
AD	 0.5080	 0.4400
AF	 0.7260	 0.5420
AH	 0.5600	 0.4580
AI	 0.6920	 0.4940
AJ	 0.8400	 0.6050
AK	 0.8160	 0.5860
AL	 0.8180	 0.5880
AM	 0.7410	 0.5650
AN	 0.8060	 0.5930
AO	 0.7780	 0.5840
AP	 0.7390	 0.5690
AQ	 0.7070	 0.5270
AR	 0.7360	 0.5350
AS	 0.8530	 0.6110
AT	 0.8310	 0.5920
AU	 0.8280	 0.5970
AV	 0.8060	 0.5920
AW	 0.8430	 0.6000
AX	 0.7470	 0.5690
AY	 0.6940	 0.5510
AZ	 0.7230	 0.5540
BA	 0.7260	 0.5180
BB	 0.8480	 0.6100
BC	 0.7980	 0.5800
BD	 0.8110	 0.5840
BE	 0.7540	 0.5700
BF	 0.8090	 0.5900
BG	 0.7600	 0.5730
BH	 0.7780	 0.5710
BI	 0.6840	 0.5300
BJ	 0.7390	 0.5380
BK	 0.8290	 0.6080



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Chain	Atom inclusion	Q-score
BL	 0.8290	 0.5920
BM	 0.8050	 0.5830
BN	 0.7740	 0.5800
BO	 0.7120	 0.5470
BP	 0.7870	 0.5790
BQ	 0.6170	 0.5370
BR	 0.7130	 0.5270
BS	 0.7000	 0.5330
BT	 0.8510	 0.6130
BU	 0.8240	 0.5930
BV	 0.8090	 0.5910
BW	 0.7980	 0.6010
BX	 0.7710	 0.5760
BY	 0.7720	 0.5720
BZ	 0.7100	 0.5560
CA	 0.7100	 0.5180
CB	 0.5830	 0.5240
CC	 0.7450	 0.5540
CD	 0.8050	 0.5780
CE	 0.7380	 0.5450
CF	 0.6970	 0.5170
CG	 0.7470	 0.5570
CH	 0.6870	 0.5270
CI	 0.6380	 0.4890
CJ	 0.5990	 0.4940
CK	 0.6190	 0.4780
CL	 0.7810	 0.5640
CM	 0.7840	 0.5720
CN	 0.7370	 0.5460
CO	 0.7020	 0.5300
CP	 0.7180	 0.5510
CQ	 0.6760	 0.5280
CR	 0.6840	 0.5100
CS	 0.6640	 0.5190
CT	 0.5510	 0.4560
CU	 0.7510	 0.5540
CV	 0.7200	 0.5350
CW	 0.7250	 0.5360
CX	 0.6470	 0.4900
CY	 0.6160	 0.4760
CZ	 0.6200	 0.4430