



Full wwPDB EM Validation Report ⓘ

Nov 12, 2024 – 01:33 AM EST

PDB ID : 8FXP
EMDB ID : EMD-29540
Title : Structure of capsid of Agrobacterium phage Milano
Authors : Sonani, R.R.; Wang, F.; Esteves, N.C.; Kelly, R.J.; Sebastian, A.; Kreutzberger, M.A.B.; Leiman, P.G.; Scharf, B.E.; Egelman, E.H.
Deposited on : 2023-01-25
Resolution : 4.04 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

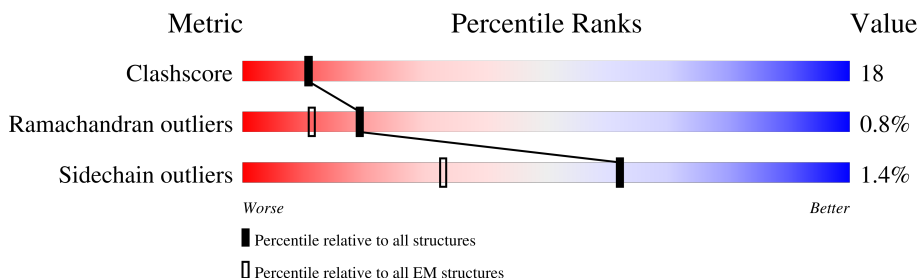
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.04 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.









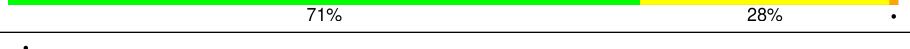
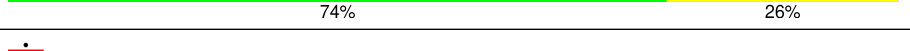
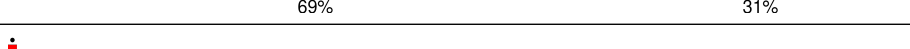
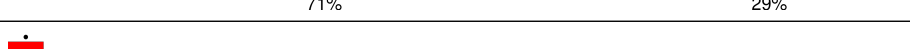
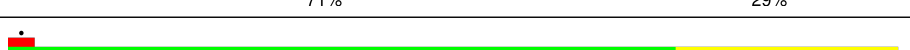

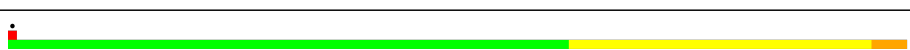

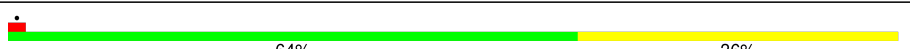




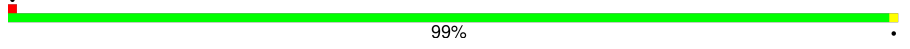
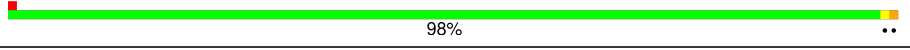
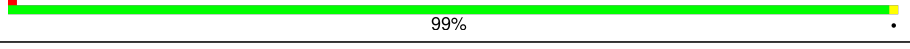
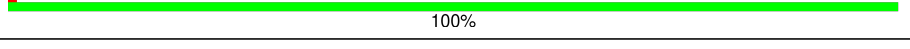
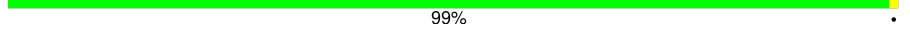

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	217	
1	0A	217	
1	0B	217	
1	0C	217	
1	0D	217	
1	f	217	
2	0E	137	
2	0F	137	

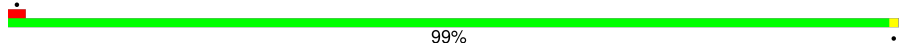
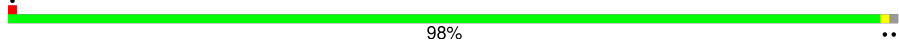
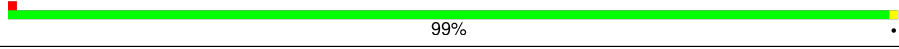
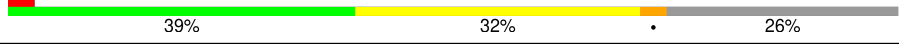
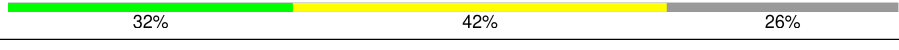
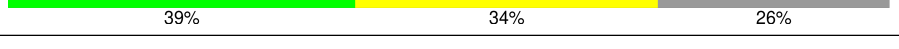

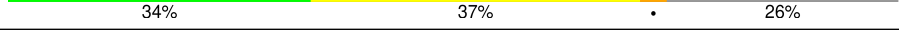
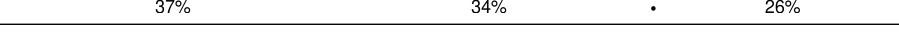
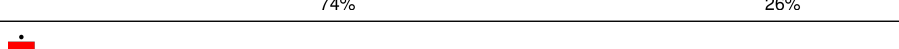
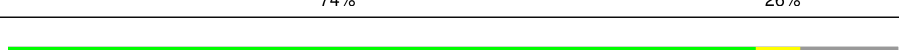

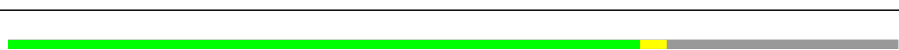
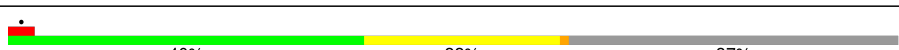
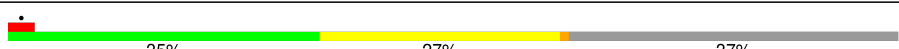
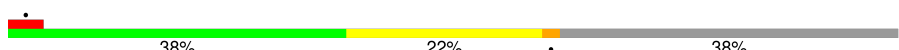
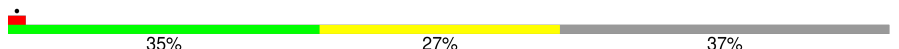
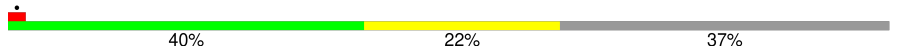
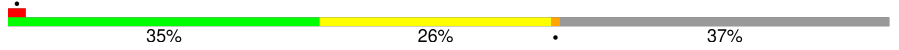

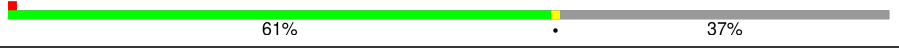
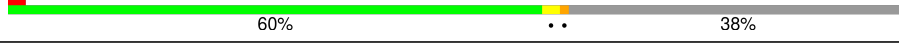



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Mol	Chain	Length	Quality of chain
2	0G	137	
2	0H	137	
2	1	137	
2	2	137	
2	3	137	
2	4	137	
2	5	137	
2	6	137	
2	7	137	
2	8	137	
2	9	137	
2	AD	137	
2	AE	137	
2	AH	137	
2	AI	137	
2	AK	137	
2	AL	137	
2	AM	137	
2	AN	137	
2	l	137	
2	m	137	
2	p	137	
2	q	137	
2	s	137	
2	t	137	

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Mol	Chain	Length	Quality of chain
2	u	137	
2	v	137	
2	z	137	
3	AO	38	
3	AP	38	
3	AQ	38	
3	AR	38	
3	AS	38	
3	AT	38	
3	a	38	
3	b	38	
3	c	38	
3	d	38	
3	e	38	
4	AA	465	
4	AB	465	
4	AC	465	
4	AF	465	
4	AG	465	
4	AJ	465	
4	g	465	
4	h	465	
4	i	465	
4	j	465	
4	k	465	

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Mol	Chain	Length	Quality of chain
4	n	465	
4	o	465	
4	r	465	
4	w	465	
4	x	465	
4	y	465	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 72532 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 Linking protein 1, gp16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	19	Total	C	N	O	S	0	0
			133	79	27	24	3		
1	f	22	Total	C	N	O	S	0	0
			158	97	30	27	4		
1	0A	19	Total	C	N	O	S	0	0
			133	79	27	24	3		
1	0B	19	Total	C	N	O	S	0	0
			133	79	27	24	3		
1	0C	19	Total	C	N	O	S	0	0
			133	79	27	24	3		
1	0D	19	Total	C	N	O	S	0	0
			133	79	27	24	3		

- Molecule 2 is a protein called Minor capsid protein, gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	3	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	4	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	8	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	9	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	m	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	p	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	q	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	s	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	t	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	u	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
2	v	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
2	z	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	0E	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	0F	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	AD	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	AE	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	AH	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	AI	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	AK	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	AL	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	AM	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
2	AN	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
2	0G	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
2	0H	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		

- Molecule 3 is a protein called Linking protein 2, gp128.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	b	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	c	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
3	d	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
3	e	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	AO	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	AP	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	AR	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	AS	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	AQ	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
3	AT	28	Total	C	N	O	S	0	0
			209	131	40	33	5		

- Molecule 4 is a protein called Major capsid protein, gp9.

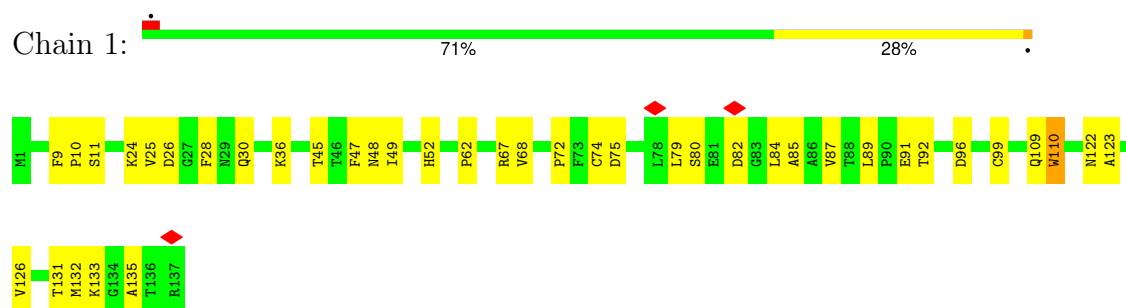
Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	h	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	i	289	Total	C	N	O	S	0	0
			2264	1434	387	427	16		
4	j	289	Total	C	N	O	S	0	0
			2264	1434	387	427	16		
4	k	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
4	n	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	o	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	r	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		

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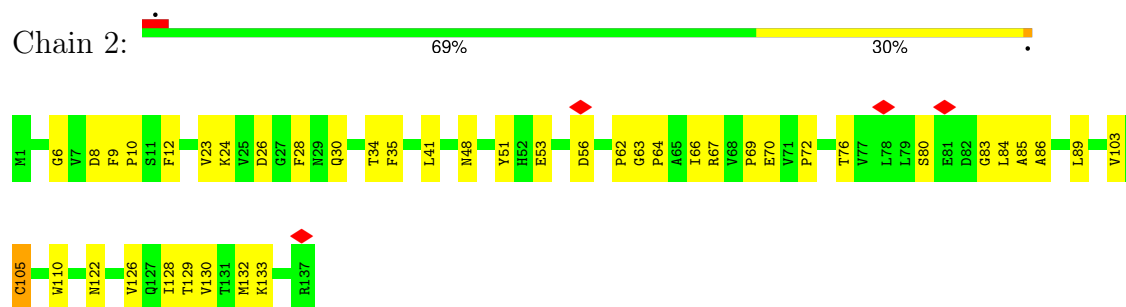
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	w	289	Total	C	N	O	S	0	0
			2264	1434	387	427	16		
4	x	289	Total	C	N	O	S	0	0
			2264	1434	387	427	16		
4	y	289	Total	C	N	O	S	0	0
			2264	1434	387	427	16		
4	AA	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	AB	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	AC	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
4	AF	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	AG	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
4	AJ	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		

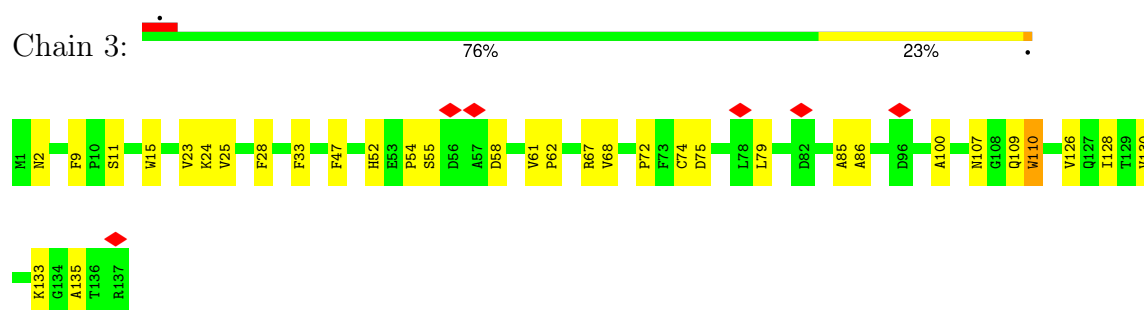
- Molecule 2: Minor capsid protein, gp10



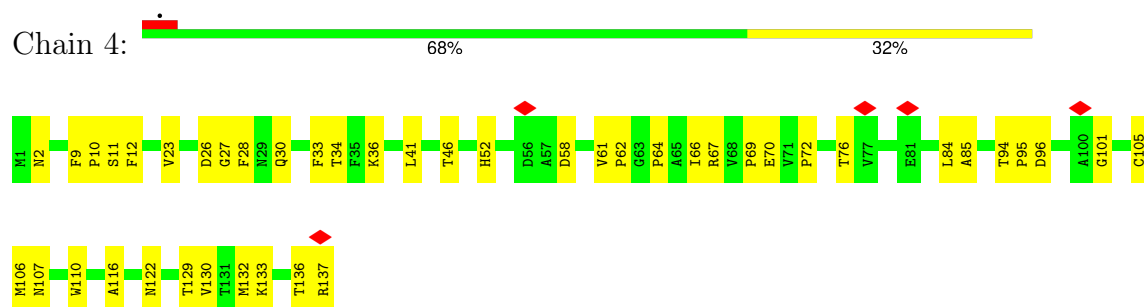
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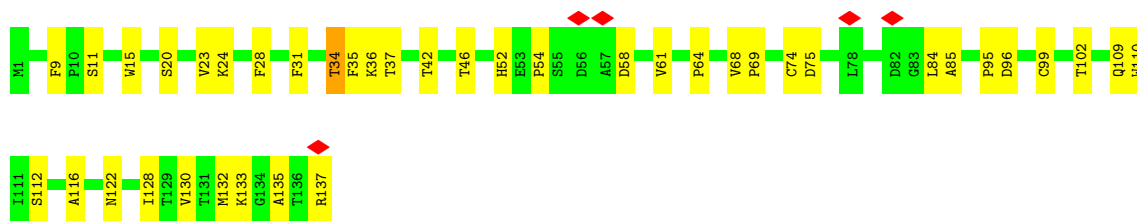


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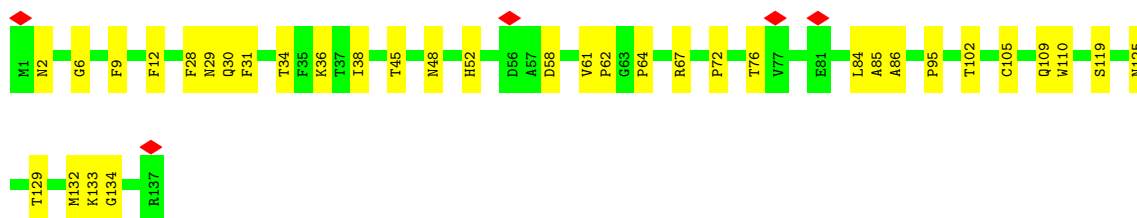


- Molecule 2: Minor capsid protein, gp10

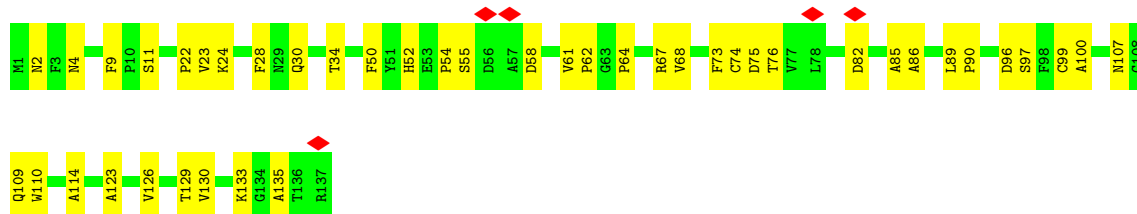




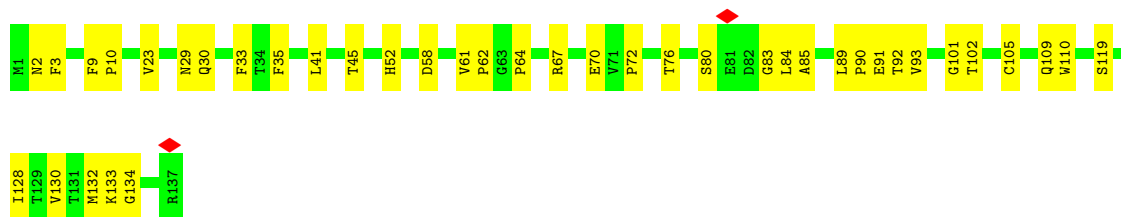
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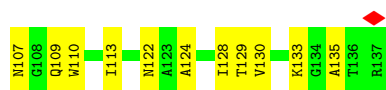


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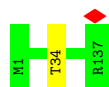




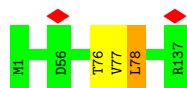
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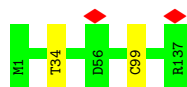
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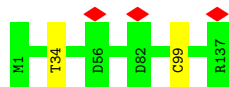
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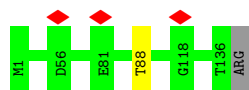


- Molecule 2: Minor capsid protein, gp10



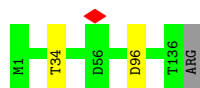
- Molecule 2: Minor capsid protein, gp10

Chain u:  99%



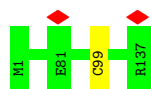
- Molecule 2: Minor capsid protein, gp10

Chain v:  98%



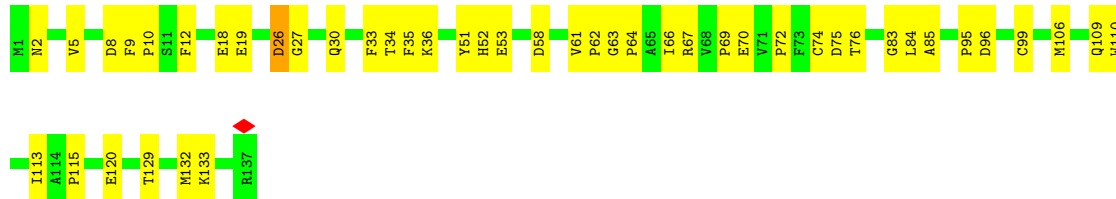
- Molecule 2: Minor capsid protein, gp10

Chain z:  99%




- Molecule 2: Minor capsid protein, gp10

Chain 0E:  66%




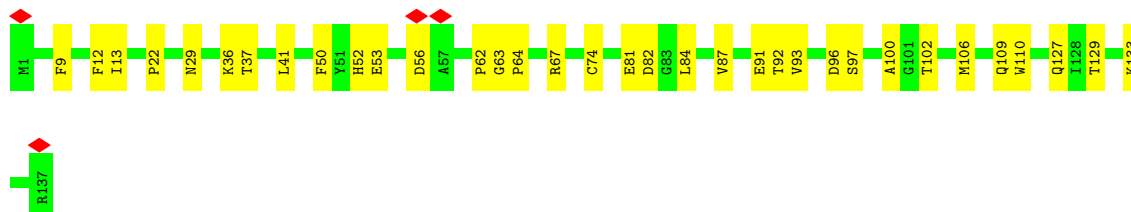
- Molecule 2: Minor capsid protein, gp10

Chain 0F:  75%

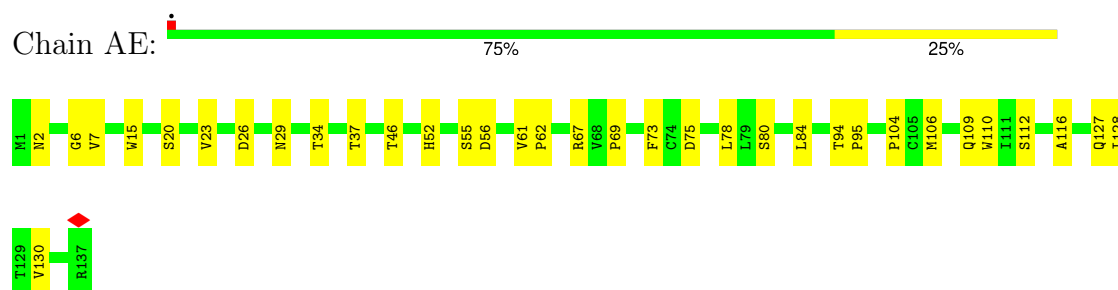


- Molecule 2: Minor capsid protein, gp10

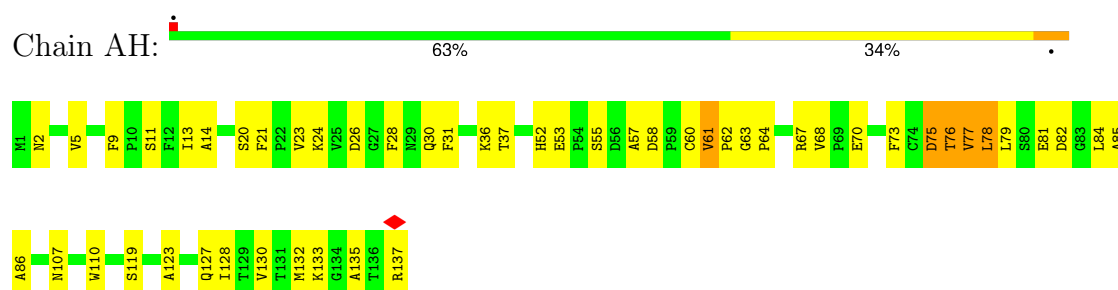
Chain AD:  75%



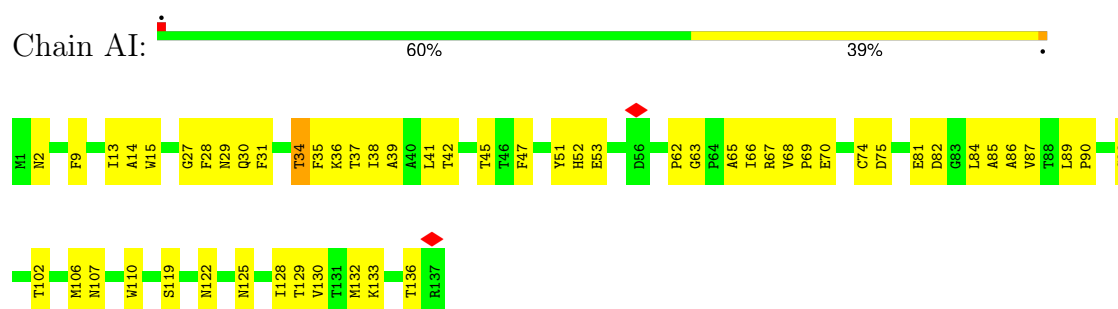
- Molecule 2: Minor capsid protein, gp10



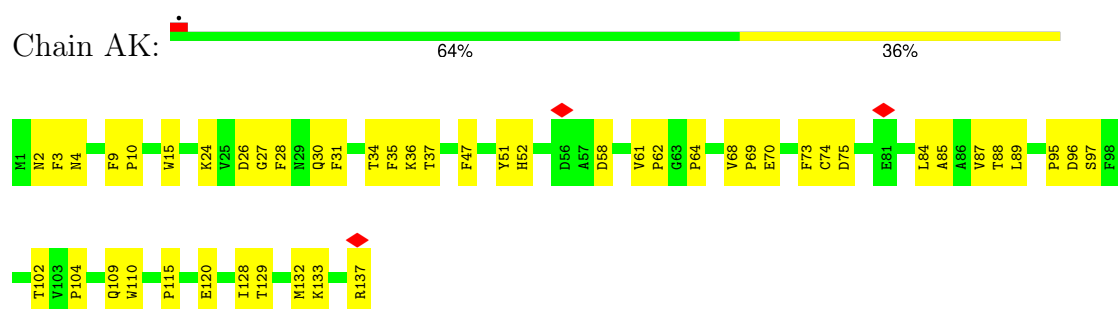
- Molecule 2: Minor capsid protein, gp10



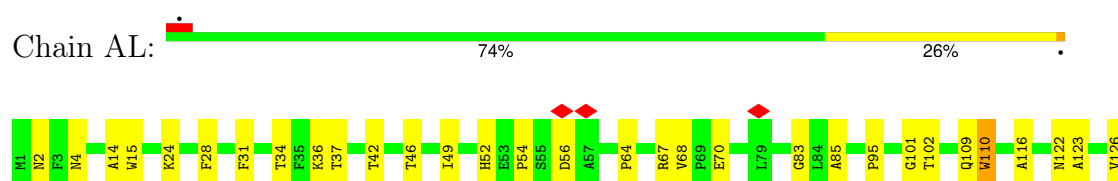
- Molecule 2: Minor capsid protein, gp10



- Molecule 2: Minor capsid protein, gp10



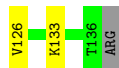
- Molecule 2: Minor capsid protein, gp10





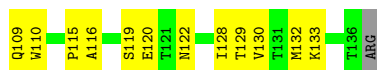
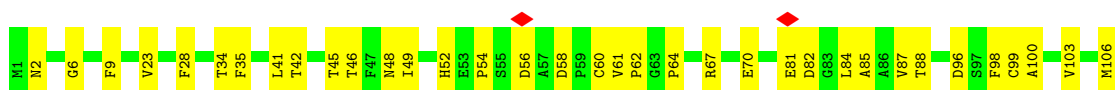
- Molecule 2: Minor capsid protein, gp10

Chain AM: 73% 26%



- Molecule 2: Minor capsid protein, gp10

Chain AN: 65% 34%



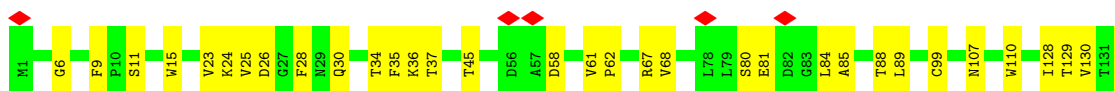
- Molecule 2: Minor capsid protein, gp10

Chain 0G: 74% 26%



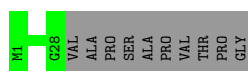
- Molecule 2: Minor capsid protein, gp10

Chain 0H: 74% 26%

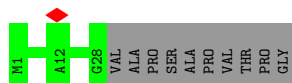


- Molecule 3: Linking protein 2, gp128

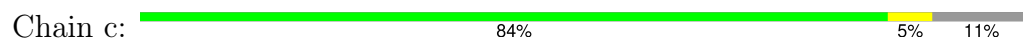
Chain a: 74% 26%



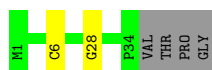
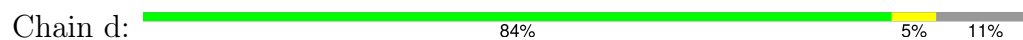
- Molecule 3: Linking protein 2, gp128



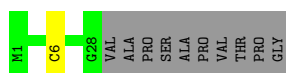
- Molecule 3: Linking protein 2, gp128



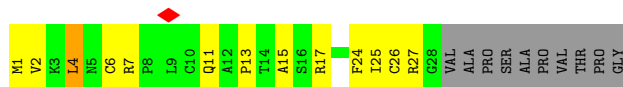
- Molecule 3: Linking protein 2, gp128



- Molecule 3: Linking protein 2, gp128



- Molecule 3: Linking protein 2, gp128

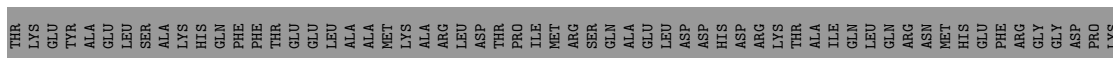


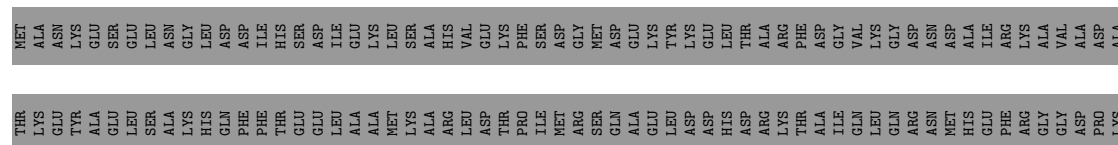
- Molecule 3: Linking protein 2, gp128

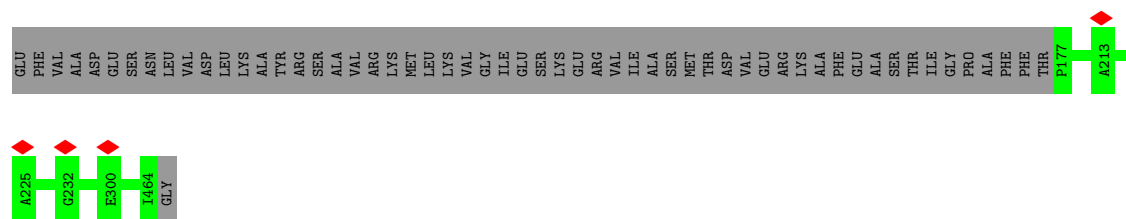


- Molecule 3: Linking protein 2, gp128



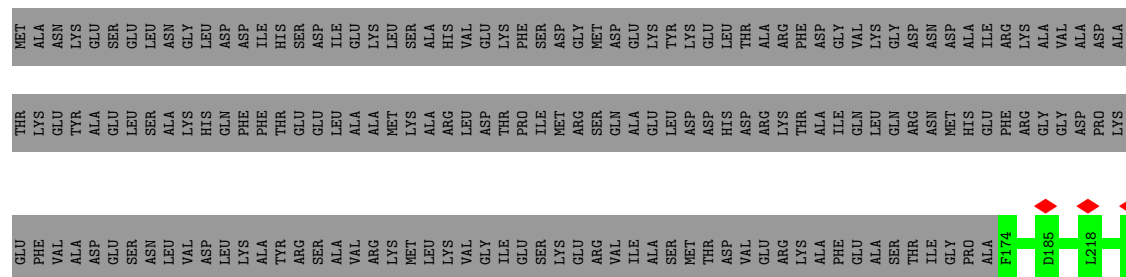






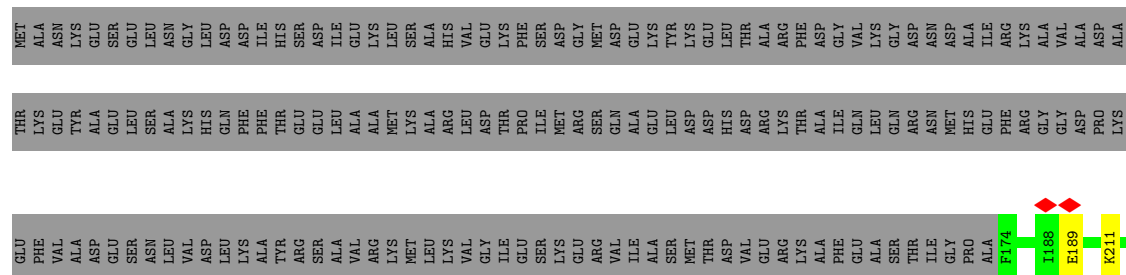
- Molecule 4: Major capsid protein, gp9

Chain n: 62% 37%



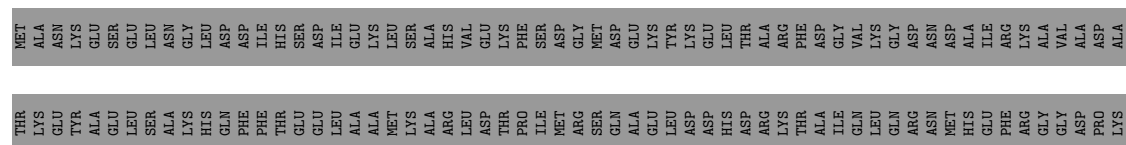
- Molecule 4: Major capsid protein, gp9

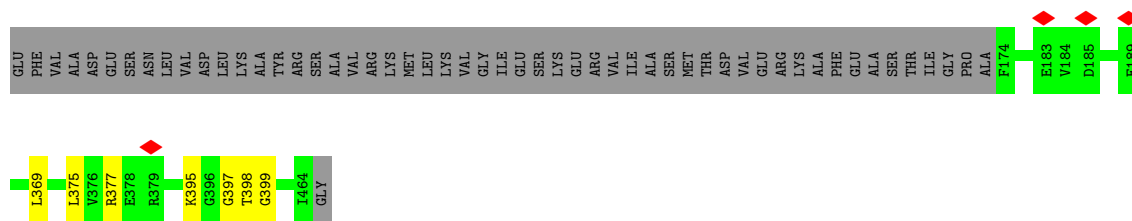
Chain o: 62% 37%



- Molecule 4: Major capsid protein, gp9

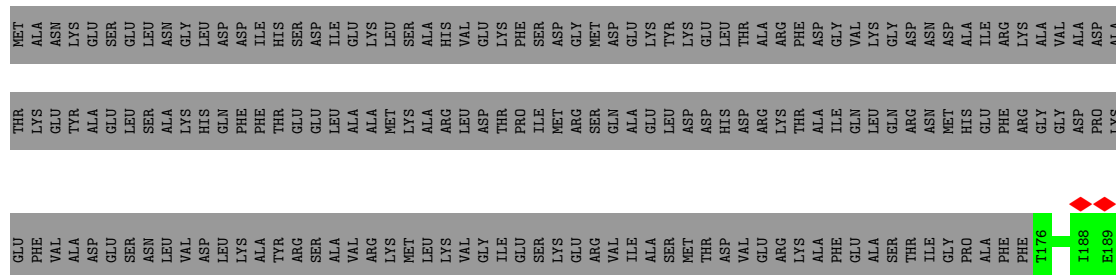
Chain r: 61% 37%





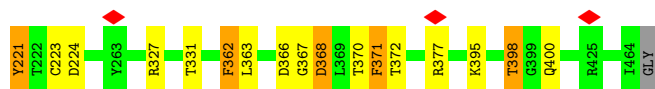
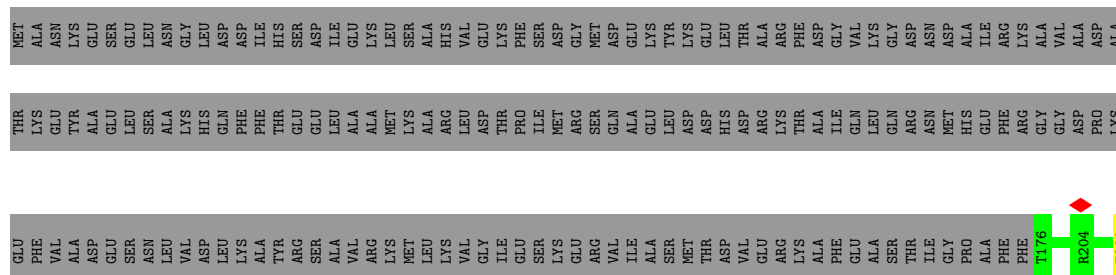
• Molecule 4: Major capsid protein, gp9

Chain w: 59% 38%



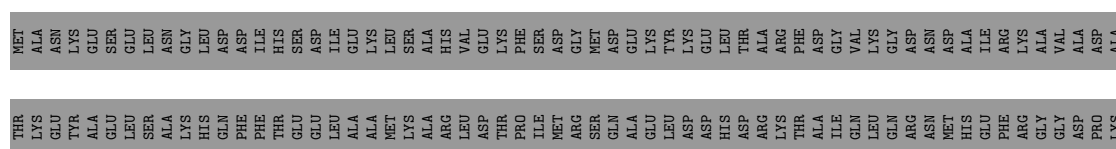
• Molecule 4: Major capsid protein, gp9

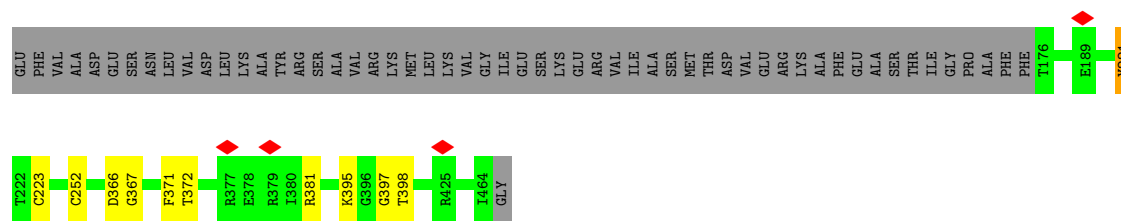
Chain x: 58% 38%



• Molecule 4: Major capsid protein, gp9

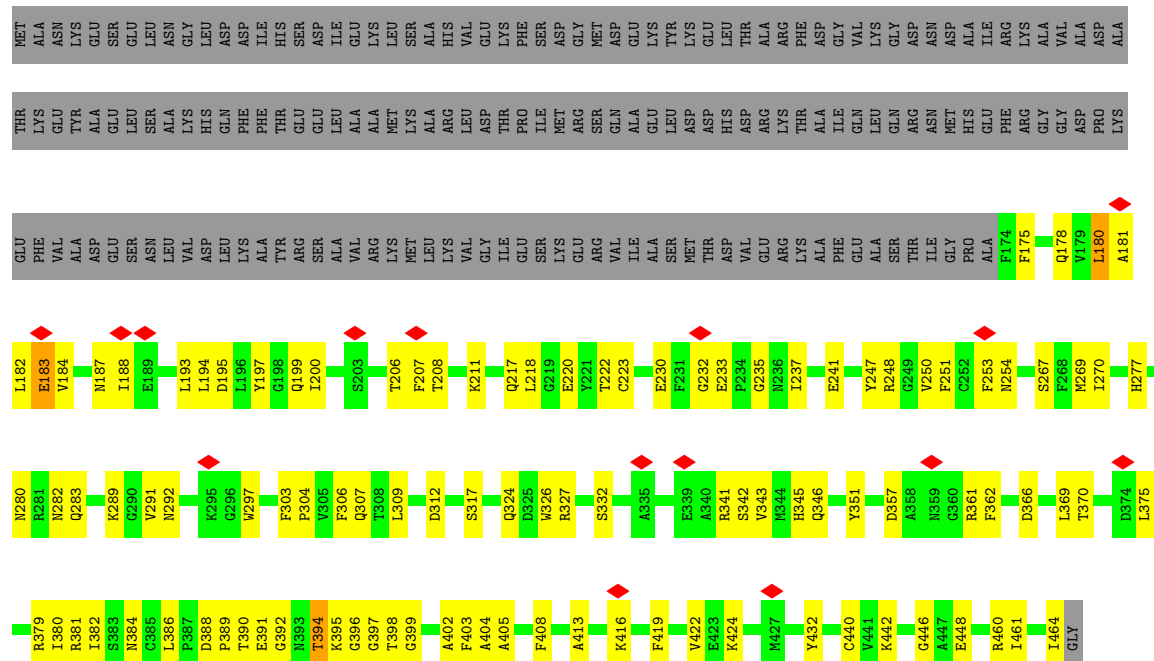
Chain y: 60% 38%





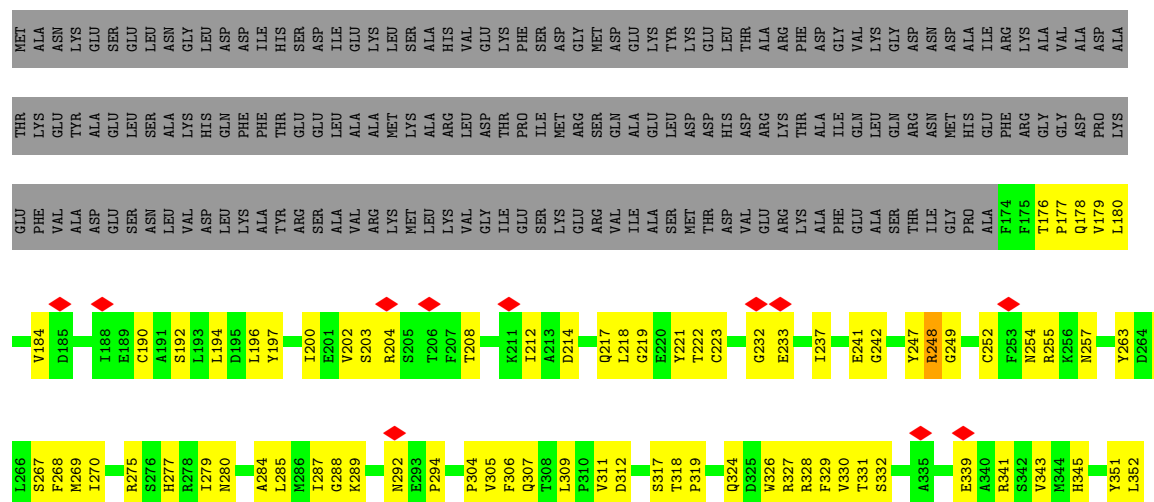
• Molecule 4: Major capsid protein, gp9

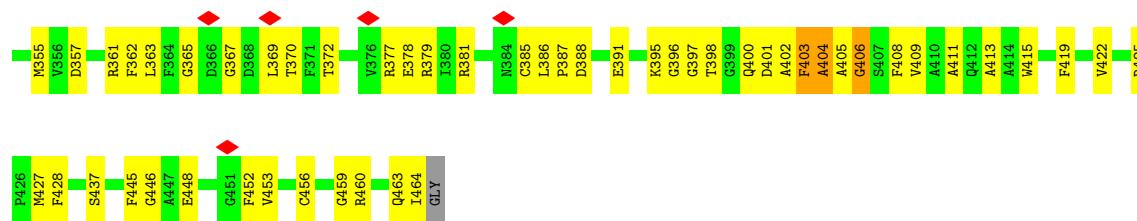
Chain AA: 40% 22% 37%



• Molecule 4: Major capsid protein, gp9

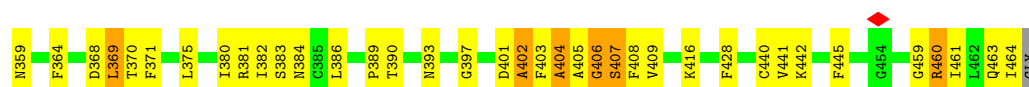
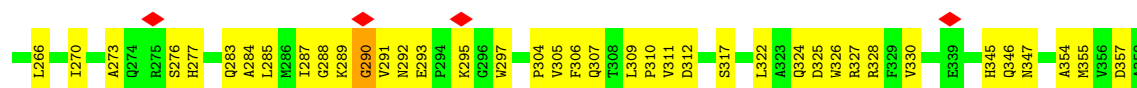
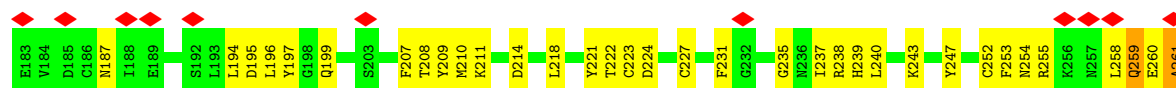
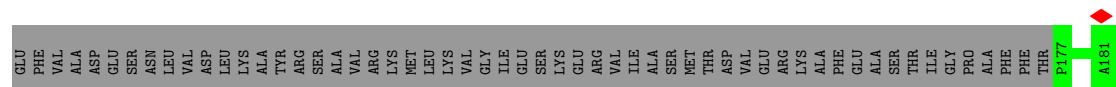
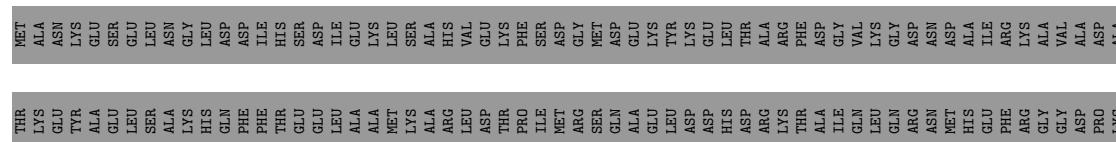
Chain AB: 35% 27% 37%





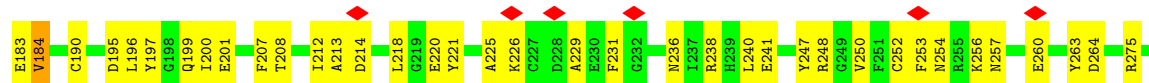
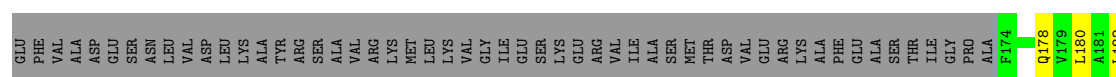
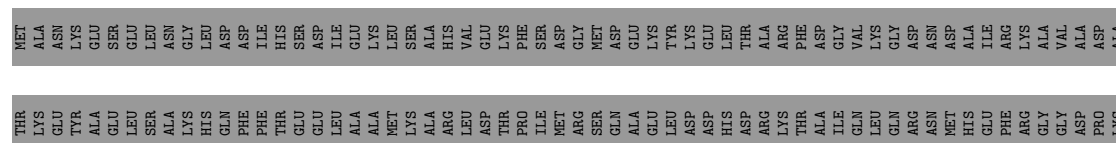
- Molecule 4: Major capsid protein, gp9

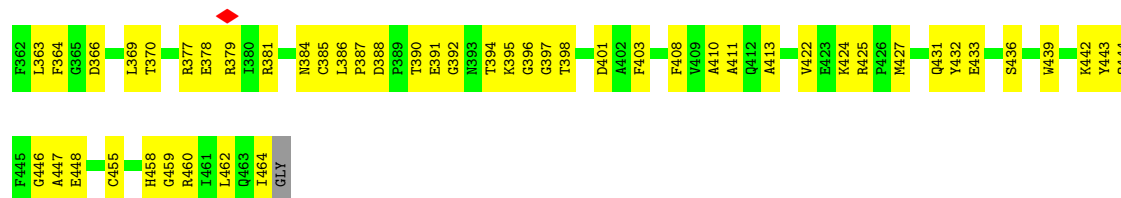
Chain AC: 38% 22% 38%



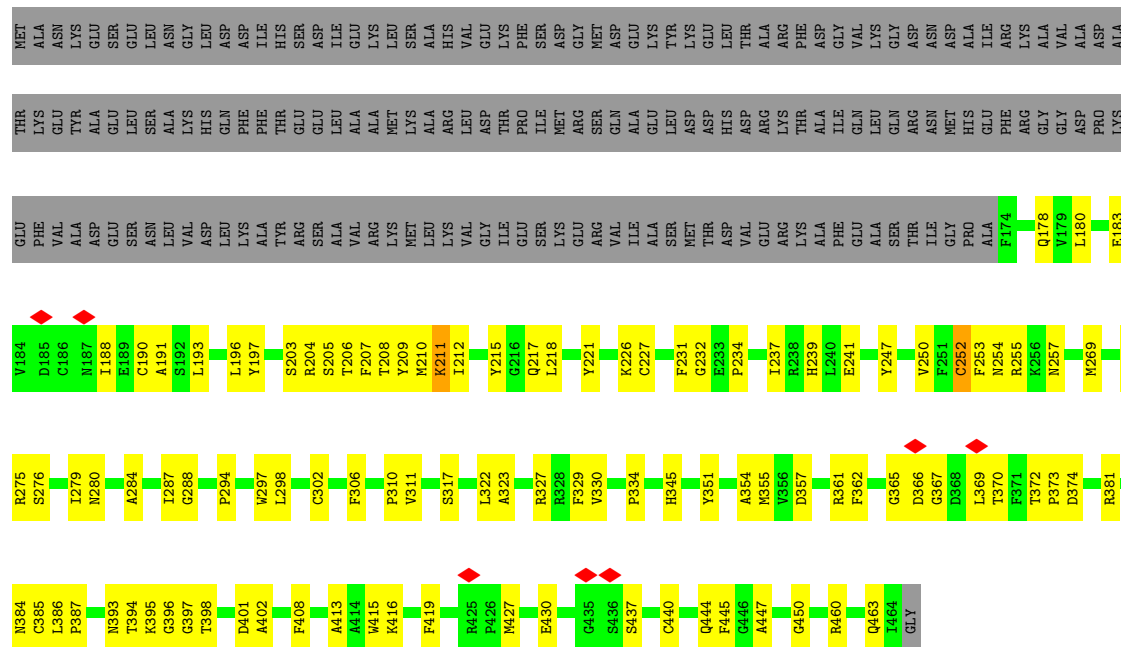
- Molecule 4: Major capsid protein, gp9

Chain AF: 35% 27% 37%

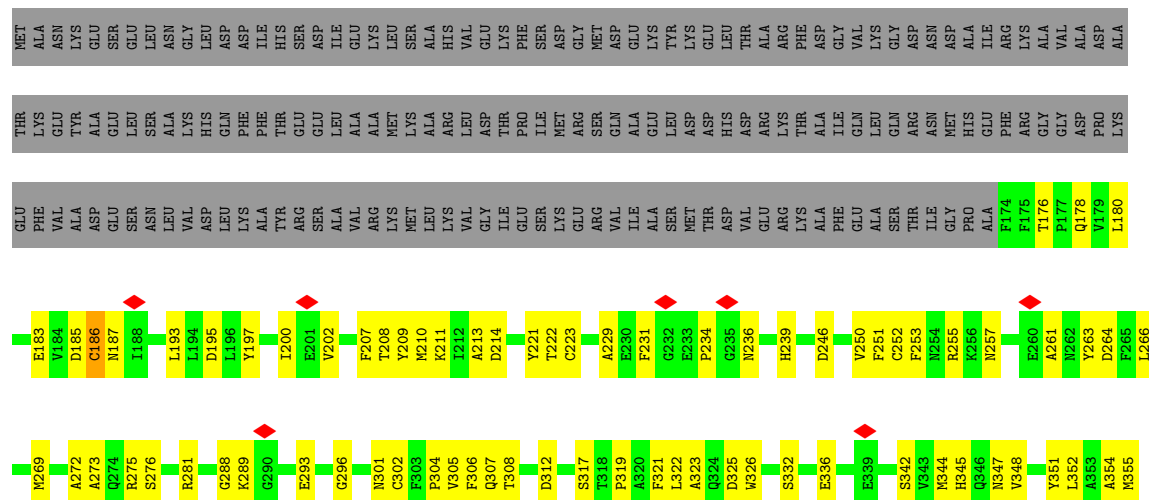


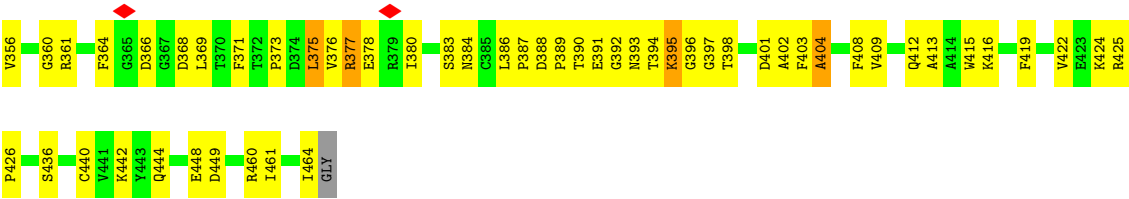


• Molecule 4: Major capsid protein, gp9



• Molecule 4: Major capsid protein, gp9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	15740	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.120	Depositor
Minimum map value	-0.429	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	1105.92, 1105.92, 1105.92	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.44, 1.44, 1.44	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.40	0/134	0.65	0/180
1	0A	0.23	0/134	0.58	0/180
1	0B	0.33	0/134	0.70	0/180
1	0C	0.31	0/134	0.67	0/180
1	0D	0.28	0/134	0.62	0/180
1	f	0.29	0/160	0.49	0/215
2	0E	0.29	0/1052	0.48	0/1443
2	0F	0.27	0/1052	0.50	0/1443
2	0G	0.31	0/1052	0.47	0/1443
2	0H	0.27	0/1052	0.49	0/1443
2	1	0.28	0/1052	0.54	0/1443
2	2	0.27	0/1052	0.48	0/1443
2	3	0.29	0/1052	0.51	0/1443
2	4	0.28	0/1052	0.48	0/1443
2	5	0.30	0/1052	0.52	0/1443
2	6	0.28	0/1052	0.47	0/1443
2	7	0.28	0/1052	0.51	1/1443 (0.1%)
2	8	0.27	0/1052	0.48	0/1443
2	9	0.28	0/1052	0.52	0/1443
2	AD	0.27	0/1052	0.49	0/1443
2	AE	0.28	0/1052	0.48	0/1443
2	AH	0.38	0/1052	0.56	0/1443
2	AI	0.27	0/1052	0.49	0/1443
2	AK	0.27	0/1052	0.46	0/1443
2	AL	0.27	0/1052	0.52	0/1443
2	AM	0.27	0/1040	0.51	0/1429
2	AN	0.26	0/1040	0.49	0/1429
2	l	0.29	0/1052	0.52	0/1443
2	m	0.29	0/1052	0.48	0/1443
2	p	0.32	0/1052	0.51	0/1443
2	q	0.29	0/1052	0.49	0/1443
2	s	0.28	0/1052	0.49	0/1443
2	t	0.30	0/1052	0.53	0/1443
2	u	0.28	0/1040	0.53	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	v	0.28	0/1040	0.52	1/1429 (0.1%)
2	z	0.28	0/1052	0.48	0/1443
3	AO	0.34	0/213	0.72	1/288 (0.3%)
3	AP	0.28	0/213	0.59	0/288
3	AQ	0.29	0/213	0.64	0/288
3	AR	0.31	0/213	0.62	0/288
3	AS	0.31	0/213	0.66	0/288
3	AT	0.29	0/213	0.53	0/288
3	a	0.28	0/213	0.45	0/288
3	b	0.26	0/213	0.48	0/288
3	c	0.28	0/252	0.49	0/344
3	d	0.30	0/252	0.53	0/344
3	e	0.26	0/213	0.48	0/288
4	AA	0.29	0/2344	0.51	0/3171
4	AB	0.31	0/2344	0.53	1/3171 (0.0%)
4	AC	0.31	0/2313	0.55	0/3128
4	AF	0.29	0/2344	0.49	0/3171
4	AG	0.28	0/2344	0.48	0/3171
4	AJ	0.31	0/2344	0.52	0/3171
4	g	0.28	0/2344	0.46	0/3171
4	h	0.30	0/2344	0.52	0/3171
4	i	0.31	0/2320	0.51	0/3139
4	j	0.31	0/2320	0.53	0/3139
4	k	0.27	0/2313	0.45	0/3128
4	n	0.26	0/2344	0.46	0/3171
4	o	0.27	0/2344	0.47	0/3171
4	r	0.28	0/2344	0.49	1/3171 (0.0%)
4	w	0.32	0/2320	0.53	0/3139
4	x	0.32	0/2320	0.55	0/3139
4	y	0.31	0/2320	0.54	0/3139
All	All	0.29	0/74429	0.51	5/101290 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AO	4	LEU	CB-CG-CD1	-5.70	101.31	111.00
2	v	96	ASP	CB-CG-OD1	5.18	122.97	118.30
2	7	82	ASP	CB-CG-OD1	5.14	122.92	118.30
4	AB	248	ARG	NE-CZ-NH1	-5.12	117.74	120.30
4	r	369	LEU	CA-CB-CG	5.09	127.00	115.30

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	0	133	0	136	5	0
1	0A	133	0	135	5	0
1	0B	133	0	136	5	0
1	0C	133	0	135	8	0
1	0D	133	0	135	1	0
1	f	158	0	158	0	0
2	0E	1023	0	975	31	0
2	0F	1023	0	974	28	0
2	0G	1023	0	975	28	0
2	0H	1023	0	975	27	0
2	1	1023	0	974	33	0
2	2	1023	0	976	30	0
2	3	1023	0	975	25	0
2	4	1023	0	975	29	0
2	5	1023	0	975	28	0
2	6	1023	0	974	27	0
2	7	1023	0	975	34	0
2	8	1023	0	975	27	0
2	9	1023	0	975	30	0
2	AD	1023	0	976	29	0
2	AE	1023	0	974	25	0
2	AH	1023	0	976	53	0
2	AI	1023	0	976	46	0
2	AK	1023	0	975	39	0
2	AL	1023	0	976	26	0
2	AM	1011	0	963	29	0
2	AN	1011	0	962	48	0
2	l	1023	0	974	0	0
2	m	1023	0	974	0	0
2	p	1023	0	975	0	0
2	q	1023	0	974	0	0
2	s	1023	0	974	0	0
2	t	1023	0	975	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	u	1011	0	961	0	0
2	v	1011	0	961	0	0
2	z	1023	0	975	0	0
3	AO	209	0	226	11	0
3	AP	209	0	226	23	0
3	AQ	209	0	226	16	0
3	AR	209	0	225	18	0
3	AS	209	0	226	17	0
3	AT	209	0	225	14	0
3	a	209	0	223	0	0
3	b	209	0	223	0	0
3	c	246	0	261	0	0
3	d	246	0	260	0	0
3	e	209	0	222	0	0
4	AA	2286	0	2155	105	0
4	AB	2286	0	2154	116	0
4	AC	2257	0	2131	114	0
4	AF	2286	0	2155	122	0
4	AG	2286	0	2156	93	0
4	AJ	2286	0	2155	125	0
4	g	2286	0	2154	0	0
4	h	2286	0	2153	0	0
4	i	2264	0	2135	0	0
4	j	2264	0	2136	0	0
4	k	2257	0	2131	0	0
4	n	2286	0	2153	0	0
4	o	2286	0	2154	0	0
4	r	2286	0	2155	0	0
4	w	2264	0	2136	0	0
4	x	2264	0	2136	0	0
4	y	2264	0	2136	0	0
All	All	72532	0	69057	1221	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 18.

All (1221) 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)
4:AJ:397:GLY:HA3	4:AJ:401:ASP:HB3	1.23	1.14
2:AH:55:SER:HB3	2:AH:61:VAL:HG23	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AH:58:ASP:HB3	2:AH:61:VAL:HG22	1.49	0.93
2:0F:62:PRO:HB3	2:0F:110:TRP:HE1	1.34	0.92
2:0G:74:CYS:SG	2:0G:75:ASP:N	2.42	0.92
4:AG:218:LEU:HA	4:AG:232:GLY:HA3	1.52	0.88
4:AC:258:LEU:HD23	4:AC:259:GLN:H	1.41	0.86
2:AH:73:PHE:HD2	2:AH:76:THR:HG1	1.22	0.85
4:AF:327:ARG:HG3	4:AG:370:THR:HA	1.60	0.84
4:AJ:253:PHE:HZ	4:AJ:269:MET:HG3	1.45	0.82
2:AD:97:SER:HA	3:AR:8:PRO:HA	1.63	0.79
4:AF:307:GLN:HE22	3:AS:15:ALA:HB1	1.47	0.79
4:AA:181:ALA:HB3	4:AJ:209:TYR:CB	2.12	0.79
4:AC:291:VAL:HG22	4:AC:292:ASN:HD22	1.48	0.78
4:AF:306:PHE:HA	3:AS:16:SER:HB2	1.66	0.78
2:0F:24:LYS:HA	2:0F:110:TRP:HB3	1.64	0.78
2:AH:9:PHE:HE1	2:AH:133:LYS:HG2	1.48	0.77
2:6:67:ARG:HG2	2:6:84:LEU:HD13	1.65	0.77
4:AG:211:LYS:HA	4:AJ:183:GLU:HG3	1.66	0.77
4:AA:327:ARG:HG3	4:AB:370:THR:HA	1.67	0.77
4:AA:375:LEU:HD12	4:AA:380:ILE:HB	1.67	0.77
2:AN:23:VAL:HG21	2:AN:130:VAL:HG11	1.67	0.76
2:2:67:ARG:HH22	2:2:86:ALA:HB2	1.50	0.76
4:AA:309:LEU:HB2	3:AQ:27:ARG:HH11	1.51	0.75
4:AF:229:ALA:HB3	4:AG:250:VAL:HG13	1.66	0.75
4:AG:204:ARG:NH1	4:AJ:176:THR:O	2.20	0.75
2:5:24:LYS:HA	2:5:110:TRP:HB3	1.69	0.74
4:AG:212:ILE:HG22	4:AG:237:ILE:HD12	1.70	0.74
2:9:62:PRO:HA	2:9:110:TRP:HZ2	1.53	0.74
2:4:34:THR:HG21	2:5:11:SER:H	1.52	0.73
4:AA:207:PHE:HB2	4:AB:180:LEU:HD22	1.70	0.73
2:5:74:CYS:SG	2:5:75:ASP:N	2.60	0.73
4:AG:197:TYR:HH	4:AG:297:TRP:HE1	1.32	0.73
2:0H:24:LYS:HA	2:0H:110:TRP:HB3	1.68	0.73
4:AA:398:THR:HA	4:AA:403:PHE:HB2	1.69	0.73
1:0B:16:VAL:HG22	1:0B:18:PRO:HD3	1.70	0.73
2:5:46:THR:HG23	2:5:116:ALA:HB3	1.71	0.73
4:AC:375:LEU:HD12	4:AC:380:ILE:HB	1.71	0.72
3:AT:4:LEU:O	3:AT:5:ASN:OD1	2.07	0.72
2:9:68:VAL:HG13	2:9:85:ALA:HB3	1.71	0.72
4:AA:187:ASN:HD21	4:AJ:214:ASP:HA	1.53	0.72
2:AL:46:THR:HG23	2:AL:116:ALA:HB3	1.70	0.72
2:AN:67:ARG:HE	2:AN:84:LEU:HB2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AG:190:CYS:SG	4:AG:191:ALA:N	2.63	0.72
4:AA:208:THR:HG22	4:AA:241:GLU:HG2	1.72	0.72
4:AF:190:CYS:SG	4:AF:385:CYS:N	2.63	0.72
2:AN:70:GLU:HB3	2:AN:85:ALA:HB2	1.70	0.72
2:2:67:ARG:HG2	2:2:84:LEU:HD13	1.71	0.72
4:AA:181:ALA:HB3	4:AJ:209:TYR:HB3	1.72	0.72
2:AD:67:ARG:HG2	2:AD:84:LEU:HD22	1.71	0.71
2:1:26:ASP:OD2	2:1:109:GLN:NE2	2.24	0.71
4:AA:230:GLU:OE1	4:AA:230:GLU:N	2.23	0.71
2:0H:62:PRO:HB3	2:0H:110:TRP:HE1	1.54	0.71
1:0A:16:VAL:HG22	1:0A:18:PRO:HD3	1.73	0.71
4:AF:360:GLY:HA2	3:AO:24:PHE:HZ	1.56	0.71
1:0:7:CYS:SG	2:2:24:LYS:NZ	2.64	0.71
2:4:10:PRO:HD2	2:4:132:MET:HB2	1.73	0.71
4:AF:337:TYR:HE1	4:AG:188:ILE:HD13	1.56	0.70
2:AN:67:ARG:NH2	2:AN:85:ALA:O	2.24	0.70
4:AC:258:LEU:O	4:AC:260:GLU:N	2.24	0.70
4:AC:197:TYR:O	4:AC:199:GLN:NE2	2.25	0.70
2:AK:73:PHE:HE2	2:AK:104:PRO:HG3	1.55	0.70
4:AC:207:PHE:HB2	4:AF:180:LEU:HD22	1.73	0.70
2:7:99:CYS:HA	1:0A:3:CYS:HB2	1.72	0.69
4:AG:394:THR:O	4:AG:401:ASP:HB2	1.92	0.69
2:8:30:GLN:HB2	2:8:133:LYS:HB3	1.73	0.69
4:AF:394:THR:HG23	4:AF:395:LYS:HG2	1.73	0.69
2:1:24:LYS:HA	2:1:110:TRP:HB3	1.74	0.69
2:AD:67:ARG:HD3	2:AD:84:LEU:HD13	1.74	0.69
4:AA:397:GLY:H	4:AA:402:ALA:HB1	1.58	0.69
2:AD:52:HIS:HB2	2:AD:110:TRP:HB2	1.75	0.68
4:AC:306:PHE:HB3	3:AR:18:LEU:HD11	1.75	0.68
2:AD:100:ALA:HB1	2:AE:6:GLY:HA3	1.74	0.68
4:AJ:319:PRO:HG2	4:AJ:402:ALA:HB1	1.75	0.68
2:8:67:ARG:NH1	2:8:85:ALA:O	2.27	0.68
4:AF:455:CYS:SG	4:AF:458:HIS:NE2	2.66	0.68
2:0E:67:ARG:NH1	2:0E:85:ALA:O	2.27	0.68
4:AA:307:GLN:HG3	3:AT:15:ALA:HB1	1.75	0.68
2:AM:81:GLU:HG2	2:AM:82:ASP:H	1.59	0.68
2:7:97:SER:HA	1:0A:5:ASN:HD22	1.59	0.68
2:AH:81:GLU:HG2	2:AH:82:ASP:H	1.59	0.68
2:1:25:VAL:HG12	2:1:110:TRP:HA	1.74	0.67
2:AI:81:GLU:HG2	2:AI:82:ASP:H	1.57	0.67
2:AK:97:SER:HA	3:AQ:8:PRO:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AB:202:VAL:HG22	4:AB:203:SER:H	1.60	0.67
4:AC:389:PRO:HG3	4:AC:409:VAL:HA	1.75	0.67
4:AJ:390:THR:HA	4:AJ:395:LYS:HB2	1.75	0.67
2:6:30:GLN:HB2	2:6:133:LYS:HB3	1.76	0.67
4:AF:427:MET:HG3	4:AF:447:ALA:HB2	1.75	0.67
4:AC:210:MET:SD	4:AC:239:HIS:ND1	2.67	0.67
4:AG:397:GLY:N	4:AG:401:ASP:O	2.26	0.67
4:AC:197:TYR:HE2	4:AC:285:LEU:HD13	1.59	0.67
2:2:103:VAL:O	2:3:2:ASN:ND2	2.28	0.67
2:5:23:VAL:HG21	2:5:130:VAL:HG11	1.77	0.66
4:AB:217:GLN:O	4:AB:233:GLU:N	2.29	0.66
2:6:67:ARG:HH22	2:6:86:ALA:HB2	1.59	0.66
2:AN:45:THR:HG21	2:AN:122:ASN:HB2	1.77	0.66
2:3:24:LYS:HA	2:3:110:TRP:HB3	1.77	0.66
2:6:52:HIS:HB2	2:6:110:TRP:HB2	1.78	0.66
4:AJ:398:THR:HB	3:AP:22:PRO:HG3	1.77	0.66
2:0H:25:VAL:HG12	2:0H:110:TRP:HA	1.77	0.66
4:AF:240:LEU:HA	2:AH:135:ALA:HB3	1.77	0.66
4:AF:324:GLN:NE2	4:AG:354:ALA:O	2.22	0.66
2:AN:48:ASN:HB3	2:AN:67:ARG:HH12	1.60	0.66
4:AB:355:MET:HB3	4:AB:363:LEU:HD13	1.78	0.66
2:AI:52:HIS:HB2	2:AI:110:TRP:HB2	1.77	0.66
4:AJ:373:PRO:HG2	4:AJ:375:LEU:HD13	1.78	0.66
4:AJ:389:PRO:HG3	4:AJ:409:VAL:HA	1.76	0.66
4:AB:427:MET:HA	4:AB:446:GLY:O	1.96	0.66
4:AG:255:ARG:NH2	4:AG:437:SER:O	2.27	0.66
2:0F:58:ASP:HB3	2:0F:61:VAL:HG12	1.77	0.65
2:0H:36:LYS:NZ	2:0H:37:THR:O	2.29	0.65
4:AA:369:LEU:HD23	4:AA:370:THR:HG23	1.79	0.65
4:AC:325:ASP:OD2	3:AO:27:ARG:NH1	2.30	0.65
2:9:68:VAL:HG23	2:9:107:ASN:HD21	1.62	0.65
4:AB:357:ASP:OD1	4:AB:361:ARG:N	2.29	0.65
4:AA:197:TYR:O	4:AA:199:GLN:NE2	2.29	0.65
4:AF:330:VAL:HG23	4:AF:331:THR:HG23	1.79	0.65
2:2:23:VAL:HG11	2:2:130:VAL:HG11	1.78	0.65
2:4:41:LEU:HD22	2:4:122:ASN:HB3	1.79	0.64
2:0F:25:VAL:HG22	2:0F:110:TRP:HA	1.77	0.64
2:AH:28:PHE:HD2	2:AH:132:MET:HG2	1.62	0.64
2:0G:67:ARG:NH1	2:0G:85:ALA:O	2.31	0.64
4:AA:181:ALA:HB3	4:AJ:209:TYR:CG	2.32	0.64
2:AH:52:HIS:HB2	2:AH:110:TRP:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0F:30:GLN:HB2	2:0F:133:LYS:HB3	1.80	0.64
2:AK:35:PHE:HB2	2:AK:99:CYS:HB3	1.79	0.64
2:9:30:GLN:HB2	2:9:133:LYS:HB3	1.80	0.64
4:AG:396:GLY:N	4:AG:401:ASP:O	2.31	0.64
2:AH:62:PRO:HA	2:AH:110:TRP:CE3	2.33	0.64
2:AK:69:PRO:HA	2:AK:84:LEU:HA	1.79	0.64
4:AA:247:TYR:HB2	4:AA:446:GLY:HA2	1.79	0.63
4:AJ:347:ASN:ND2	4:AJ:392:GLY:O	2.31	0.63
2:AK:74:CYS:SG	2:AK:75:ASP:N	2.71	0.63
2:AL:24:LYS:HA	2:AL:110:TRP:HB3	1.81	0.63
2:AD:102:THR:OG1	2:AE:2:ASN:ND2	2.32	0.63
4:AF:377:ARG:HH11	4:AF:378:GLU:HG2	1.63	0.63
2:AN:46:THR:HG23	2:AN:116:ALA:HB3	1.80	0.63
2:1:28:PHE:HA	2:1:135:ALA:HB2	1.81	0.63
1:0C:7:CYS:SG	1:0C:8:GLY:N	2.71	0.63
4:AC:211:LYS:HG3	4:AF:184:VAL:HG22	1.80	0.63
4:AB:402:ALA:O	4:AB:403:PHE:HB3	1.98	0.63
4:AF:254:ASN:HB3	4:AF:257:ASN:HB3	1.79	0.63
4:AG:193:LEU:HD23	4:AG:381:ARG:HH11	1.63	0.63
2:AK:24:LYS:HE2	2:AK:26:ASP:HB3	1.81	0.63
2:AL:49:ILE:O	2:AL:67:ARG:NH2	2.32	0.63
2:AL:15:TRP:HB3	2:AL:128:ILE:HB	1.81	0.63
2:1:68:VAL:HG13	2:1:85:ALA:HB3	1.81	0.62
2:1:74:CYS:SG	2:1:75:ASP:N	2.72	0.62
2:7:68:VAL:HG23	2:7:107:ASN:HD21	1.64	0.62
4:AC:306:PHE:HE2	4:AC:460:ARG:HG2	1.63	0.62
4:AF:247:TYR:O	4:AF:446:GLY:HA2	1.98	0.62
4:AA:184:VAL:HG13	4:AJ:211:LYS:HD3	1.81	0.62
4:AC:284:ALA:O	4:AC:288:GLY:N	2.29	0.62
4:AJ:332:SER:O	4:AJ:460:ARG:NH1	2.32	0.62
2:3:62:PRO:HB3	2:3:110:TRP:HE1	1.63	0.62
2:7:24:LYS:HA	2:7:110:TRP:HB3	1.79	0.62
4:AA:247:TYR:HH	4:AA:277:HIS:CE1	2.15	0.62
4:AF:182:LEU:HD23	4:AF:183:GLU:H	1.64	0.62
4:AF:413:ALA:HB2	4:AF:459:GLY:HA2	1.80	0.62
2:5:54:PRO:HD3	2:5:109:GLN:HG3	1.82	0.62
2:AH:58:ASP:C	2:AH:60:CYS:H	2.03	0.62
2:AE:37:THR:HG23	2:AE:95:PRO:HA	1.81	0.62
2:AN:49:ILE:HD11	2:AN:87:VAL:HG23	1.82	0.62
4:AA:312:ASP:HA	4:AA:317:SER:HA	1.81	0.62
4:AJ:395:LYS:O	4:AJ:403:PHE:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AN:48:ASN:HB3	2:AN:67:ARG:NH1	2.15	0.62
2:AE:55:SER:HB3	2:AE:61:VAL:HG13	1.82	0.62
2:AK:30:GLN:HB2	2:AK:133:LYS:HB3	1.81	0.62
4:AC:328:ARG:NH1	3:AR:19:VAL:O	2.32	0.61
2:3:15:TRP:HB3	2:3:128:ILE:HB	1.82	0.61
2:4:23:VAL:HG11	2:4:130:VAL:HG11	1.81	0.61
4:AC:258:LEU:CD2	4:AC:259:GLN:H	2.11	0.61
2:AH:58:ASP:HB3	2:AH:61:VAL:CG2	2.26	0.61
2:9:24:LYS:HA	2:9:110:TRP:HB3	1.82	0.61
2:7:28:PHE:CD1	2:7:135:ALA:HB2	2.35	0.61
2:9:25:VAL:HG22	2:9:110:TRP:HA	1.82	0.61
4:AA:200:ILE:HB	4:AA:422:VAL:HG12	1.83	0.61
4:AF:361:ARG:NH1	4:AF:366:ASP:OD2	2.33	0.61
4:AJ:312:ASP:HA	4:AJ:317:SER:HA	1.82	0.61
2:1:30:GLN:HB2	2:1:133:LYS:HB3	1.83	0.61
2:AD:87:VAL:HG23	3:AR:2:VAL:HG11	1.83	0.61
4:AG:427:MET:HA	4:AG:447:ALA:HB2	1.82	0.61
2:AN:96:ASP:OD1	3:AP:10:CYS:HB2	2.01	0.61
2:0F:26:ASP:OD2	2:0F:109:GLN:NE2	2.34	0.61
4:AG:190:CYS:SG	4:AG:385:CYS:N	2.74	0.61
4:AA:397:GLY:N	4:AA:402:ALA:HB1	2.15	0.61
2:2:41:LEU:HD22	2:2:122:ASN:HB3	1.82	0.60
4:AA:361:ARG:NH1	4:AA:366:ASP:OD2	2.33	0.60
2:AI:69:PRO:HA	2:AI:84:LEU:HB3	1.81	0.60
2:AK:27:GLY:HA2	2:AK:137:ARG:HD3	1.83	0.60
4:AF:432:TYR:HB2	4:AF:444:GLN:HG3	1.83	0.60
2:AI:14:ALA:HB2	2:AI:130:VAL:HG23	1.83	0.60
4:AC:255:ARG:H	4:AC:258:LEU:HD13	1.66	0.60
4:AJ:361:ARG:NH1	4:AJ:366:ASP:OD2	2.34	0.60
2:AK:36:LYS:NZ	2:AK:37:THR:O	2.33	0.60
2:AE:7:VAL:HB	3:AR:5:ASN:HD22	1.66	0.60
4:AJ:319:PRO:HB3	4:AJ:464:ILE:HG21	1.84	0.60
2:6:36:LYS:NZ	2:6:95:PRO:O	2.35	0.60
2:1:62:PRO:HB3	2:1:110:TRP:HE1	1.66	0.60
2:0F:28:PHE:CD1	2:0F:135:ALA:HB2	2.37	0.60
4:AA:217:GLN:OE1	4:AB:280:ASN:ND2	2.35	0.60
2:2:67:ARG:NH1	2:2:85:ALA:O	2.34	0.60
2:7:62:PRO:HA	2:7:110:TRP:CZ2	2.36	0.60
4:AF:240:LEU:HD12	2:AH:137:ARG:H	1.67	0.60
2:AI:67:ARG:HH22	2:AI:86:ALA:HB2	1.66	0.60
4:AJ:396:GLY:HA2	4:AJ:403:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:68:VAL:HG23	2:3:107:ASN:HD21	1.67	0.60
2:AH:75:ASP:O	2:AH:76:THR:C	2.39	0.60
4:AA:303:PHE:HD2	4:AA:461:ILE:HG12	1.66	0.60
2:AK:52:HIS:HB2	2:AK:110:TRP:HB2	1.84	0.60
2:6:31:PHE:HB3	2:6:132:MET:HG3	1.84	0.59
2:2:34:THR:HG21	2:3:11:SER:H	1.67	0.59
2:AH:76:THR:O	2:AH:77:VAL:C	2.41	0.59
2:AN:46:THR:HA	2:AN:88:THR:HA	1.85	0.59
2:5:37:THR:HG23	2:5:95:PRO:HA	1.84	0.59
2:0E:115:PRO:HB2	2:0E:120:GLU:HG2	1.85	0.59
4:AA:309:LEU:HB2	3:AQ:27:ARG:NH1	2.18	0.59
2:6:30:GLN:HG2	2:7:2:ASN:HA	1.84	0.59
4:AC:214:ASP:O	4:AC:235:GLY:HA3	2.02	0.59
2:AE:7:VAL:HB	3:AR:5:ASN:ND2	2.17	0.59
4:AG:366:ASP:OD1	4:AJ:361:ARG:NH2	2.35	0.59
4:AJ:288:GLY:O	4:AJ:296:GLY:N	2.33	0.59
2:5:68:VAL:HG13	2:5:85:ALA:HB3	1.85	0.59
3:AO:6:CYS:SG	3:AO:7:ARG:N	2.76	0.59
2:4:70:GLU:HB3	2:4:85:ALA:HA	1.84	0.59
4:AC:221:TYR:OH	4:AF:281:ARG:HA	2.02	0.59
4:AF:221:TYR:CD1	4:AG:247:TYR:HB3	2.38	0.59
4:AA:218:LEU:O	4:AA:220:GLU:HG2	2.03	0.59
4:AA:222:THR:HG21	4:AB:248:ARG:HG2	1.85	0.59
2:AE:67:ARG:HG2	2:AE:84:LEU:HD22	1.82	0.59
2:AH:2:ASN:ND2	2:AI:102:THR:OG1	2.35	0.59
4:AG:393:ASN:HB3	3:AS:18:LEU:HA	1.85	0.59
2:AH:73:PHE:HD2	2:AH:76:THR:OG1	1.83	0.59
2:AN:34:THR:OG1	2:AN:129:THR:OG1	2.21	0.59
2:4:11:SER:H	2:5:34:THR:HG21	1.67	0.59
2:6:58:ASP:HB3	2:6:61:VAL:HG22	1.85	0.59
1:0B:3:CYS:SG	1:0B:4:ARG:N	2.75	0.59
4:AF:345:HIS:HB3	4:AF:348:VAL:HG23	1.84	0.59
4:AF:250:VAL:HG23	4:AF:444:GLN:HG2	1.84	0.58
2:4:36:LYS:NZ	2:4:95:PRO:O	2.33	0.58
2:1:49:ILE:O	2:1:67:ARG:NH2	2.36	0.58
2:7:68:VAL:HG13	2:7:85:ALA:HB3	1.85	0.58
2:0F:9:PHE:CE1	2:0F:133:LYS:HG2	2.38	0.58
4:AF:332:SER:O	4:AF:460:ARG:NH1	2.36	0.58
2:0H:58:ASP:HB3	2:0H:61:VAL:HG12	1.84	0.58
2:0E:35:PHE:HB2	2:0E:99:CYS:HB2	1.86	0.58
4:AB:405:ALA:O	4:AB:406:GLY:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AH:30:GLN:HB2	2:AH:133:LYS:HB3	1.85	0.58
4:AF:354:ALA:O	3:AR:21:PRO:HG2	2.03	0.58
4:AJ:390:THR:HG22	4:AJ:403:PHE:HE1	1.68	0.58
2:AN:99:CYS:HA	3:AP:6:CYS:HA	1.85	0.58
4:AB:398:THR:HB	4:AB:402:ALA:HB3	1.84	0.58
4:AJ:348:VAL:HG22	4:AJ:390:THR:HG23	1.86	0.58
2:7:62:PRO:HA	2:7:110:TRP:HZ2	1.69	0.58
2:9:69:PRO:HA	2:9:84:LEU:HA	1.86	0.58
4:AA:326:TRP:HE1	4:AB:369:LEU:HB3	1.68	0.58
2:AD:52:HIS:ND1	2:AD:64:PRO:O	2.34	0.58
2:0G:72:PRO:HA	3:AT:1:MET:HG3	1.85	0.58
2:6:6:GLY:HA3	2:7:100:ALA:HB1	1.86	0.58
4:AB:190:CYS:SG	4:AB:385:CYS:N	2.76	0.58
4:AC:357:ASP:HB2	4:AF:360:GLY:HA3	1.85	0.58
4:AF:345:HIS:CD2	4:AF:388:ASP:HB2	2.39	0.58
2:0H:30:GLN:HB2	2:0H:133:LYS:HB3	1.86	0.58
2:6:12:PHE:O	2:6:129:THR:OG1	2.20	0.58
2:7:54:PRO:HD3	2:7:109:GLN:HG3	1.86	0.58
4:AB:309:LEU:HD22	3:AO:17:ARG:HH21	1.69	0.58
2:7:55:SER:HB3	2:7:61:VAL:HG13	1.86	0.57
4:AF:225:ALA:HB3	2:AM:105:CYS:SG	2.44	0.57
2:AH:62:PRO:HB3	2:AH:110:TRP:CG	2.39	0.57
2:AL:68:VAL:HG13	2:AL:85:ALA:HB3	1.85	0.57
4:AF:240:LEU:CD1	2:AH:137:ARG:H	2.18	0.57
2:AH:9:PHE:CE1	2:AH:133:LYS:HG2	2.35	0.57
2:AK:68:VAL:O	2:AK:85:ALA:N	2.35	0.57
2:5:35:PHE:HD2	2:5:99:CYS:HB3	1.68	0.57
4:AA:291:VAL:HG21	2:0H:107:ASN:HA	1.85	0.57
2:AN:9:PHE:HE1	2:AN:133:LYS:HG3	1.69	0.57
2:AN:67:ARG:HH21	2:AN:84:LEU:HG	1.70	0.57
1:0C:8:GLY:O	1:0C:9:ALA:C	2.42	0.57
4:AB:196:LEU:HB3	4:AB:415:TRP:HB2	1.86	0.57
4:AC:231:PHE:CE1	4:AF:250:VAL:HG13	2.39	0.57
4:AJ:301:ASN:O	3:AQ:11:GLN:NE2	2.38	0.57
2:0G:115:PRO:HB2	2:0G:120:GLU:HG2	1.85	0.57
2:1:52:HIS:HB2	2:1:110:TRP:CD1	2.39	0.57
4:AA:181:ALA:O	4:AA:182:LEU:HB2	2.03	0.57
4:AC:312:ASP:HA	4:AC:317:SER:HA	1.87	0.57
4:AC:406:GLY:N	4:AC:464:ILE:HB	2.20	0.57
4:AF:347:ASN:ND2	4:AF:392:GLY:O	2.37	0.57
2:7:89:LEU:HD12	2:7:90:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AA:341:ARG:HD3	4:AA:379:ARG:HG3	1.87	0.57
4:AG:254:ASN:HB3	4:AG:257:ASN:HB2	1.86	0.57
4:AJ:195:ASP:O	4:AJ:416:LYS:NZ	2.37	0.57
2:6:48:ASN:OD1	2:6:67:ARG:NH2	2.38	0.57
1:0B:9:ALA:O	1:0B:10:ALA:C	2.42	0.57
4:AA:220:GLU:HA	4:AB:247:TYR:CE1	2.40	0.56
4:AG:221:TYR:HD1	4:AJ:293:GLU:HG2	1.70	0.56
4:AJ:202:VAL:HG13	4:AJ:424:LYS:HB2	1.86	0.56
2:AD:96:ASP:O	3:AR:9:LEU:N	2.37	0.56
4:AB:208:THR:HA	4:AB:241:GLU:HA	1.86	0.56
4:AB:406:GLY:HA2	4:AB:464:ILE:H	1.68	0.56
4:AF:431:GLN:NE2	4:AF:433:GLU:OE1	2.38	0.56
4:AG:207:PHE:O	4:AG:241:GLU:HB2	2.06	0.56
2:AH:70:GLU:HA	2:AH:85:ALA:HB2	1.87	0.56
4:AJ:264:ASP:OD1	4:AJ:266:LEU:N	2.38	0.56
2:0G:58:ASP:HB3	2:0G:61:VAL:HG22	1.88	0.56
2:0G:89:LEU:HD23	3:AT:4:LEU:HD13	1.86	0.56
2:0H:9:PHE:CE1	2:0H:133:LYS:HG2	2.40	0.56
4:AA:253:PHE:HZ	4:AA:269:MET:HG3	1.71	0.56
2:AM:4:ASN:ND2	3:AP:3:LYS:HD2	2.21	0.56
2:4:26:ASP:HB3	2:4:137:ARG:HH12	1.70	0.56
2:7:52:HIS:ND1	2:7:64:PRO:O	2.31	0.56
4:AJ:364:PHE:HB3	4:AJ:371:PHE:CE1	2.41	0.56
4:AC:194:LEU:O	4:AC:199:GLN:NE2	2.29	0.56
4:AF:220:GLU:O	4:AG:247:TYR:HB2	2.06	0.56
4:AG:247:TYR:CE1	4:AG:447:ALA:HB3	2.41	0.56
2:AL:34:THR:OG1	2:AL:129:THR:OG1	2.24	0.56
2:0H:34:THR:OG1	2:0H:129:THR:OG1	2.23	0.56
2:7:74:CYS:SG	2:7:75:ASP:N	2.79	0.56
2:0E:58:ASP:HB3	2:0E:61:VAL:HG22	1.86	0.56
4:AA:195:ASP:N	4:AA:195:ASP:OD1	2.39	0.56
2:3:67:ARG:HH12	2:3:86:ALA:HB2	1.71	0.56
4:AB:305:VAL:HG13	3:AO:15:ALA:HA	1.88	0.56
4:AB:319:PRO:HB2	4:AB:403:PHE:CE2	2.41	0.56
4:AB:328:ARG:HH21	4:AC:393:ASN:HD22	1.53	0.56
4:AC:309:LEU:HD13	4:AC:310:PRO:HD2	1.88	0.56
2:5:28:PHE:CD1	2:5:135:ALA:HB2	2.41	0.55
2:AK:89:LEU:HD23	3:AQ:4:LEU:HD13	1.86	0.55
4:AC:347:ASN:ND2	4:AC:390:THR:O	2.39	0.55
2:0E:70:GLU:N	2:0E:83:GLY:O	2.39	0.55
4:AA:342:SER:OG	4:AA:379:ARG:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AB:324:GLN:NE2	4:AC:354:ALA:O	2.39	0.55
2:1:67:ARG:HG2	2:1:84:LEU:HD23	1.89	0.55
2:6:52:HIS:ND1	2:6:64:PRO:O	2.40	0.55
4:AB:377:ARG:NH2	4:AB:378:GLU:OE2	2.35	0.55
4:AB:254:ASN:HB3	4:AB:257:ASN:HB2	1.88	0.55
2:AI:15:TRP:HB3	2:AI:128:ILE:HB	1.88	0.55
2:AM:67:ARG:HB3	2:AM:84:LEU:HG	1.88	0.55
4:AB:267:SER:O	4:AB:270:ILE:HG22	2.07	0.55
2:4:72:PRO:HB2	2:4:76:THR:HG21	1.89	0.55
4:AC:289:LYS:N	4:AC:293:GLU:OE1	2.36	0.55
4:AF:226:LYS:HD3	2:AM:71:VAL:HG13	1.89	0.55
4:AF:288:GLY:O	4:AF:296:GLY:N	2.30	0.55
2:3:28:PHE:CD1	2:3:135:ALA:HB2	2.42	0.55
4:AB:329:PHE:O	4:AB:460:ARG:NH2	2.40	0.55
4:AB:395:LYS:NZ	4:AB:401:ASP:O	2.35	0.55
2:AI:36:LYS:NZ	2:AI:37:THR:O	2.38	0.55
2:AH:67:ARG:HH21	2:AH:86:ALA:HB2	1.70	0.54
2:AK:4:ASN:HD21	2:AL:101:GLY:HA2	1.71	0.54
4:AA:398:THR:OG1	4:AA:399:GLY:N	2.39	0.54
4:AF:213:ALA:HB3	4:AF:236:ASN:HB3	1.88	0.54
4:AG:274:GLN:HG2	4:AG:427:MET:SD	2.47	0.54
4:AJ:376:VAL:O	4:AJ:378:GLU:N	2.40	0.54
2:AL:137:ARG:NH1	3:AQ:9:LEU:O	2.40	0.54
2:0H:35:PHE:HB2	2:0H:99:CYS:SG	2.48	0.54
2:1:48:ASN:HB3	2:1:67:ARG:HH22	1.72	0.54
2:0F:24:LYS:HE3	2:0F:26:ASP:HB3	1.89	0.54
4:AC:307:GLN:HE21	3:AR:17:ARG:HB3	1.70	0.54
2:0G:28:PHE:CD2	2:0G:132:MET:HG2	2.42	0.54
2:6:45:THR:HG23	2:6:119:SER:HB2	1.88	0.54
4:AF:197:TYR:O	4:AF:199:GLN:NE2	2.40	0.54
2:0G:96:ASP:N	2:0G:96:ASP:OD1	2.38	0.54
4:AC:196:LEU:HD21	4:AC:381:ARG:HD2	1.90	0.54
4:AF:309:LEU:HD11	3:AR:27:ARG:HD3	1.89	0.54
4:AF:357:ASP:OD1	4:AF:361:ARG:N	2.30	0.54
4:AJ:200:ILE:HB	4:AJ:422:VAL:HG12	1.88	0.54
2:9:52:HIS:ND1	2:9:64:PRO:O	2.41	0.54
1:0C:6:LEU:O	1:0C:7:CYS:C	2.46	0.54
2:AD:74:CYS:SG	4:AF:252:CYS:HB3	2.48	0.54
4:AB:255:ARG:NH2	4:AB:437:SER:O	2.41	0.54
2:AM:2:ASN:ND2	2:AN:103:VAL:O	2.33	0.54
2:0G:100:ALA:HB1	2:0H:6:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:9:ALA:O	1:0:10:ALA:C	2.46	0.54
4:AA:398:THR:O	4:AA:402:ALA:HB3	2.08	0.54
4:AC:404:ALA:O	4:AC:464:ILE:HG13	2.08	0.54
3:AO:11:GLN:HG2	3:AO:13:PRO:HD3	1.90	0.54
4:AF:322:LEU:HD12	3:AR:27:ARG:NH2	2.22	0.54
4:AG:210:MET:HG2	4:AG:239:HIS:ND1	2.23	0.54
2:AH:75:ASP:HA	2:AH:77:VAL:HG23	1.89	0.54
2:1:36:LYS:HE2	2:1:96:ASP:HA	1.89	0.54
4:AG:193:LEU:HD23	4:AG:381:ARG:NH1	2.23	0.54
2:AL:54:PRO:HD3	2:AL:109:GLN:HG3	1.89	0.54
2:AN:81:GLU:HG2	2:AN:82:ASP:H	1.72	0.54
2:5:36:LYS:NZ	2:5:37:THR:O	2.34	0.53
4:AC:255:ARG:HA	4:AC:258:LEU:HB3	1.89	0.53
2:AD:82:ASP:OD1	2:AD:82:ASP:N	2.41	0.53
4:AF:231:PHE:HB3	4:AG:250:VAL:O	2.08	0.53
4:AF:377:ARG:O	4:AF:379:ARG:NH1	2.41	0.53
4:AG:252:CYS:SG	2:AI:74:CYS:HB3	2.48	0.53
2:0F:62:PRO:HB3	2:0F:110:TRP:NE1	2.16	0.53
4:AC:227:CYS:O	4:AF:248:ARG:NH1	2.42	0.53
2:7:96:ASP:O	1:0A:5:ASN:ND2	2.41	0.53
4:AA:391:GLU:OE2	4:AA:404:ALA:HB2	2.08	0.53
4:AB:221:TYR:HE2	4:AC:293:GLU:HG2	1.72	0.53
4:AF:195:ASP:OD1	4:AF:196:LEU:HD12	2.09	0.53
4:AJ:302:CYS:HA	3:AQ:11:GLN:NE2	2.24	0.53
2:0G:12:PHE:O	2:0G:129:THR:OG1	2.21	0.53
4:AF:398:THR:H	3:AR:22:PRO:HG3	1.73	0.53
2:AH:23:VAL:HG11	2:AH:130:VAL:HG11	1.89	0.53
2:9:28:PHE:CD1	2:9:135:ALA:HB2	2.43	0.53
2:0E:74:CYS:SG	2:0E:75:ASP:N	2.82	0.53
4:AA:394:THR:O	4:AA:395:LYS:C	2.44	0.53
4:AG:387:PRO:HD2	4:AG:408:PHE:HD1	1.73	0.53
2:3:54:PRO:HD3	2:3:109:GLN:HG3	1.89	0.53
1:0C:16:VAL:O	1:0C:17:GLN:HG3	2.09	0.53
2:0E:36:LYS:NZ	2:0E:95:PRO:O	2.41	0.53
4:AC:223:CYS:SG	4:AC:224:ASP:N	2.81	0.53
2:AD:41:LEU:HD11	2:AD:93:VAL:HG12	1.91	0.53
2:AI:45:THR:HG23	2:AI:119:SER:HB2	1.90	0.53
3:AR:1:MET:HE3	3:AR:2:VAL:HG23	1.91	0.53
3:AT:6:CYS:O	3:AT:7:ARG:HB3	2.09	0.53
2:6:9:PHE:HA	2:6:132:MET:O	2.09	0.53
2:7:23:VAL:HG21	2:7:130:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:34:THR:OG1	2:7:129:THR:OG1	2.24	0.53
2:AI:69:PRO:HB3	2:AI:84:LEU:HD23	1.89	0.53
4:AA:180:LEU:N	4:AJ:208:THR:O	2.42	0.53
4:AC:290:GLY:H	4:AC:295:LYS:HD3	1.73	0.53
4:AG:253:PHE:HZ	4:AG:269:MET:HG3	1.74	0.53
4:AJ:255:ARG:NE	4:AJ:440:CYS:O	2.38	0.53
2:AN:42:THR:OG1	2:AN:122:ASN:ND2	2.33	0.53
2:0H:23:VAL:HG21	2:0H:130:VAL:HG11	1.90	0.53
4:AF:336:GLU:OE1	4:AF:336:GLU:N	2.36	0.53
4:AJ:322:LEU:HD11	3:AP:24:PHE:HD1	1.74	0.53
2:AL:28:PHE:HA	2:AL:135:ALA:HA	1.91	0.53
2:5:9:PHE:CE1	2:5:133:LYS:HG2	2.44	0.52
4:AG:275:ARG:O	4:AG:279:ILE:HG12	2.09	0.52
2:AI:35:PHE:HB2	2:AI:99:CYS:HB2	1.90	0.52
2:4:30:GLN:HB2	2:4:133:LYS:HB3	1.91	0.52
2:9:9:PHE:CE1	2:9:133:LYS:HG2	2.45	0.52
2:0E:34:THR:HG21	2:0F:11:SER:H	1.74	0.52
4:AB:214:ASP:HA	4:AC:187:ASN:HD21	1.75	0.52
4:AF:431:GLN:HA	4:AF:443:TYR:HA	1.92	0.52
2:AK:115:PRO:HB2	2:AK:120:GLU:HG2	1.91	0.52
2:0F:15:TRP:HB3	2:0F:128:ILE:HB	1.91	0.52
4:AJ:403:PHE:O	4:AJ:404:ALA:CB	2.57	0.52
2:AE:20:SER:HG	2:AE:112:SER:HG	1.43	0.52
4:AG:217:GLN:HA	4:AJ:276:SER:HB3	1.91	0.52
2:AM:76:THR:HG23	2:AM:78:LEU:H	1.74	0.52
2:AN:62:PRO:HB3	2:AN:110:TRP:CG	2.44	0.52
2:3:23:VAL:HG11	2:3:130:VAL:HG11	1.91	0.52
2:6:109:GLN:HB2	2:6:110:TRP:CE3	2.45	0.52
4:AB:219:GLY:HA3	4:AC:247:TYR:CZ	2.44	0.52
2:AE:62:PRO:HB3	2:AE:110:TRP:CG	2.44	0.52
4:AG:334:PRO:HD3	4:AG:460:ARG:HH22	1.73	0.52
4:AJ:281:ARG:NE	4:AJ:449:ASP:OD2	2.31	0.52
2:1:11:SER:HA	2:1:132:MET:HE1	1.91	0.52
4:AA:303:PHE:HZ	4:AA:413:ALA:HB2	1.73	0.52
4:AJ:375:LEU:O	4:AJ:377:ARG:N	2.43	0.52
4:AC:359:ASN:N	4:AF:359:ASN:OD1	2.43	0.52
2:2:69:PRO:HA	2:2:84:LEU:HA	1.91	0.52
2:5:35:PHE:HD1	2:5:128:ILE:HG23	1.74	0.52
4:AJ:222:THR:HG23	4:AJ:223:CYS:O	2.10	0.52
4:AA:208:THR:O	4:AB:180:LEU:HD23	2.09	0.52
4:AA:304:PRO:O	4:AA:461:ILE:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AA:332:SER:O	4:AA:460:ARG:NH2	2.42	0.52
4:AB:203:SER:OG	4:AB:204:ARG:N	2.41	0.52
2:AD:106:MET:SD	2:AD:106:MET:N	2.82	0.52
4:AF:275:ARG:O	4:AF:279:ILE:HG12	2.10	0.52
4:AF:321:PHE:CZ	4:AF:326:TRP:HB2	2.45	0.52
2:AH:76:THR:HG22	2:AH:77:VAL:N	2.24	0.52
4:AB:254:ASN:OD1	4:AB:255:ARG:N	2.43	0.52
4:AB:398:THR:OG1	4:AB:400:GLN:O	2.28	0.52
4:AC:405:ALA:O	4:AC:406:GLY:C	2.48	0.52
2:AI:29:ASN:HD22	2:AI:30:GLN:HG3	1.76	0.51
4:AA:211:LYS:HG3	4:AB:184:VAL:HG23	1.91	0.51
4:AF:341:ARG:HH12	4:AF:379:ARG:HH21	1.57	0.51
2:AI:62:PRO:HB3	2:AI:110:TRP:CG	2.46	0.51
4:AJ:305:VAL:HG22	4:AJ:461:ILE:HB	1.91	0.51
2:AL:70:GLU:N	2:AL:83:GLY:O	2.38	0.51
4:AA:178:GLN:O	4:AJ:207:PHE:HA	2.10	0.51
4:AA:391:GLU:OE1	4:AA:396:GLY:HA3	2.10	0.51
2:AD:12:PHE:O	2:AD:129:THR:OG1	2.23	0.51
2:AH:31:PHE:HB3	2:AH:132:MET:HG3	1.92	0.51
4:AJ:210:MET:SD	4:AJ:239:HIS:ND1	2.83	0.51
3:AO:1:MET:SD	3:AO:2:VAL:N	2.83	0.51
2:1:9:PHE:CE1	2:1:133:LYS:HG2	2.44	0.51
4:AB:197:TYR:CD1	4:AB:419:PHE:HB3	2.44	0.51
4:AG:351:TYR:HE2	3:AS:19:VAL:HG11	1.76	0.51
2:AH:78:LEU:C	2:AH:79:LEU:HD22	2.31	0.51
2:AK:73:PHE:CE2	2:AK:104:PRO:HG3	2.42	0.51
2:0E:26:ASP:OD2	2:0E:26:ASP:N	2.44	0.51
4:AA:343:VAL:HG12	4:AA:381:ARG:HB3	1.93	0.51
4:AA:384:ASN:ND2	4:AJ:336:GLU:OE2	2.42	0.51
4:AC:311:VAL:HG21	4:AC:322:LEU:HD11	1.92	0.51
2:AH:13:ILE:HG12	2:AI:13:ILE:HG12	1.93	0.51
2:AH:127:GLN:NE2	2:AI:13:ILE:H	2.09	0.51
2:1:11:SER:HB2	2:1:131:THR:HG23	1.91	0.51
2:0F:68:VAL:HG23	2:0F:107:ASN:HD21	1.75	0.51
4:AA:357:ASP:OD2	4:AB:361:ARG:NH2	2.44	0.51
4:AB:352:LEU:HD11	4:AC:369:LEU:HD21	1.93	0.51
4:AF:252:CYS:SG	4:AF:253:PHE:N	2.84	0.51
4:AG:306:PHE:O	4:AG:463:GLN:N	2.40	0.51
2:AH:5:VAL:HG11	2:AI:133:LYS:HD2	1.92	0.51
2:AN:87:VAL:HG22	3:AP:2:VAL:HG11	1.93	0.51
2:2:64:PRO:HG2	2:2:66:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AB:327:ARG:HH12	4:AC:370:THR:C	2.13	0.51
4:AC:345:HIS:NE2	4:AC:384:ASN:O	2.44	0.51
4:AF:345:HIS:CD2	4:AF:384:ASN:HA	2.45	0.51
2:AI:13:ILE:HA	2:AI:129:THR:HG22	1.92	0.51
2:AN:81:GLU:HG2	2:AN:82:ASP:N	2.25	0.51
4:AB:217:GLN:NE2	4:AC:276:SER:OG	2.44	0.51
4:AF:432:TYR:HD2	4:AF:442:LYS:HD2	1.74	0.51
4:AB:357:ASP:HB2	4:AC:359:ASN:O	2.10	0.51
4:AB:396:GLY:H	4:AB:403:PHE:H	1.58	0.51
4:AF:306:PHE:HA	3:AS:16:SER:CB	2.38	0.51
4:AG:254:ASN:OD1	4:AG:255:ARG:N	2.39	0.51
4:AJ:197:TYR:HD1	4:AJ:419:PHE:HB3	1.77	0.51
2:AN:28:PHE:CG	2:AN:132:MET:HB3	2.46	0.51
2:OG:30:GLN:HB2	2:OG:133:LYS:HB3	1.93	0.51
2:1:48:ASN:HB3	2:1:67:ARG:NH2	2.26	0.50
2:3:52:HIS:HB2	2:3:110:TRP:CD1	2.46	0.50
2:9:34:THR:OG1	2:9:129:THR:OG1	2.27	0.50
4:AG:310:PRO:HB2	4:AG:317:SER:HB2	1.93	0.50
2:AI:41:LEU:HD11	2:AI:89:LEU:HD11	1.92	0.50
2:AI:53:GLU:O	2:AI:63:GLY:N	2.38	0.50
2:AI:70:GLU:HB2	2:AI:85:ALA:HB2	1.92	0.50
2:AN:52:HIS:ND1	2:AN:64:PRO:O	2.43	0.50
2:2:28:PHE:CD1	2:2:132:MET:HB3	2.46	0.50
2:AH:61:VAL:O	2:AH:62:PRO:C	2.48	0.50
2:4:94:THR:OG1	2:4:96:ASP:OD2	2.24	0.50
4:AA:357:ASP:OD1	4:AA:361:ARG:N	2.44	0.50
4:AB:428:PHE:O	4:AB:445:PHE:HA	2.12	0.50
2:AK:96:ASP:HB2	3:AQ:9:LEU:HG	1.92	0.50
2:AM:35:PHE:HB2	2:AM:99:CYS:SG	2.51	0.50
2:AI:38:ILE:HG22	2:AI:125:ASN:HB3	1.93	0.50
4:AA:230:GLU:CG	4:AB:249:GLY:HA2	2.41	0.50
4:AB:218:LEU:HB2	4:AC:273:ALA:HA	1.93	0.50
4:AC:222:THR:HG21	4:AF:248:ARG:HB2	1.94	0.50
4:AF:312:ASP:HA	4:AF:317:SER:HA	1.92	0.50
4:AG:386:LEU:HD13	4:AG:408:PHE:HE1	1.76	0.50
2:AH:62:PRO:HD3	2:AH:110:TRP:CE2	2.46	0.50
2:7:123:ALA:HA	2:7:126:VAL:HG12	1.93	0.50
4:AA:432:TYR:HD2	4:AA:442:LYS:HD2	1.77	0.50
4:AC:258:LEU:HD23	4:AC:259:GLN:N	2.20	0.50
4:AF:390:THR:OG1	4:AF:394:THR:O	2.25	0.50
2:AN:9:PHE:HD1	2:AN:133:LYS:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0H:15:TRP:HB3	2:0H:128:ILE:HB	1.92	0.50
2:9:41:LEU:HD22	2:9:122:ASN:HB3	1.92	0.50
2:0F:68:VAL:HG13	2:0F:85:ALA:HB3	1.94	0.50
2:AL:14:ALA:HB2	2:AL:130:VAL:HG23	1.92	0.50
2:2:10:PRO:HD2	2:2:132:MET:HB2	1.94	0.50
2:0E:26:ASP:CG	2:0E:27:GLY:H	2.15	0.50
4:AA:207:PHE:HA	4:AB:178:GLN:O	2.12	0.50
4:AB:287:ILE:HD12	4:AB:289:LYS:HZ1	1.77	0.50
2:AH:52:HIS:ND1	2:AH:64:PRO:O	2.41	0.50
4:AG:237:ILE:HG21	4:AJ:263:TYR:OH	2.12	0.50
4:AG:357:ASP:OD1	4:AG:361:ARG:N	2.45	0.50
2:AM:16:ASP:OD1	2:AM:17:GLY:N	2.45	0.50
2:1:28:PHE:HA	2:1:135:ALA:CB	2.42	0.49
2:5:52:HIS:HB2	2:5:110:TRP:CD1	2.47	0.49
4:AC:397:GLY:HA3	4:AC:402:ALA:HA	1.94	0.49
4:AF:408:PHE:HE2	4:AF:411:ALA:HB2	1.76	0.49
2:AN:98:PHE:HD1	3:AP:9:LEU:HD11	1.77	0.49
2:4:52:HIS:HB2	2:4:110:TRP:HB2	1.94	0.49
2:6:67:ARG:NH1	2:6:85:ALA:O	2.45	0.49
4:AB:453:VAL:HG21	4:AB:456:CYS:HB3	1.94	0.49
4:AC:304:PRO:HD2	4:AC:459:GLY:O	2.12	0.49
2:AI:84:LEU:H	2:AI:84:LEU:HD12	1.77	0.49
2:0G:35:PHE:HB2	2:0G:99:CYS:HB2	1.94	0.49
2:0G:97:SER:HA	3:AT:8:PRO:HA	1.93	0.49
2:8:2:ASN:ND2	2:9:103:VAL:O	2.43	0.49
2:9:97:SER:HA	1:0C:5:ASN:HD21	1.76	0.49
2:4:64:PRO:HG2	2:4:66:ILE:HD11	1.93	0.49
4:AB:403:PHE:O	4:AB:404:ALA:HB2	2.11	0.49
2:AH:58:ASP:C	2:AH:60:CYS:N	2.66	0.49
2:AK:51:TYR:HD1	2:AK:68:VAL:HG22	1.77	0.49
2:0G:18:GLU:HG2	2:0G:19:GLU:HG2	1.94	0.49
4:AF:432:TYR:CD2	4:AF:442:LYS:HD2	2.47	0.49
2:AM:74:CYS:SG	2:AM:75:ASP:N	2.86	0.49
2:AN:62:PRO:HB3	2:AN:110:TRP:CD2	2.47	0.49
2:2:48:ASN:OD1	2:2:67:ARG:NH2	2.46	0.49
2:4:67:ARG:NH2	2:4:85:ALA:O	2.45	0.49
4:AA:250:VAL:HG13	4:AJ:229:ALA:HB3	1.95	0.49
4:AB:326:TRP:HE1	4:AC:369:LEU:HD11	1.78	0.49
4:AC:305:VAL:HG23	4:AC:461:ILE:HG13	1.94	0.49
2:AE:56:ASP:OD1	2:AE:56:ASP:N	2.45	0.49
2:AI:68:VAL:HG13	2:AI:85:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AM:75:ASP:N	2:AM:75:ASP:OD2	2.44	0.49
3:AS:15:ALA:O	3:AS:16:SER:HB2	2.12	0.49
2:8:2:ASN:ND2	2:9:102:THR:OG1	2.46	0.49
2:0F:56:ASP:OD1	2:0F:56:ASP:N	2.46	0.49
4:AA:280:ASN:HA	4:AA:283:GLN:HG2	1.94	0.49
4:AB:388:ASP:OD2	4:AB:391:GLU:N	2.45	0.49
4:AC:407:SER:O	4:AC:408:PHE:C	2.51	0.49
4:AF:282:ASN:O	4:AF:286:MET:HG2	2.12	0.49
4:AJ:342:SER:HA	4:AJ:412:GLN:HA	1.94	0.49
4:AJ:344:MET:N	4:AJ:344:MET:SD	2.86	0.49
2:AN:67:ARG:NE	2:AN:84:LEU:HD12	2.27	0.49
2:4:58:ASP:HB3	2:4:61:VAL:HG22	1.93	0.49
4:AA:206:THR:O	4:AB:178:GLN:HB3	2.12	0.49
4:AB:194:LEU:HD11	4:AB:285:LEU:HD21	1.94	0.49
2:AE:78:LEU:HG	2:AE:80:SER:H	1.77	0.49
4:AJ:396:GLY:HA2	4:AJ:403:PHE:CD2	2.48	0.49
4:AF:207:PHE:HB3	4:AG:178:GLN:HE21	1.78	0.49
4:AG:276:SER:O	4:AG:280:ASN:ND2	2.38	0.49
4:AJ:197:TYR:CD1	4:AJ:419:PHE:HB3	2.48	0.49
4:AJ:345:HIS:CD2	4:AJ:388:ASP:HB2	2.48	0.49
4:AA:217:GLN:N	4:AA:233:GLU:OE2	2.41	0.48
4:AA:309:LEU:HD11	3:AT:19:VAL:HG12	1.94	0.48
4:AA:346:GLN:HB3	4:AA:382:ILE:HG21	1.94	0.48
2:AN:87:VAL:HG22	3:AP:2:VAL:HG21	1.93	0.48
4:AB:406:GLY:H	4:AB:464:ILE:HB	1.77	0.48
4:AF:395:LYS:HE3	4:AF:401:ASP:HA	1.95	0.48
4:AG:398:THR:H	3:AS:22:PRO:HG2	1.79	0.48
2:AM:100:ALA:HB1	2:AN:6:GLY:HA3	1.96	0.48
1:0D:16:VAL:HG22	1:0D:18:PRO:HD3	1.94	0.48
4:AA:267:SER:HA	4:AA:270:ILE:HD12	1.94	0.48
4:AA:324:GLN:HA	4:AB:362:PHE:HZ	1.79	0.48
4:AB:400:GLN:NE2	4:AB:401:ASP:H	2.11	0.48
4:AF:397:GLY:N	4:AF:401:ASP:O	2.34	0.48
2:AM:103:VAL:O	2:AN:2:ASN:ND2	2.40	0.48
2:8:9:PHE:HA	2:8:132:MET:O	2.13	0.48
4:AB:200:ILE:HD11	4:AB:422:VAL:HG22	1.95	0.48
2:AD:56:ASP:N	2:AD:56:ASP:OD1	2.45	0.48
4:AJ:246:ASP:HA	4:AJ:448:GLU:HB3	1.95	0.48
2:AM:79:LEU:HD23	2:AM:79:LEU:H	1.77	0.48
2:0H:80:SER:OG	2:0H:81:GLU:N	2.46	0.48
2:4:69:PRO:HA	2:4:84:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:54:PRO:HD3	2:9:109:GLN:HG3	1.95	0.48
4:AA:291:VAL:HG22	4:AA:292:ASN:ND2	2.29	0.48
4:AB:306:PHE:HE2	4:AB:460:ARG:HB3	1.78	0.48
4:AC:266:LEU:O	4:AC:270:ILE:HG12	2.14	0.48
2:8:58:ASP:HB3	2:8:61:VAL:HG22	1.96	0.48
2:8:67:ARG:HB3	2:8:84:LEU:HD12	1.94	0.48
2:0F:29:ASN:OD1	2:0F:29:ASN:N	2.47	0.48
4:AB:311:VAL:HG12	3:AT:27:ARG:HG2	1.95	0.48
4:AC:390:THR:HG22	4:AC:393:ASN:HA	1.96	0.48
2:AD:9:PHE:CE1	2:AD:133:LYS:HG2	2.49	0.48
4:AJ:322:LEU:HD21	3:AP:24:PHE:HE1	1.79	0.48
2:0H:68:VAL:HG13	2:0H:85:ALA:HB3	1.96	0.48
2:5:15:TRP:HB3	2:5:128:ILE:HB	1.96	0.48
4:AA:188:ILE:HD11	4:AJ:336:GLU:HG3	1.95	0.48
4:AF:226:LYS:HZ2	2:AM:71:VAL:HG22	1.79	0.48
2:AI:28:PHE:CG	2:AI:132:MET:HB3	2.49	0.48
4:AJ:360:GLY:HA2	3:AS:25:ILE:HG12	1.96	0.48
2:8:29:ASN:OD1	2:8:30:GLN:NE2	2.47	0.48
4:AA:345:HIS:CD2	4:AA:388:ASP:HB2	2.48	0.48
4:AC:255:ARG:CZ	4:AC:441:VAL:HB	2.43	0.48
4:AC:327:ARG:HA	4:AC:330:VAL:HG12	1.95	0.48
4:AF:208:THR:HG22	4:AF:241:GLU:HG3	1.94	0.48
4:AF:264:ASP:OD1	4:AF:264:ASP:N	2.46	0.48
2:AK:88:THR:H	3:AQ:2:VAL:HG12	1.78	0.48
2:AM:30:GLN:HB2	2:AM:133:LYS:HB3	1.94	0.48
2:AM:52:HIS:ND1	2:AM:64:PRO:O	2.46	0.48
2:7:22:PRO:HB3	2:7:110:TRP:CD1	2.49	0.48
4:AG:180:LEU:HD23	4:AG:180:LEU:H	1.77	0.48
2:AI:81:GLU:HG2	2:AI:82:ASP:N	2.27	0.48
2:3:47:PHE:HZ	2:3:126:VAL:HG11	1.78	0.48
2:5:36:LYS:HE2	2:5:96:ASP:HA	1.96	0.48
2:8:41:LEU:HD12	2:8:93:VAL:H	1.79	0.48
4:AA:222:THR:HG22	4:AB:247:TYR:HA	1.95	0.48
4:AG:322:LEU:HB2	4:AG:355:MET:HE1	1.96	0.48
4:AG:365:GLY:O	4:AG:367:GLY:N	2.44	0.48
2:AH:119:SER:O	2:AH:123:ALA:N	2.47	0.48
2:AN:52:HIS:HB2	2:AN:110:TRP:HB2	1.96	0.48
2:1:91:GLU:HG3	2:1:92:THR:H	1.78	0.47
4:AB:365:GLY:O	4:AB:367:GLY:N	2.43	0.47
4:AB:406:GLY:N	4:AB:464:ILE:HB	2.29	0.47
4:AB:463:GLN:HG2	4:AB:464:ILE:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0E:106:MET:SD	2:0E:106:MET:N	2.84	0.47
4:AC:252:CYS:SG	4:AC:253:PHE:N	2.87	0.47
4:AG:294:PRO:HG3	4:AG:450:GLY:HA2	1.95	0.47
4:AG:351:TYR:OH	4:AG:396:GLY:O	2.27	0.47
2:AI:42:THR:OG1	2:AI:122:ASN:ND2	2.44	0.47
4:AJ:371:PHE:CZ	4:AJ:373:PRO:HB3	2.49	0.47
2:AM:68:VAL:O	2:AM:84:LEU:HB3	2.14	0.47
2:AN:115:PRO:HB2	2:AN:120:GLU:HG3	1.96	0.47
2:2:24:LYS:HE2	2:2:26:ASP:HB3	1.96	0.47
2:8:80:SER:O	2:8:83:GLY:N	2.42	0.47
2:8:89:LEU:HD12	2:8:90:PRO:HD2	1.94	0.47
2:9:15:TRP:HB3	2:9:128:ILE:HB	1.96	0.47
4:AF:396:GLY:H	3:AR:19:VAL:HG11	1.78	0.47
2:AH:53:GLU:O	2:AH:63:GLY:N	2.46	0.47
4:AJ:345:HIS:CD2	4:AJ:384:ASN:HA	2.49	0.47
2:3:58:ASP:HB3	2:3:61:VAL:HG12	1.97	0.47
2:3:72:PRO:HB3	2:3:79:LEU:HD21	1.95	0.47
2:AD:91:GLU:HG2	2:AD:92:THR:H	1.78	0.47
2:AD:109:GLN:HB2	2:AD:110:TRP:CE3	2.49	0.47
4:AA:351:TYR:CD2	3:AQ:21:PRO:HG3	2.50	0.47
4:AB:247:TYR:HD2	4:AB:277:HIS:HD2	1.62	0.47
4:AB:284:ALA:O	4:AB:288:GLY:N	2.42	0.47
2:AE:75:ASP:OD1	2:AE:75:ASP:N	2.46	0.47
4:AF:343:VAL:HG12	4:AF:381:ARG:HB3	1.96	0.47
4:AJ:356:VAL:HG21	3:AS:25:ILE:HD11	1.96	0.47
4:AJ:397:GLY:HA3	4:AJ:401:ASP:CB	2.17	0.47
4:AA:332:SER:O	4:AA:332:SER:OG	2.33	0.47
4:AB:328:ARG:NH2	4:AC:393:ASN:HD22	2.12	0.47
4:AC:197:TYR:CE2	4:AC:285:LEU:HD13	2.45	0.47
4:AC:252:CYS:HA	4:AC:442:LYS:HA	1.96	0.47
2:AH:14:ALA:HB3	2:AH:128:ILE:O	2.14	0.47
2:1:72:PRO:HB3	2:1:79:LEU:HD21	1.96	0.47
2:7:67:ARG:NH1	2:7:86:ALA:HB2	2.28	0.47
2:0E:12:PHE:O	2:0E:129:THR:OG1	2.21	0.47
4:AA:182:LEU:H	4:AJ:209:TYR:HB2	1.78	0.47
4:AA:193:LEU:HD23	4:AA:193:LEU:H	1.77	0.47
2:AD:81:GLU:HG2	2:AD:82:ASP:H	1.79	0.47
4:AG:193:LEU:HA	4:AG:381:ARG:HH12	1.80	0.47
4:AG:208:THR:N	4:AJ:178:GLN:O	2.48	0.47
4:AG:395:LYS:HE2	4:AG:401:ASP:HA	1.95	0.47
2:AH:24:LYS:HE2	2:AH:26:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AH:78:LEU:H	2:AH:79:LEU:HD22	1.79	0.47
2:AN:49:ILE:H	2:AN:67:ARG:HH12	1.63	0.47
2:3:55:SER:HB3	2:3:61:VAL:HG13	1.97	0.47
2:4:2:ASN:ND2	2:5:102:THR:OG1	2.48	0.47
2:9:91:GLU:HG3	2:9:92:THR:H	1.80	0.47
4:AA:180:LEU:O	4:AJ:209:TYR:HB3	2.15	0.47
4:AF:182:LEU:HD22	4:AF:184:VAL:HG12	1.96	0.47
4:AF:410:ALA:HB3	4:AF:462:LEU:HB3	1.96	0.47
4:AG:215:TYR:CD2	4:AJ:272:ALA:HA	2.50	0.47
2:0G:10:PRO:HA	2:0H:34:THR:HG21	1.95	0.47
2:0G:52:HIS:HB2	2:0G:110:TRP:HB2	1.97	0.47
2:8:62:PRO:HG3	2:8:110:TRP:CD1	2.49	0.47
2:0E:18:GLU:HG2	2:0E:19:GLU:HG2	1.96	0.47
4:AB:397:GLY:O	3:AT:22:PRO:HD3	2.14	0.47
4:AJ:213:ALA:HB3	4:AJ:236:ASN:HB2	1.97	0.47
4:AJ:345:HIS:HA	4:AJ:383:SER:O	2.14	0.47
4:AJ:393:ASN:O	3:AP:19:VAL:HG22	2.15	0.47
2:AL:36:LYS:NZ	2:AL:37:THR:O	2.48	0.47
2:AN:45:THR:HB	2:AN:119:SER:HB2	1.97	0.47
2:2:12:PHE:O	2:2:129:THR:OG1	2.27	0.47
2:2:72:PRO:HB2	2:2:76:THR:HG21	1.97	0.47
2:3:25:VAL:HG22	2:3:110:TRP:HA	1.97	0.47
2:8:30:GLN:O	2:8:133:LYS:N	2.48	0.47
4:AB:304:PRO:HD3	4:AB:456:CYS:O	2.15	0.47
4:AC:208:THR:OG1	4:AC:240:LEU:O	2.20	0.47
4:AF:377:ARG:NH1	4:AF:378:GLU:HG2	2.30	0.47
2:AM:67:ARG:HD3	2:AM:84:LEU:HB2	1.97	0.47
2:3:74:CYS:SG	2:3:75:ASP:N	2.88	0.46
2:8:52:HIS:HB2	2:8:110:TRP:HB2	1.97	0.46
2:0E:8:ASP:OD1	2:0E:8:ASP:N	2.48	0.46
2:AI:47:PHE:HB2	2:AI:87:VAL:HG12	1.97	0.46
4:AJ:376:VAL:C	4:AJ:378:GLU:N	2.68	0.46
2:5:42:THR:OG1	2:5:122:ASN:ND2	2.48	0.46
2:8:35:PHE:HD1	2:8:128:ILE:HG12	1.80	0.46
2:0E:64:PRO:HG2	2:0E:66:ILE:HD11	1.97	0.46
4:AA:230:GLU:HG2	4:AB:249:GLY:HA2	1.96	0.46
4:AC:208:THR:O	4:AF:180:LEU:HD23	2.15	0.46
4:AC:310:PRO:HB2	4:AC:317:SER:HG	1.80	0.46
2:AD:22:PRO:HB2	2:AD:62:PRO:HG3	1.97	0.46
2:AM:68:VAL:O	2:AM:85:ALA:N	2.48	0.46
2:9:97:SER:HA	1:0C:5:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0F:34:THR:OG1	2:0F:129:THR:OG1	2.28	0.46
4:AF:321:PHE:HZ	4:AF:326:TRP:HB2	1.80	0.46
4:AF:386:LEU:HD13	4:AF:408:PHE:CE1	2.50	0.46
2:AH:73:PHE:CD2	2:AH:76:THR:OG1	2.64	0.46
2:2:70:GLU:OE2	2:2:80:SER:N	2.43	0.46
2:0E:30:GLN:HB2	2:0E:133:LYS:HB3	1.96	0.46
4:AA:369:LEU:HG	4:AJ:326:TRP:HE1	1.81	0.46
4:AC:291:VAL:HG23	2:AE:106:MET:HG2	1.97	0.46
4:AC:346:GLN:HA	4:AC:382:ILE:HD11	1.98	0.46
2:AE:52:HIS:HB2	2:AE:110:TRP:HB2	1.96	0.46
4:AJ:376:VAL:O	4:AJ:377:ARG:C	2.54	0.46
2:AK:47:PHE:HB2	2:AK:87:VAL:HG23	1.97	0.46
2:AK:58:ASP:HB3	2:AK:61:VAL:HG22	1.97	0.46
2:AM:45:THR:O	2:AM:88:THR:OG1	2.21	0.46
3:AQ:2:VAL:HG23	3:AQ:3:LYS:N	2.30	0.46
2:8:10:PRO:HA	2:9:34:THR:HG21	1.98	0.46
4:AB:192:SER:C	4:AB:194:LEU:H	2.19	0.46
4:AB:332:SER:HB3	4:AB:460:ARG:HH22	1.80	0.46
4:AG:302:CYS:HA	3:AP:11:GLN:HE22	1.79	0.46
2:AI:90:PRO:HD3	3:AS:4:LEU:HD13	1.96	0.46
4:AJ:378:GLU:O	4:AJ:380:ILE:HG12	2.16	0.46
2:0G:96:ASP:O	3:AT:9:LEU:N	2.48	0.46
2:0G:62:PRO:HG3	2:0G:110:TRP:CD1	2.51	0.46
2:4:33:PHE:HB2	2:4:101:GLY:O	2.15	0.46
2:5:20:SER:HG	2:5:112:SER:HG	1.57	0.46
2:6:28:PHE:CD1	2:6:132:MET:HB3	2.51	0.46
4:AA:362:PHE:N	4:AA:366:ASP:OD1	2.47	0.46
4:AF:200:ILE:O	4:AF:422:VAL:HA	2.16	0.46
4:AJ:397:GLY:O	4:AJ:402:ALA:N	2.49	0.46
2:AN:56:ASP:OD1	2:AN:56:ASP:N	2.48	0.46
2:1:11:SER:HA	2:1:132:MET:CE	2.46	0.46
2:9:14:ALA:HB2	2:9:130:VAL:HG23	1.98	0.46
4:AA:208:THR:OG1	4:AB:179:VAL:HA	2.15	0.46
4:AB:197:TYR:HD1	4:AB:419:PHE:HB3	1.81	0.46
4:AB:217:GLN:NE2	4:AB:219:GLY:O	2.41	0.46
4:AB:343:VAL:HG12	4:AB:381:ARG:HB2	1.96	0.46
4:AF:391:GLU:HB2	4:AF:395:LYS:HB2	1.97	0.46
2:0H:68:VAL:HG23	2:0H:107:ASN:HD21	1.80	0.46
3:AS:17:ARG:HA	3:AS:17:ARG:HD2	1.70	0.46
2:4:9:PHE:HA	2:4:132:MET:O	2.16	0.46
4:AC:195:ASP:N	4:AC:195:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AF:221:TYR:HD1	4:AG:247:TYR:HB3	1.77	0.46
4:AF:291:VAL:HG22	4:AF:292:ASN:OD1	2.15	0.46
4:AJ:386:LEU:HD23	4:AJ:408:PHE:CZ	2.51	0.46
2:9:2:ASN:OD1	2:9:2:ASN:N	2.49	0.46
2:9:17:GLY:O	2:9:124:ALA:HA	2.16	0.46
4:AC:260:GLU:O	4:AC:261:ALA:HB2	2.16	0.46
2:AD:36:LYS:HB3	2:AD:127:GLN:HG3	1.99	0.46
2:AE:67:ARG:HD3	2:AE:84:LEU:HD13	1.98	0.46
4:AG:284:ALA:O	4:AG:288:GLY:N	2.42	0.46
2:AI:39:ALA:HB3	2:AI:125:ASN:HD22	1.80	0.46
2:AK:62:PRO:HG3	2:AK:110:TRP:CD1	2.50	0.46
2:2:103:VAL:HG12	2:2:105:CYS:H	1.81	0.45
2:6:29:ASN:ND2	2:6:134:GLY:HA3	2.31	0.45
2:0F:45:THR:O	2:0F:88:THR:HA	2.16	0.45
4:AB:307:GLN:NE2	3:AO:17:ARG:HD2	2.31	0.45
2:AI:29:ASN:ND2	2:AI:30:GLN:HG3	2.31	0.45
2:4:12:PHE:O	2:4:129:THR:OG1	2.24	0.45
4:AA:386:LEU:HD23	4:AA:386:LEU:HA	1.83	0.45
4:AG:329:PHE:HB2	3:AP:18:LEU:HD21	1.98	0.45
2:AI:106:MET:SD	2:AI:106:MET:N	2.82	0.45
2:8:72:PRO:HB2	2:8:76:THR:HG21	1.98	0.45
2:0E:72:PRO:HB2	2:0E:76:THR:HG21	1.99	0.45
4:AB:341:ARG:HA	4:AB:379:ARG:HB3	1.97	0.45
4:AC:247:TYR:HE2	4:AC:277:HIS:HB2	1.80	0.45
4:AC:255:ARG:HA	4:AC:258:LEU:HD22	1.98	0.45
4:AC:322:LEU:HD23	3:AO:24:PHE:HB2	1.98	0.45
4:AJ:425:ARG:HD2	4:AJ:426:PRO:HD2	1.97	0.45
2:AK:37:THR:HB	2:AK:95:PRO:HA	1.98	0.45
2:AK:52:HIS:ND1	2:AK:64:PRO:O	2.49	0.45
2:3:68:VAL:HG13	2:3:85:ALA:HB3	1.98	0.45
2:4:52:HIS:ND1	2:4:64:PRO:O	2.49	0.45
2:7:73:PHE:HD2	2:7:75:ASP:H	1.64	0.45
2:0E:5:VAL:HG23	2:0F:131:THR:HG23	1.98	0.45
4:AB:194:LEU:HA	4:AB:197:TYR:HD2	1.80	0.45
4:AC:401:ASP:O	4:AC:402:ALA:C	2.54	0.45
2:AD:9:PHE:CD1	2:AD:133:LYS:HA	2.52	0.45
4:AG:311:VAL:HG22	3:AS:27:ARG:NH2	2.32	0.45
4:AJ:395:LYS:HA	4:AJ:395:LYS:NZ	2.31	0.45
2:AM:6:GLY:HA3	2:AN:100:ALA:HB1	1.98	0.45
2:1:49:ILE:HD11	2:1:87:VAL:HG13	1.98	0.45
2:8:33:PHE:HB2	2:8:101:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0E:52:HIS:ND1	2:0E:64:PRO:O	2.47	0.45
4:AC:291:VAL:O	4:AC:293:GLU:HG3	2.16	0.45
4:AC:368:ASP:O	4:AC:370:THR:HG22	2.17	0.45
4:AC:409:VAL:HG23	4:AC:463:GLN:HA	1.97	0.45
4:AG:209:TYR:HB3	4:AJ:180:LEU:HD12	1.98	0.45
2:AH:68:VAL:O	2:AH:84:LEU:HA	2.17	0.45
2:AH:81:GLU:HG2	2:AH:82:ASP:N	2.30	0.45
4:AJ:368:ASP:O	4:AJ:369:LEU:HG	2.16	0.45
2:2:62:PRO:HG3	2:2:110:TRP:CD2	2.51	0.45
2:8:3:PHE:N	2:9:30:GLN:OE1	2.35	0.45
2:8:91:GLU:HG3	2:8:92:THR:HG23	1.99	0.45
2:0E:9:PHE:HA	2:0E:132:MET:O	2.16	0.45
2:AN:82:ASP:N	2:AN:82:ASP:OD1	2.50	0.45
2:0G:99:CYS:HA	3:AT:5:ASN:O	2.17	0.45
2:3:62:PRO:HB3	2:3:110:TRP:NE1	2.31	0.45
2:9:22:PRO:HB3	2:9:110:TRP:CD1	2.52	0.45
4:AA:424:LYS:HB3	4:AA:448:GLU:HG2	1.98	0.45
4:AC:221:TYR:CD2	4:AF:293:GLU:HG3	2.52	0.45
4:AC:428:PHE:O	4:AC:445:PHE:HB2	2.17	0.45
4:AG:204:ARG:HH12	4:AJ:178:GLN:N	2.14	0.45
4:AG:231:PHE:HD1	4:AJ:251:PHE:HA	1.82	0.45
2:AH:13:ILE:HG23	2:AI:13:ILE:HD11	1.98	0.45
4:AJ:250:VAL:HG12	4:AJ:444:GLN:HA	1.99	0.45
2:AN:81:GLU:N	2:AN:81:GLU:OE2	2.50	0.45
2:2:53:GLU:O	2:2:63:GLY:N	2.50	0.45
4:AA:324:GLN:HA	4:AB:362:PHE:CZ	2.52	0.45
4:AC:195:ASP:O	4:AC:416:LYS:NZ	2.37	0.45
4:AJ:306:PHE:CE2	4:AJ:460:ARG:HD3	2.52	0.45
2:AM:91:GLU:OE2	2:AM:92:THR:N	2.39	0.45
2:3:2:ASN:OD1	2:3:2:ASN:N	2.50	0.45
2:7:58:ASP:O	2:7:61:VAL:HG12	2.17	0.45
4:AB:214:ASP:HA	4:AC:187:ASN:ND2	2.30	0.45
4:AB:241:GLU:OE1	4:AB:242:GLY:N	2.50	0.45
4:AB:386:LEU:HD23	4:AB:408:PHE:CE2	2.52	0.45
4:AF:197:TYR:OH	4:AF:297:TRP:NE1	2.35	0.45
4:AJ:371:PHE:CE2	4:AJ:373:PRO:HB3	2.52	0.45
2:AK:10:PRO:HA	2:AL:34:THR:HG21	1.99	0.45
2:AL:56:ASP:N	2:AL:56:ASP:OD1	2.50	0.45
2:4:106:MET:SD	2:4:106:MET:N	2.90	0.45
2:7:73:PHE:CE2	2:7:76:THR:HG23	2.51	0.45
2:8:45:THR:HG23	2:8:119:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:41:LEU:HD23	2:9:41:LEU:HA	1.88	0.45
2:0F:52:HIS:HB2	2:0F:110:TRP:CD1	2.52	0.45
4:AA:254:ASN:HA	4:AA:440:CYS:HA	1.98	0.45
4:AG:197:TYR:HD1	4:AG:419:PHE:HB3	1.80	0.45
2:0G:87:VAL:HG22	3:AT:2:VAL:HG21	1.99	0.45
4:AB:212:ILE:HG22	4:AB:237:ILE:HD13	2.00	0.44
4:AB:218:LEU:HA	4:AB:232:GLY:HA3	1.99	0.44
4:AB:222:THR:OG1	4:AB:223:CYS:N	2.50	0.44
4:AB:326:TRP:O	4:AB:330:VAL:HG23	2.17	0.44
4:AF:363:LEU:O	4:AG:367:GLY:HA3	2.17	0.44
4:AJ:387:PRO:HD2	4:AJ:408:PHE:CE1	2.53	0.44
4:AA:248:ARG:HB2	4:AJ:222:THR:HG21	1.98	0.44
4:AG:218:LEU:HD11	4:AJ:273:ALA:HB2	1.99	0.44
4:AJ:195:ASP:OD1	4:AJ:195:ASP:N	2.50	0.44
2:AN:35:PHE:HD1	2:AN:128:ILE:HG12	1.82	0.44
2:0H:67:ARG:NE	2:0H:84:LEU:HD12	2.32	0.44
2:6:38:ILE:HG12	2:6:125:ASN:HA	2.00	0.44
4:AB:413:ALA:HB3	4:AB:415:TRP:CE2	2.52	0.44
4:AF:218:LEU:HD12	4:AG:445:PHE:CE1	2.52	0.44
4:AF:390:THR:HB	4:AF:403:PHE:HE2	1.81	0.44
2:AI:9:PHE:CE1	2:AI:133:LYS:HB2	2.52	0.44
2:0G:8:ASP:OD1	2:0G:8:ASP:N	2.49	0.44
4:AB:339:GLU:OE1	4:AB:379:ARG:NH2	2.50	0.44
2:AE:73:PHE:CZ	2:AE:104:PRO:HG3	2.53	0.44
2:AK:70:GLU:HB3	2:AK:85:ALA:HA	1.98	0.44
2:1:132:MET:N	2:1:132:MET:SD	2.90	0.44
2:8:23:VAL:HG21	2:8:130:VAL:HG21	1.99	0.44
2:0E:2:ASN:OD1	2:0E:2:ASN:N	2.50	0.44
4:AC:208:THR:HG22	4:AF:178:GLN:O	2.18	0.44
4:AC:254:ASN:O	4:AC:255:ARG:HB2	2.17	0.44
4:AF:201:GLU:OE1	4:AF:201:GLU:N	2.51	0.44
4:AG:351:TYR:CE2	3:AS:19:VAL:HG11	2.52	0.44
2:AH:36:LYS:NZ	2:AH:37:THR:O	2.39	0.44
2:AK:2:ASN:HB2	2:AL:31:PHE:H	1.82	0.44
2:AL:123:ALA:O	2:AL:126:VAL:HG12	2.18	0.44
2:0G:52:HIS:ND1	2:0G:64:PRO:O	2.50	0.44
2:2:8:ASP:HB3	2:2:9:PHE:CD2	2.52	0.44
4:AA:182:LEU:O	4:AA:183:GLU:HB2	2.16	0.44
2:AE:69:PRO:HA	2:AE:84:LEU:HD23	2.00	0.44
4:AG:255:ARG:NH2	4:AG:440:CYS:O	2.50	0.44
4:AJ:308:THR:HG1	3:AP:27:ARG:HH12	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:45:THR:HG22	2:1:122:ASN:HB3	2.00	0.44
2:2:6:GLY:HA3	2:3:100:ALA:HB1	1.98	0.44
4:AA:389:PRO:HG3	4:AA:408:PHE:O	2.17	0.44
4:AJ:186:CYS:O	4:AJ:187:ASN:C	2.56	0.44
4:AJ:395:LYS:HB3	4:AJ:403:PHE:CD1	2.53	0.44
2:8:70:GLU:HG3	2:8:83:GLY:O	2.17	0.44
2:9:20:SER:OG	2:9:113:ILE:O	2.27	0.44
4:AB:200:ILE:HD11	4:AB:452:PHE:HE1	1.83	0.44
4:AB:345:HIS:CD2	4:AB:388:ASP:HB3	2.53	0.44
4:AC:253:PHE:HB3	4:AC:258:LEU:HD11	2.00	0.44
4:AC:327:ARG:HE	4:AF:370:THR:HA	1.83	0.44
4:AJ:306:PHE:CD1	3:AQ:16:SER:HB3	2.53	0.44
4:AJ:351:TYR:CE2	3:AP:21:PRO:HD3	2.53	0.44
2:5:28:PHE:CD1	2:5:132:MET:HB3	2.53	0.43
4:AA:394:THR:OG1	4:AA:395:LYS:N	2.50	0.43
4:AB:372:THR:O	4:AB:372:THR:OG1	2.35	0.43
4:AC:324:GLN:HB2	4:AF:354:ALA:HB1	2.00	0.43
4:AC:406:GLY:C	4:AC:463:GLN:HE21	2.21	0.43
4:AJ:403:PHE:O	4:AJ:404:ALA:HB3	2.18	0.43
2:AN:49:ILE:N	2:AN:67:ARG:HH12	2.15	0.43
2:5:58:ASP:O	2:5:61:VAL:HG12	2.18	0.43
2:0F:132:MET:SD	2:0F:132:MET:N	2.91	0.43
4:AG:215:TYR:OH	4:AJ:275:ARG:HD3	2.18	0.43
4:AJ:307:GLN:N	4:AJ:307:GLN:OE1	2.51	0.43
2:AK:2:ASN:ND2	2:AL:102:THR:OG1	2.51	0.43
1:0:15:LEU:HB3	1:0:17:GLN:HE22	1.82	0.43
2:3:9:PHE:CE1	2:3:133:LYS:HG2	2.54	0.43
2:4:34:THR:HG21	2:5:11:SER:N	2.28	0.43
1:0B:5:ASN:O	1:0B:6:LEU:HD22	2.18	0.43
4:AB:327:ARG:NH1	4:AC:370:THR:C	2.72	0.43
4:AB:387:PRO:HG2	4:AB:408:PHE:HB3	2.00	0.43
2:AK:9:PHE:HA	2:AK:132:MET:O	2.19	0.43
2:1:99:CYS:HA	1:0B:3:CYS:HB3	2.01	0.43
2:0F:67:ARG:NE	2:0F:84:LEU:HD12	2.34	0.43
4:AC:322:LEU:O	4:AC:325:ASP:HB2	2.18	0.43
2:AD:37:THR:HG21	2:AD:93:VAL:HG13	2.00	0.43
4:AG:208:THR:HG22	4:AJ:178:GLN:O	2.18	0.43
2:AM:56:ASP:OD1	2:AM:56:ASP:N	2.47	0.43
2:AM:58:ASP:HB3	2:AM:61:VAL:HG22	2.00	0.43
4:AB:403:PHE:CG	4:AB:404:ALA:N	2.87	0.43
4:AC:252:CYS:SG	4:AC:440:CYS:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AF:214:ASP:N	4:AF:214:ASP:OD1	2.52	0.43
2:AH:28:PHE:CD1	2:AH:135:ALA:HA	2.54	0.43
4:AJ:391:GLU:H	4:AJ:395:LYS:HB2	1.82	0.43
2:AK:109:GLN:HB2	2:AK:110:TRP:CE3	2.53	0.43
2:5:52:HIS:ND1	2:5:64:PRO:O	2.51	0.43
2:AI:69:PRO:HD2	2:AI:107:ASN:ND2	2.33	0.43
4:AJ:323:ALA:HB2	4:AJ:355:MET:SD	2.59	0.43
4:AJ:351:TYR:CD2	3:AP:21:PRO:HD3	2.53	0.43
2:2:122:ASN:O	2:2:126:VAL:HG23	2.18	0.43
4:AA:289:LYS:O	4:AA:291:VAL:N	2.45	0.43
4:AB:265:PHE:O	4:AB:269:MET:HG2	2.18	0.43
4:AC:416:LYS:HD3	4:AC:416:LYS:HA	1.67	0.43
2:AD:96:ASP:OD1	3:AR:10:CYS:HB2	2.18	0.43
4:AG:370:THR:OG1	4:AG:372:THR:HG23	2.18	0.43
4:AJ:416:LYS:HA	4:AJ:416:LYS:HD3	1.75	0.43
2:0H:28:PHE:CD2	2:0H:132:MET:HG2	2.53	0.43
2:2:30:GLN:HB2	2:2:133:LYS:HB3	2.00	0.43
4:AC:311:VAL:CG2	4:AC:322:LEU:HD11	2.49	0.43
4:AF:334:PRO:HG2	4:AF:337:TYR:CE2	2.54	0.43
2:AH:78:LEU:O	2:AH:79:LEU:HD22	2.19	0.43
4:AJ:255:ARG:HH21	4:AJ:436:SER:HB2	1.83	0.43
4:AJ:394:THR:HA	3:AP:19:VAL:HG22	2.01	0.43
2:AN:41:LEU:HD11	2:AN:122:ASN:HB3	2.01	0.43
2:6:34:THR:HG21	2:7:11:SER:H	1.84	0.43
4:AA:222:THR:O	4:AB:292:ASN:ND2	2.36	0.43
4:AB:327:ARG:O	4:AB:331:THR:HG23	2.19	0.43
2:AD:53:GLU:O	2:AD:63:GLY:N	2.50	0.43
2:AD:82:ASP:O	2:AD:84:LEU:HG	2.19	0.43
4:AF:238:ARG:CD	3:AS:7:ARG:HD2	2.49	0.43
4:AG:196:LEU:HD12	4:AG:415:TRP:CG	2.54	0.43
4:AG:252:CYS:N	2:AI:75:ASP:OD2	2.52	0.43
4:AG:255:ARG:HH21	4:AG:440:CYS:C	2.22	0.43
2:AI:62:PRO:HB3	2:AI:110:TRP:CD2	2.53	0.43
3:AO:25:ILE:O	3:AO:26:CYS:HB2	2.19	0.43
2:1:45:THR:OG1	2:1:89:LEU:HB2	2.19	0.43
2:4:28:PHE:CD1	2:4:132:MET:HB3	2.54	0.43
4:AA:175:PHE:HD2	2:AK:3:PHE:CZ	2.37	0.43
4:AA:237:ILE:HD12	4:AB:263:TYR:CE2	2.54	0.43
4:AB:409:VAL:HG23	4:AB:463:GLN:HA	2.00	0.43
4:AC:209:TYR:HD1	4:AF:180:LEU:HD21	1.83	0.43
4:AF:386:LEU:HD13	4:AF:408:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AG:197:TYR:CD1	4:AG:419:PHE:HB3	2.54	0.43
4:AG:387:PRO:HD2	4:AG:408:PHE:CD1	2.52	0.43
2:AI:41:LEU:HD23	2:AI:41:LEU:H	1.84	0.43
2:AK:28:PHE:CD2	2:AK:132:MET:HG2	2.54	0.43
2:AM:68:VAL:HG13	2:AM:85:ALA:HB3	2.01	0.43
2:AN:58:ASP:HB3	2:AN:61:VAL:HG12	2.01	0.43
2:0H:62:PRO:HB3	2:0H:110:TRP:NE1	2.28	0.43
3:AQ:12:ALA:HB1	3:AQ:13:PRO:HD2	1.99	0.43
2:1:28:PHE:CD1	2:1:132:MET:HB3	2.54	0.42
4:AA:194:LEU:HD21	4:AA:282:ASN:OD1	2.19	0.42
4:AB:275:ARG:O	4:AB:279:ILE:HG12	2.18	0.42
4:AF:256:LYS:O	4:AF:260:GLU:HG2	2.19	0.42
4:AF:324:GLN:HB3	3:AR:27:ARG:NH1	2.34	0.42
4:AG:205:SER:OG	4:AG:206:THR:N	2.51	0.42
4:AJ:305:VAL:HG13	4:AJ:461:ILE:HB	2.00	0.42
4:AJ:397:GLY:O	4:AJ:398:THR:C	2.56	0.42
2:AM:9:PHE:CD1	2:AM:133:LYS:HA	2.54	0.42
2:7:109:GLN:HB2	2:7:110:TRP:CE3	2.55	0.42
2:0F:28:PHE:HD1	2:0F:135:ALA:HB2	1.81	0.42
4:AA:223:CYS:HA	4:AB:292:ASN:ND2	2.34	0.42
4:AG:397:GLY:N	4:AG:402:ALA:HA	2.35	0.42
1:0:15:LEU:HB3	1:0:17:GLN:NE2	2.34	0.42
2:2:70:GLU:HG2	2:2:83:GLY:C	2.40	0.42
4:AA:306:PHE:CE1	4:AA:460:ARG:HD3	2.54	0.42
4:AA:324:GLN:NE2	3:AT:21:PRO:O	2.42	0.42
2:AD:13:ILE:HD12	2:AE:127:GLN:HB3	2.00	0.42
4:AF:357:ASP:OD1	4:AF:360:GLY:N	2.52	0.42
2:AI:31:PHE:HB3	2:AI:132:MET:HG3	2.00	0.42
4:AJ:304:PRO:HG2	4:AJ:460:ARG:HG2	2.01	0.42
2:7:9:PHE:CE1	2:7:133:LYS:HG2	2.53	0.42
2:0E:30:GLN:HG3	2:0F:2:ASN:HA	2.01	0.42
4:AB:176:THR:HA	4:AB:177:PRO:HD3	1.85	0.42
4:AJ:325:ASP:OD2	3:AP:27:ARG:NH1	2.52	0.42
2:0G:109:GLN:HB2	2:0G:110:TRP:CE3	2.55	0.42
2:1:80:SER:O	2:1:82:ASP:N	2.53	0.42
2:3:47:PHE:CZ	2:3:126:VAL:HG11	2.55	0.42
2:6:28:PHE:HA	2:6:134:GLY:O	2.19	0.42
1:0C:2:ASP:OD1	1:0C:2:ASP:N	2.51	0.42
2:0E:62:PRO:HG3	2:0E:110:TRP:CD1	2.55	0.42
4:AB:312:ASP:HA	4:AB:317:SER:HA	2.01	0.42
4:AC:238:ARG:NH2	4:AC:240:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AC:406:GLY:HA2	4:AC:463:GLN:HG2	2.00	0.42
4:AF:433:GLU:O	4:AF:436:SER:OG	2.31	0.42
4:AG:203:SER:OG	4:AG:204:ARG:HG2	2.20	0.42
4:AG:430:GLU:HG3	4:AG:444:GLN:O	2.20	0.42
2:AK:34:THR:OG1	2:AK:129:THR:HG23	2.20	0.42
2:AL:54:PRO:HD3	2:AL:109:GLN:CG	2.49	0.42
2:AN:100:ALA:N	3:AP:5:ASN:O	2.51	0.42
2:4:26:ASP:OD1	2:4:137:ARG:NH2	2.42	0.42
2:6:2:ASN:HA	2:7:30:GLN:HG2	2.02	0.42
2:6:102:THR:OG1	2:7:4:ASN:HA	2.19	0.42
4:AB:221:TYR:HD1	4:AC:247:TYR:HB2	1.84	0.42
4:AB:351:TYR:CE2	3:AT:21:PRO:HG3	2.54	0.42
4:AC:209:TYR:HB3	4:AF:180:LEU:HG	2.02	0.42
4:AC:355:MET:HB2	4:AC:364:PHE:HD2	1.85	0.42
4:AF:313:VAL:HG12	3:AR:25:ILE:HG12	2.00	0.42
4:AG:416:LYS:HA	4:AG:416:LYS:HD3	1.74	0.42
2:AH:67:ARG:NE	2:AH:84:LEU:HB3	2.35	0.42
2:AI:51:TYR:CE1	2:AI:66:ILE:HB	2.55	0.42
4:AJ:257:ASN:O	4:AJ:261:ALA:HB2	2.20	0.42
4:AA:218:LEU:HD23	4:AA:232:GLY:HA3	2.02	0.42
4:AA:416:LYS:HD3	4:AA:416:LYS:HA	1.73	0.42
4:AC:383:SER:OG	4:AC:384:ASN:N	2.53	0.42
4:AC:402:ALA:O	4:AC:404:ALA:N	2.53	0.42
2:AI:82:ASP:O	2:AI:84:LEU:HD12	2.19	0.42
4:AJ:344:MET:HA	4:AJ:386:LEU:HD22	2.00	0.42
2:AK:99:CYS:SG	3:AQ:4:LEU:HB3	2.60	0.42
3:AS:2:VAL:HG12	3:AS:3:LYS:O	2.20	0.42
1:0C:5:ASN:OD1	1:0C:5:ASN:N	2.52	0.42
4:AB:406:GLY:HA2	4:AB:464:ILE:HB	2.01	0.42
4:AF:212:ILE:HG13	4:AG:183:GLU:OE1	2.20	0.42
2:0H:28:PHE:CD1	2:0H:135:ALA:HB2	2.55	0.42
2:7:73:PHE:O	2:7:76:THR:OG1	2.36	0.42
2:8:29:ASN:ND2	2:8:134:GLY:HA3	2.34	0.42
4:AF:250:VAL:HA	4:AF:443:TYR:O	2.20	0.42
4:AF:324:GLN:HA	4:AG:362:PHE:HE1	1.85	0.42
4:AF:439:TRP:CD1	4:AF:439:TRP:N	2.87	0.42
4:AJ:321:PHE:CE2	4:AJ:352:LEU:HD21	2.55	0.42
2:AL:52:HIS:ND1	2:AL:64:PRO:O	2.52	0.42
2:5:69:PRO:HA	2:5:84:LEU:HA	2.02	0.42
2:6:72:PRO:HB2	2:6:76:THR:HG21	2.02	0.42
4:AJ:253:PHE:CZ	4:AJ:269:MET:HG3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AS:15:ALA:O	3:AS:16:SER:CB	2.67	0.42
3:AQ:2:VAL:HG23	3:AQ:3:LYS:H	1.85	0.42
2:1:67:ARG:HE	2:1:84:LEU:HB3	1.85	0.41
2:7:52:HIS:HB2	2:7:110:TRP:NE1	2.35	0.41
2:7:99:CYS:SG	2:7:100:ALA:N	2.93	0.41
2:8:52:HIS:ND1	2:8:64:PRO:O	2.53	0.41
4:AC:209:TYR:O	4:AC:239:HIS:ND1	2.52	0.41
2:AD:29:ASN:OD1	2:AD:29:ASN:N	2.52	0.41
4:AF:337:TYR:CE1	4:AG:188:ILE:HD13	2.45	0.41
4:AF:425:ARG:HB3	4:AF:448:GLU:OE1	2.20	0.41
2:AH:73:PHE:H	2:AH:76:THR:CB	2.32	0.41
4:AJ:193:LEU:HD23	4:AJ:193:LEU:H	1.84	0.41
2:0G:35:PHE:HD2	2:0G:99:CYS:O	2.03	0.41
2:0H:28:PHE:HD1	2:0H:135:ALA:HB2	1.84	0.41
2:0H:89:LEU:HD23	2:0H:89:LEU:HA	1.87	0.41
2:5:54:PRO:HD3	2:5:109:GLN:CG	2.49	0.41
2:7:9:PHE:CD1	2:7:9:PHE:N	2.88	0.41
2:0E:69:PRO:HA	2:0E:84:LEU:HD23	2.02	0.41
4:AC:283:GLN:O	4:AC:287:ILE:HG22	2.19	0.41
2:AE:26:ASP:HB3	2:AE:109:GLN:OE1	2.18	0.41
2:AK:102:THR:OG1	2:AL:4:ASN:HA	2.19	0.41
2:AL:28:PHE:CD1	2:AL:135:ALA:HB2	2.55	0.41
2:0G:2:ASN:N	2:0G:2:ASN:OD1	2.51	0.41
2:0G:36:LYS:NZ	2:0G:95:PRO:O	2.49	0.41
2:1:123:ALA:O	2:1:126:VAL:HG12	2.20	0.41
2:2:35:PHE:CD1	2:2:128:ILE:HG12	2.55	0.41
4:AA:180:LEU:HD13	4:AA:180:LEU:HA	1.80	0.41
4:AA:188:ILE:HA	4:AA:188:ILE:HD12	1.79	0.41
4:AA:297:TRP:HB3	4:AA:419:PHE:CE1	2.55	0.41
4:AA:390:THR:O	4:AA:392:GLY:N	2.53	0.41
4:AA:405:ALA:HA	4:AA:464:ILE:HG21	2.02	0.41
4:AC:237:ILE:HD13	4:AF:263:TYR:CE2	2.55	0.41
4:AJ:322:LEU:HD11	3:AP:24:PHE:CD1	2.53	0.41
2:2:56:ASP:OD1	2:2:56:ASP:N	2.52	0.41
2:5:28:PHE:CG	2:5:135:ALA:HB2	2.55	0.41
2:6:62:PRO:HG3	2:6:110:TRP:CD1	2.54	0.41
2:9:68:VAL:HG23	2:9:107:ASN:ND2	2.31	0.41
4:AA:235:GLY:H	4:AB:268:PHE:HE2	1.68	0.41
4:AC:371:PHE:CZ	4:AF:369:LEU:HD11	2.55	0.41
2:1:62:PRO:HB3	2:1:110:TRP:NE1	2.31	0.41
2:2:51:TYR:HA	2:2:110:TRP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:31:PHE:HA	2:5:132:MET:HA	2.03	0.41
2:AE:15:TRP:HB3	2:AE:128:ILE:HB	2.01	0.41
2:AH:20:SER:OG	2:AH:21:PHE:N	2.53	0.41
2:AH:31:PHE:H	2:AI:2:ASN:HB2	1.85	0.41
2:AI:52:HIS:CE1	2:AI:65:ALA:HB2	2.55	0.41
2:AM:2:ASN:OD1	2:AM:2:ASN:N	2.54	0.41
2:AN:98:PHE:CZ	3:AP:7:ARG:HB3	2.56	0.41
1:0:15:LEU:HD13	1:0:15:LEU:HA	1.75	0.41
2:1:47:PHE:CZ	2:1:126:VAL:HG11	2.55	0.41
2:4:62:PRO:HG3	2:4:110:TRP:CD1	2.56	0.41
2:9:73:PHE:N	2:9:76:THR:OG1	2.43	0.41
2:0E:10:PRO:HA	2:0F:34:THR:HG21	2.01	0.41
2:0F:67:ARG:NH1	2:0F:86:ALA:HB2	2.35	0.41
4:AB:425:ARG:O	4:AB:448:GLU:N	2.41	0.41
4:AC:197:TYR:OH	4:AC:297:TRP:NE1	2.49	0.41
4:AC:326:TRP:HZ2	4:AC:380:ILE:HD11	1.85	0.41
4:AC:383:SER:HB3	4:AC:386:LEU:HG	2.02	0.41
4:AJ:424:LYS:HD2	4:AJ:448:GLU:OE2	2.21	0.41
2:AL:42:THR:OG1	2:AL:122:ASN:ND2	2.43	0.41
4:AA:251:PHE:HA	4:AJ:231:PHE:HD1	1.85	0.41
4:AC:211:LYS:HE3	4:AC:238:ARG:HB2	2.01	0.41
2:AE:94:THR:HA	2:AE:95:PRO:HD3	1.94	0.41
4:AF:364:PHE:HE1	4:AG:369:LEU:H	1.69	0.41
4:AF:387:PRO:HD2	4:AF:408:PHE:CD1	2.55	0.41
2:AH:68:VAL:HG23	2:AH:107:ASN:OD1	2.20	0.41
2:AL:36:LYS:HZ1	2:AL:95:PRO:HB3	1.85	0.41
2:AN:54:PRO:HD3	2:AN:109:GLN:OE1	2.21	0.41
2:0H:24:LYS:HE3	2:0H:26:ASP:HB3	2.03	0.41
2:4:27:GLY:O	2:4:136:THR:OG1	2.32	0.41
2:6:58:ASP:HB3	2:6:61:VAL:CG2	2.50	0.41
2:0E:51:TYR:HA	2:0E:110:TRP:O	2.21	0.41
2:0E:53:GLU:O	2:0E:63:GLY:N	2.53	0.41
4:AB:318:THR:HA	4:AB:319:PRO:HD3	1.91	0.41
4:AF:387:PRO:HG2	4:AF:408:PHE:HB3	2.02	0.41
2:AI:27:GLY:O	2:AI:136:THR:OG1	2.32	0.41
4:AJ:252:CYS:HB2	4:AJ:442:LYS:HG2	2.03	0.41
2:AK:31:PHE:HB3	2:AK:132:MET:HG3	2.02	0.41
2:AN:106:MET:SD	2:AN:106:MET:N	2.83	0.41
3:AP:17:ARG:HG3	3:AP:17:ARG:HH11	1.85	0.41
2:1:47:PHE:HZ	2:1:126:VAL:HG11	1.86	0.41
2:6:109:GLN:HB2	2:6:110:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:50:PHE:HE2	2:7:114:ALA:HB3	1.85	0.41
2:0E:109:GLN:HB2	2:0E:110:TRP:CE3	2.55	0.41
4:AA:269:MET:SD	4:AJ:234:PRO:HB3	2.61	0.41
4:AC:209:TYR:CD1	4:AF:180:LEU:HD21	2.55	0.41
4:AF:307:GLN:HB2	4:AF:464:ILE:C	2.41	0.41
4:AF:329:PHE:CG	4:AF:462:LEU:HD22	2.55	0.41
4:AF:391:GLU:HB2	4:AF:395:LYS:HG3	2.03	0.41
4:AF:395:LYS:HA	4:AF:401:ASP:HB2	2.03	0.41
4:AG:287:ILE:HG22	4:AG:298:LEU:HB2	2.03	0.41
4:AG:323:ALA:N	4:AG:355:MET:SD	2.94	0.41
2:0G:34:THR:HG21	2:0H:11:SER:H	1.86	0.41
2:3:54:PRO:HD3	2:3:109:GLN:CG	2.51	0.41
2:0F:67:ARG:NH2	2:0F:85:ALA:O	2.52	0.41
4:AC:243:LYS:NZ	2:AE:29:ASN:HB2	2.36	0.41
2:AH:11:SER:H	2:AI:34:THR:HG21	1.86	0.41
4:AJ:413:ALA:HB3	4:AJ:415:TRP:CE2	2.56	0.41
2:AK:99:CYS:SG	3:AQ:4:LEU:HD22	2.60	0.41
2:AL:2:ASN:N	2:AL:2:ASN:OD1	2.52	0.41
4:AA:403:PHE:CE1	4:AA:464:ILE:HD12	2.56	0.40
2:AD:50:PHE:HA	2:AD:67:ARG:HA	2.04	0.40
2:AE:52:HIS:HB2	2:AE:110:TRP:CD1	2.57	0.40
4:AG:226:LYS:HD3	4:AG:227:CYS:H	1.86	0.40
4:AG:354:ALA:HB3	3:AS:21:PRO:HD2	2.02	0.40
4:AJ:354:ALA:C	3:AP:21:PRO:HG2	2.41	0.40
4:AJ:422:VAL:O	4:AJ:449:ASP:HB2	2.21	0.40
2:AK:15:TRP:HB3	2:AK:128:ILE:HB	2.03	0.40
2:0G:64:PRO:HG2	2:0G:66:ILE:HD11	2.02	0.40
1:0A:6:LEU:HD12	1:0A:6:LEU:HA	1.93	0.40
4:AC:253:PHE:O	4:AC:440:CYS:HA	2.21	0.40
4:AG:413:ALA:HB3	4:AG:415:TRP:CE2	2.56	0.40
2:AH:9:PHE:CD1	2:AH:133:LYS:HA	2.56	0.40
2:AM:123:ALA:HA	2:AM:126:VAL:HG12	2.02	0.40
2:0H:45:THR:O	2:0H:88:THR:HA	2.21	0.40
2:2:34:THR:HG21	2:3:11:SER:N	2.34	0.40
2:4:46:THR:OG1	2:4:116:ALA:HB3	2.20	0.40
2:4:107:ASN:N	2:4:107:ASN:OD1	2.55	0.40
2:8:102:THR:OG1	2:9:4:ASN:HA	2.21	0.40
2:8:109:GLN:HB2	2:8:110:TRP:CZ3	2.57	0.40
4:AA:247:TYR:CE1	4:AJ:221:TYR:CE1	3.09	0.40
4:AB:284:ALA:HB1	4:AB:294:PRO:HD2	2.03	0.40
4:AC:322:LEU:HD13	3:AO:27:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AE:46:THR:OG1	2:AE:116:ALA:HB3	2.22	0.40
4:AF:395:LYS:HE3	4:AF:395:LYS:HB3	1.82	0.40
4:AG:234:PRO:HB3	4:AJ:269:MET:SD	2.60	0.40
4:AG:345:HIS:CD2	4:AG:384:ASN:HA	2.56	0.40
4:AJ:390:THR:O	4:AJ:390:THR:OG1	2.35	0.40
2:AN:58:ASP:OD2	2:AN:60:CYS:HB3	2.21	0.40
2:0E:33:PHE:CZ	2:0E:113:ILE:HD11	2.56	0.40
2:0E:69:PRO:HA	2:0E:84:LEU:HA	2.02	0.40
2:0E:96:ASP:OD1	2:0E:96:ASP:N	2.54	0.40
2:0F:23:VAL:HG21	2:0F:130:VAL:HG11	2.02	0.40
4:AA:178:GLN:HE22	4:AA:180:LEU:CD2	2.34	0.40
4:AA:248:ARG:HA	4:AA:248:ARG:HD2	1.95	0.40
4:AB:402:ALA:O	4:AB:403:PHE:CB	2.67	0.40
4:AB:408:PHE:HE1	4:AB:411:ALA:HB2	1.87	0.40
4:AC:310:PRO:HB2	4:AC:317:SER:OG	2.21	0.40
4:AF:424:LYS:HB3	4:AF:448:GLU:HB3	2.03	0.40
4:AG:327:ARG:HA	4:AG:330:VAL:HG12	2.02	0.40
2:AI:2:ASN:OD1	2:AI:2:ASN:N	2.55	0.40
4:AJ:185:ASP:HB3	4:AJ:187:ASN:HD22	1.86	0.40
2:AK:30:GLN:HG2	2:AL:2:ASN:HA	2.02	0.40
2:AN:98:PHE:CE1	3:AP:7:ARG:HB3	2.57	0.40
2:0H:9:PHE:N	2:0H:9:PHE:CD1	2.89	0.40
3:AR:1:MET:HB3	3:AR:2:VAL:H	1.53	0.40
2:2:35:PHE:HB3	2:2:89:LEU:HD11	2.03	0.40
4:AB:304:PRO:HD2	4:AB:459:GLY:O	2.22	0.40
4:AB:453:VAL:CG2	4:AB:456:CYS:HB3	2.52	0.40
4:AC:218:LEU:HA	4:AC:218:LEU:HD23	1.81	0.40
2:AE:23:VAL:HG21	2:AE:130:VAL:HG11	2.03	0.40
4:AJ:289:LYS:O	4:AJ:293:GLU:HB2	2.22	0.40
2:AK:89:LEU:HD23	2:AK:89:LEU:HA	1.87	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	0	17/217 (8%)	10 (59%)	6 (35%)	1 (6%)	1	16
1	0A	17/217 (8%)	13 (76%)	4 (24%)	0	100	100
1	0B	17/217 (8%)	10 (59%)	7 (41%)	0	100	100
1	0C	17/217 (8%)	9 (53%)	4 (24%)	4 (24%)	0	1
1	0D	17/217 (8%)	13 (76%)	4 (24%)	0	100	100
1	f	20/217 (9%)	18 (90%)	2 (10%)	0	100	100
2	0E	135/137 (98%)	123 (91%)	11 (8%)	1 (1%)	19	55
2	0F	135/137 (98%)	120 (89%)	15 (11%)	0	100	100
2	0G	135/137 (98%)	125 (93%)	10 (7%)	0	100	100
2	0H	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
2	1	135/137 (98%)	118 (87%)	16 (12%)	1 (1%)	19	55
2	2	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
2	3	135/137 (98%)	120 (89%)	15 (11%)	0	100	100
2	4	135/137 (98%)	120 (89%)	15 (11%)	0	100	100
2	5	135/137 (98%)	120 (89%)	15 (11%)	0	100	100
2	6	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
2	7	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
2	8	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
2	9	135/137 (98%)	121 (90%)	14 (10%)	0	100	100
2	AD	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
2	AE	135/137 (98%)	116 (86%)	19 (14%)	0	100	100
2	AH	135/137 (98%)	110 (82%)	22 (16%)	3 (2%)	5	32
2	AI	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
2	AK	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
2	AL	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
2	AM	134/137 (98%)	119 (89%)	15 (11%)	0	100	100
2	AN	134/137 (98%)	113 (84%)	21 (16%)	0	100	100
2	l	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
2	m	135/137 (98%)	116 (86%)	19 (14%)	0	100	100
2	p	135/137 (98%)	117 (87%)	16 (12%)	2 (2%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	q	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
2	s	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
2	t	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
2	u	134/137 (98%)	118 (88%)	16 (12%)	0	100	100
2	v	134/137 (98%)	116 (87%)	18 (13%)	0	100	100
2	z	135/137 (98%)	125 (93%)	10 (7%)	0	100	100
3	AO	26/38 (68%)	20 (77%)	6 (23%)	0	100	100
3	AP	26/38 (68%)	16 (62%)	9 (35%)	1 (4%)	2	22
3	AQ	26/38 (68%)	18 (69%)	7 (27%)	1 (4%)	2	22
3	AR	26/38 (68%)	17 (65%)	8 (31%)	1 (4%)	2	22
3	AS	26/38 (68%)	14 (54%)	9 (35%)	3 (12%)	0	5
3	AT	26/38 (68%)	18 (69%)	6 (23%)	2 (8%)	1	13
3	a	26/38 (68%)	23 (88%)	3 (12%)	0	100	100
3	b	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
3	c	32/38 (84%)	28 (88%)	4 (12%)	0	100	100
3	d	32/38 (84%)	27 (84%)	4 (12%)	1 (3%)	3	26
3	e	26/38 (68%)	20 (77%)	6 (23%)	0	100	100
4	AA	289/465 (62%)	241 (83%)	46 (16%)	2 (1%)	19	55
4	AB	289/465 (62%)	238 (82%)	48 (17%)	3 (1%)	13	47
4	AC	286/465 (62%)	227 (79%)	53 (18%)	6 (2%)	5	33
4	AF	289/465 (62%)	249 (86%)	40 (14%)	0	100	100
4	AG	289/465 (62%)	242 (84%)	45 (16%)	2 (1%)	19	55
4	AJ	289/465 (62%)	248 (86%)	39 (14%)	2 (1%)	19	55
4	g	289/465 (62%)	255 (88%)	34 (12%)	0	100	100
4	h	289/465 (62%)	238 (82%)	47 (16%)	4 (1%)	9	40
4	i	287/465 (62%)	240 (84%)	44 (15%)	3 (1%)	13	47
4	j	287/465 (62%)	232 (81%)	48 (17%)	7 (2%)	5	31
4	k	286/465 (62%)	262 (92%)	24 (8%)	0	100	100
4	n	289/465 (62%)	257 (89%)	32 (11%)	0	100	100
4	o	289/465 (62%)	246 (85%)	41 (14%)	2 (1%)	19	55
4	r	289/465 (62%)	251 (87%)	34 (12%)	4 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	w	287/465 (62%)	226 (79%)	53 (18%)	8 (3%)	4	28
4	x	287/465 (62%)	240 (84%)	39 (14%)	8 (3%)	4	28
4	y	287/465 (62%)	237 (83%)	46 (16%)	4 (1%)	9	40
All	All	9346/13735 (68%)	8023 (86%)	1247 (13%)	76 (1%)	19	53

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	16	VAL
4	h	191	ALA
4	h	193	LEU
4	i	212	ILE
4	i	366	ASP
4	j	212	ILE
4	j	221	TYR
4	j	370	THR
4	j	372	THR
2	p	77	VAL
2	p	78	LEU
4	w	221	TYR
4	w	373	PRO
4	y	221	TYR
4	y	398	THR
1	0C	9	ALA
1	0C	16	VAL
2	0E	26	ASP
4	AC	259	GLN
4	AJ	404	ALA
4	j	396	GLY
4	r	377	ARG
4	r	397	GLY
4	r	399	GLY
4	w	225	ALA
4	w	368	ASP
4	x	221	TYR
4	x	362	PHE
4	x	366	ASP
4	x	367	GLY
4	x	372	THR
4	y	397	GLY
4	AB	404	ALA

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Mol	Chain	Res	Type
4	AB	406	GLY
4	AC	261	ALA
4	AC	402	ALA
4	AC	406	GLY
2	AH	77	VAL
4	AJ	377	ARG
3	AR	26	CYS
3	AS	16	SER
4	j	223	CYS
4	j	225	ALA
4	o	189	GLU
4	w	222	THR
4	w	372	THR
4	x	368	ASP
4	AA	183	GLU
4	AB	403	PHE
2	AH	57	ALA
2	AH	78	LEU
3	AS	9	LEU
4	i	226	LYS
4	w	394	THR
4	y	367	GLY
1	0C	7	CYS
1	0C	8	GLY
4	AA	394	THR
4	AG	374	ASP
3	AT	7	ARG
4	h	190	CYS
4	h	192	SER
4	o	373	PRO
4	r	398	THR
4	w	371	PHE
4	x	371	PHE
4	x	398	THR
4	AC	404	ALA
3	AP	8	PRO
3	AS	10	CYS
3	AT	13	PRO
4	AG	373	PRO
2	1	10	PRO
4	AC	290	GLY
3	AQ	25	ILE

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Mol	Chain	Res	Type
3	d	28	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	14/175 (8%)	12 (86%)	2 (14%)	2	15
1	0A	14/175 (8%)	14 (100%)	0	100	100
1	0B	14/175 (8%)	13 (93%)	1 (7%)	12	35
1	0C	14/175 (8%)	12 (86%)	2 (14%)	2	15
1	0D	14/175 (8%)	12 (86%)	2 (14%)	2	15
1	f	17/175 (10%)	17 (100%)	0	100	100
2	0E	112/112 (100%)	112 (100%)	0	100	100
2	0F	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	0G	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	0H	112/112 (100%)	112 (100%)	0	100	100
2	1	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	2	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	3	112/112 (100%)	110 (98%)	2 (2%)	54	71
2	4	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	5	112/112 (100%)	110 (98%)	2 (2%)	54	71
2	6	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	7	112/112 (100%)	112 (100%)	0	100	100
2	8	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	9	112/112 (100%)	112 (100%)	0	100	100
2	AD	112/112 (100%)	112 (100%)	0	100	100
2	AE	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	AH	112/112 (100%)	109 (97%)	3 (3%)	40	61
2	AI	112/112 (100%)	111 (99%)	1 (1%)	75	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AK	112/112 (100%)	112 (100%)	0	100	100
2	AL	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	AM	111/112 (99%)	111 (100%)	0	100	100
2	AN	111/112 (99%)	111 (100%)	0	100	100
2	l	112/112 (100%)	112 (100%)	0	100	100
2	m	112/112 (100%)	111 (99%)	1 (1%)	75	83
2	p	112/112 (100%)	110 (98%)	2 (2%)	54	71
2	q	112/112 (100%)	110 (98%)	2 (2%)	54	71
2	s	112/112 (100%)	112 (100%)	0	100	100
2	t	112/112 (100%)	110 (98%)	2 (2%)	54	71
2	u	111/112 (99%)	110 (99%)	1 (1%)	75	83
2	v	111/112 (99%)	110 (99%)	1 (1%)	75	83
2	z	112/112 (100%)	111 (99%)	1 (1%)	75	83
3	AO	25/32 (78%)	24 (96%)	1 (4%)	27	49
3	AP	25/32 (78%)	25 (100%)	0	100	100
3	AQ	25/32 (78%)	24 (96%)	1 (4%)	27	49
3	AR	25/32 (78%)	25 (100%)	0	100	100
3	AS	25/32 (78%)	25 (100%)	0	100	100
3	AT	25/32 (78%)	25 (100%)	0	100	100
3	a	25/32 (78%)	25 (100%)	0	100	100
3	b	25/32 (78%)	25 (100%)	0	100	100
3	c	29/32 (91%)	27 (93%)	2 (7%)	13	35
3	d	29/32 (91%)	28 (97%)	1 (3%)	32	54
3	e	25/32 (78%)	24 (96%)	1 (4%)	27	49
4	AA	235/379 (62%)	234 (100%)	1 (0%)	89	91
4	AB	235/379 (62%)	234 (100%)	1 (0%)	89	91
4	AC	232/379 (61%)	228 (98%)	4 (2%)	56	73
4	AF	235/379 (62%)	234 (100%)	1 (0%)	89	91
4	AG	235/379 (62%)	233 (99%)	2 (1%)	75	83
4	AJ	235/379 (62%)	232 (99%)	3 (1%)	65	77
4	g	235/379 (62%)	235 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	h	235/379 (62%)	231 (98%)	4 (2%)	56	73
4	i	233/379 (62%)	223 (96%)	10 (4%)	25	48
4	j	233/379 (62%)	226 (97%)	7 (3%)	36	57
4	k	232/379 (61%)	232 (100%)	0	100	100
4	n	235/379 (62%)	234 (100%)	1 (0%)	89	91
4	o	235/379 (62%)	234 (100%)	1 (0%)	89	91
4	r	235/379 (62%)	233 (99%)	2 (1%)	75	83
4	w	233/379 (62%)	224 (96%)	9 (4%)	27	50
4	x	233/379 (62%)	218 (94%)	15 (6%)	14	37
4	y	233/379 (62%)	225 (97%)	8 (3%)	32	54
All	All	7705/11205 (69%)	7596 (99%)	109 (1%)	62	76

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	14	ARG
1	0	15	LEU
2	1	110	TRP
2	2	105	CYS
2	3	33	PHE
2	3	110	TRP
2	4	105	CYS
2	5	34	THR
2	5	137	ARG
2	6	105	CYS
2	8	105	CYS
3	c	3	LYS
3	c	23	CYS
3	d	6	CYS
3	e	6	CYS
4	h	189	GLU
4	h	192	SER
4	h	385	CYS
4	h	390	THR
4	i	211	LYS
4	i	212	ILE
4	i	220	GLU
4	i	221	TYR

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Mol	Chain	Res	Type
4	i	223	CYS
4	i	226	LYS
4	i	325	ASP
4	i	366	ASP
4	i	377	ARG
4	i	395	LYS
4	j	211	LYS
4	j	222	THR
4	j	223	CYS
4	j	226	LYS
4	j	362	PHE
4	j	363	LEU
4	j	364	PHE
2	m	34	THR
4	n	252	CYS
4	o	211	LYS
2	p	76	THR
2	p	78	LEU
2	q	34	THR
2	q	99	CYS
4	r	375	LEU
4	r	395	LYS
2	t	34	THR
2	t	99	CYS
2	u	88	THR
2	v	34	THR
4	w	220	GLU
4	w	221	TYR
4	w	223	CYS
4	w	226	LYS
4	w	243	LYS
4	w	371	PHE
4	w	374	ASP
4	w	377	ARG
4	w	395	LYS
4	x	220	GLU
4	x	221	TYR
4	x	223	CYS
4	x	224	ASP
4	x	327	ARG
4	x	331	THR
4	x	362	PHE

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Mol	Chain	Res	Type
4	x	363	LEU
4	x	368	ASP
4	x	370	THR
4	x	371	PHE
4	x	377	ARG
4	x	395	LYS
4	x	398	THR
4	x	400	GLN
4	y	221	TYR
4	y	223	CYS
4	y	252	CYS
4	y	366	ASP
4	y	371	PHE
4	y	372	THR
4	y	381	ARG
4	y	395	LYS
2	z	99	CYS
1	0B	14	ARG
1	0C	6	LEU
1	0C	14	ARG
1	0D	7	CYS
1	0D	14	ARG
2	0F	110	TRP
4	AA	180	LEU
4	AB	252	CYS
4	AC	369	LEU
4	AC	403	PHE
4	AC	407	SER
4	AC	460	ARG
2	AE	34	THR
4	AF	184	VAL
4	AG	211	LYS
4	AG	252	CYS
2	AH	61	VAL
2	AH	75	ASP
2	AH	76	THR
2	AI	34	THR
4	AJ	186	CYS
4	AJ	375	LEU
4	AJ	395	LYS
2	AL	110	TRP
2	0G	74	CYS

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Mol	Chain	Res	Type
3	AO	4	LEU
3	AQ	24	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	5	ASN
1	0	17	GLN
2	1	127	GLN
2	2	127	GLN
2	3	107	ASN
2	3	109	GLN
2	3	127	GLN
2	4	109	GLN
2	4	127	GLN
2	5	107	ASN
2	5	127	GLN
2	6	127	GLN
2	7	127	GLN
2	8	127	GLN
2	9	107	ASN
2	9	109	GLN
2	9	127	GLN
4	g	187	ASN
4	g	239	HIS
4	g	292	ASN
4	h	239	HIS
4	h	257	ASN
4	h	277	HIS
4	h	292	ASN
4	h	314	ASN
4	h	347	ASN
4	i	307	GLN
4	i	384	ASN
4	i	393	ASN
4	i	400	GLN
4	i	444	GLN
4	j	257	ASN
4	j	384	ASN
4	k	236	ASN
4	k	257	ASN
4	k	292	ASN

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Mol	Chain	Res	Type
2	l	48	ASN
2	m	127	GLN
4	n	239	HIS
4	n	277	HIS
4	n	324	GLN
4	n	393	ASN
4	o	178	GLN
4	o	314	ASN
4	o	346	GLN
4	o	431	GLN
4	o	444	GLN
2	p	48	ASN
2	p	127	GLN
4	r	199	GLN
4	r	277	HIS
4	r	282	ASN
4	r	301	ASN
4	r	400	GLN
2	s	30	GLN
2	s	127	GLN
2	t	127	GLN
2	u	127	GLN
2	v	122	ASN
4	w	178	GLN
4	w	257	ASN
4	w	283	GLN
4	w	384	ASN
4	w	444	GLN
4	x	257	ASN
4	x	359	ASN
4	x	444	GLN
4	y	257	ASN
4	y	283	GLN
2	z	127	GLN
1	0A	5	ASN
2	0E	127	GLN
2	0F	4	ASN
2	0F	127	GLN
4	AA	187	ASN
4	AA	199	GLN
4	AA	239	HIS
4	AA	292	ASN

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Mol	Chain	Res	Type
4	AA	463	GLN
4	AB	239	HIS
4	AB	257	ASN
4	AB	277	HIS
4	AB	393	ASN
4	AB	400	GLN
4	AC	262	ASN
4	AC	292	ASN
4	AC	307	GLN
2	AD	127	GLN
2	AE	127	GLN
4	AF	239	HIS
4	AF	277	HIS
4	AF	347	ASN
4	AG	178	GLN
4	AG	282	ASN
4	AG	292	ASN
4	AG	307	GLN
4	AG	384	ASN
4	AG	393	ASN
4	AG	431	GLN
4	AG	458	HIS
2	AH	48	ASN
2	AH	127	GLN
2	AI	29	ASN
4	AJ	187	ASN
4	AJ	292	ASN
4	AJ	301	ASN
4	AJ	324	GLN
2	AK	127	GLN
2	AL	127	GLN
2	AM	109	GLN
2	AN	122	ASN
2	OG	127	GLN
2	OH	127	GLN
3	AP	11	GLN
3	AR	5	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

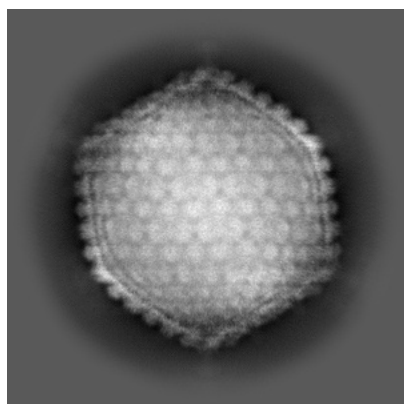
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29540. These allow visual inspection of the internal detail of the map and identification of artifacts.

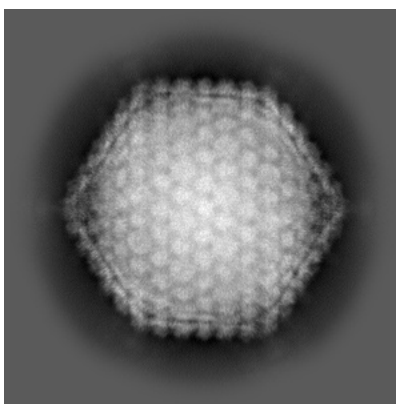
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

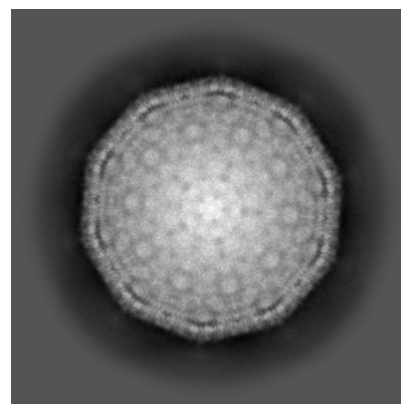
6.1.1 Primary map



X

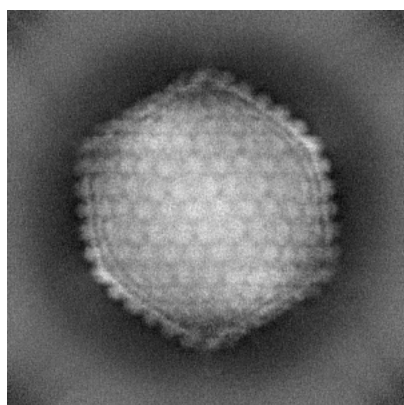


Y

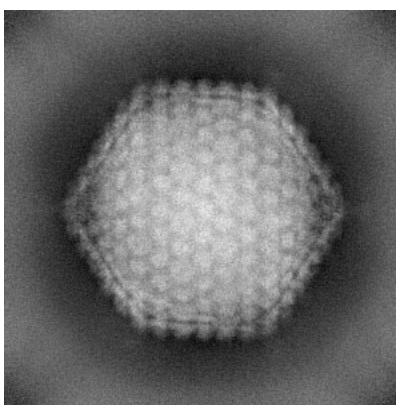


Z

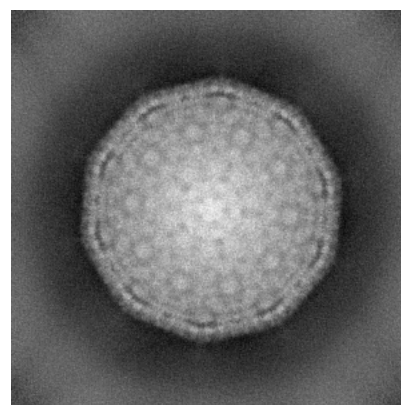
6.1.2 Raw map



X



Y

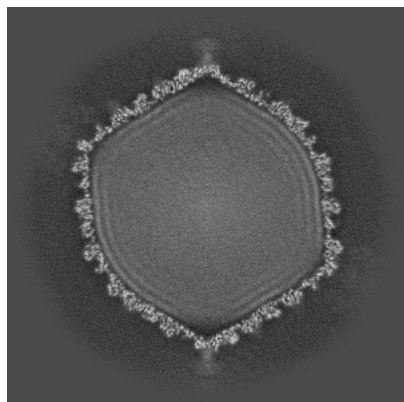


Z

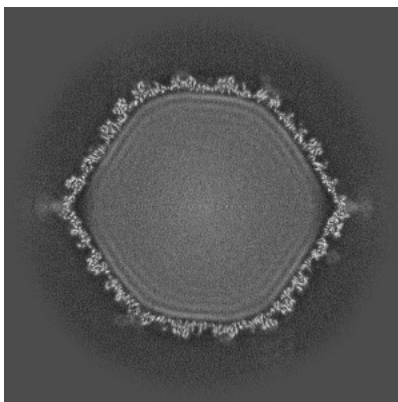
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

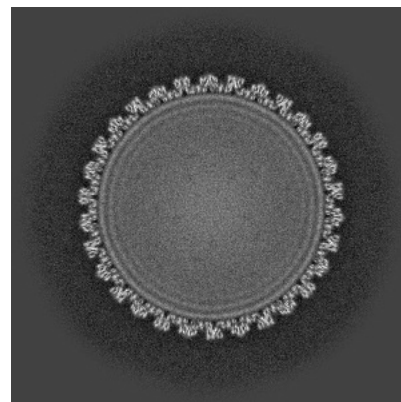
6.2.1 Primary map



X Index: 384

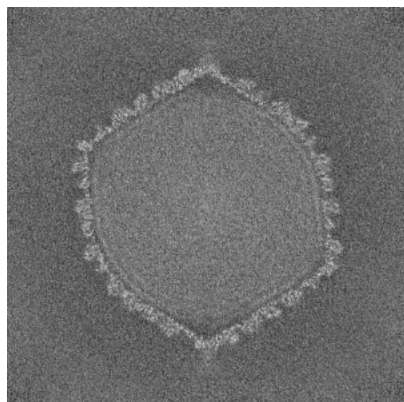


Y Index: 384

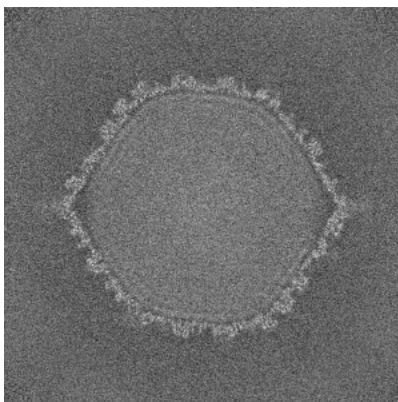


Z Index: 384

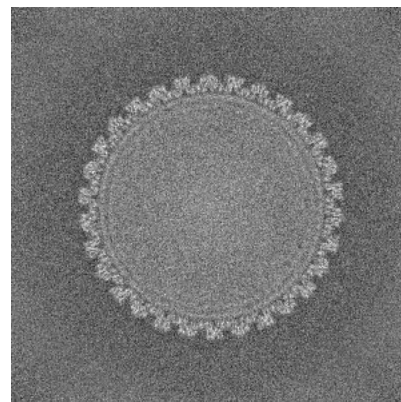
6.2.2 Raw map



X Index: 384



Y Index: 384

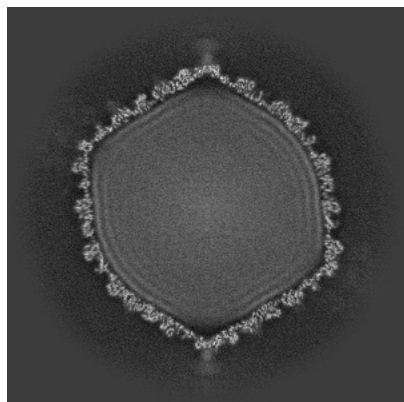


Z Index: 384

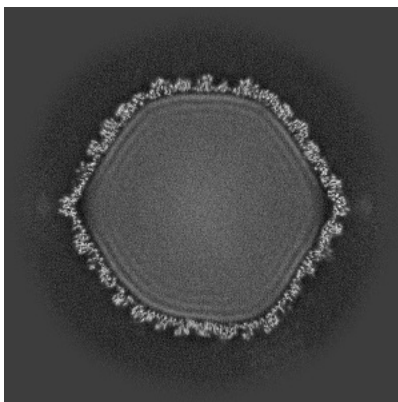
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

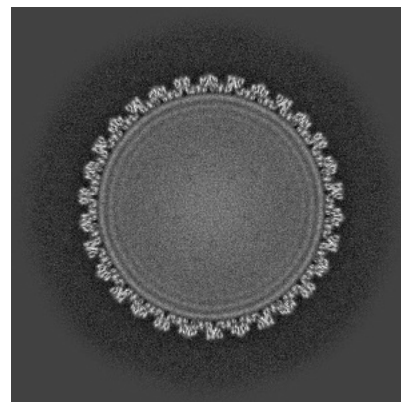
6.3.1 Primary map



X Index: 385

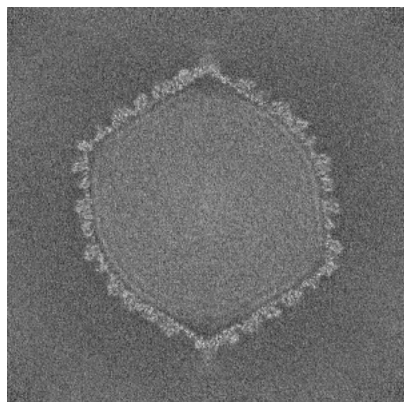


Y Index: 369

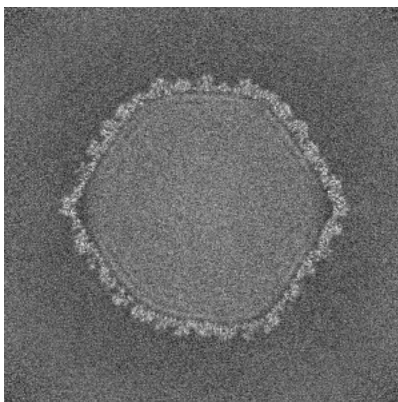


Z Index: 384

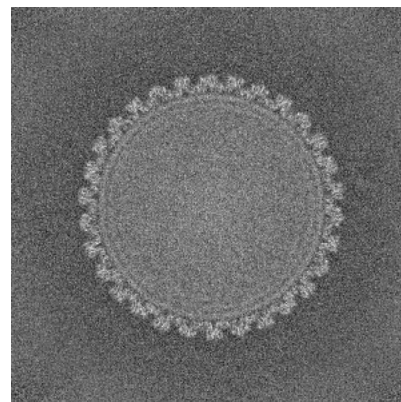
6.3.2 Raw map



X Index: 384



Y Index: 369

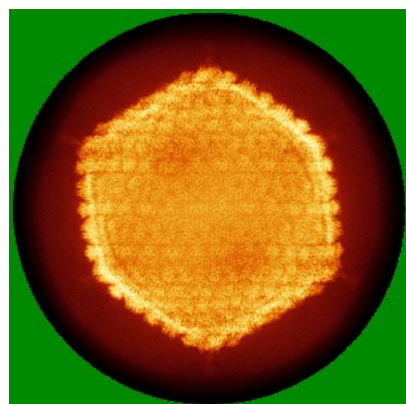


Z Index: 383

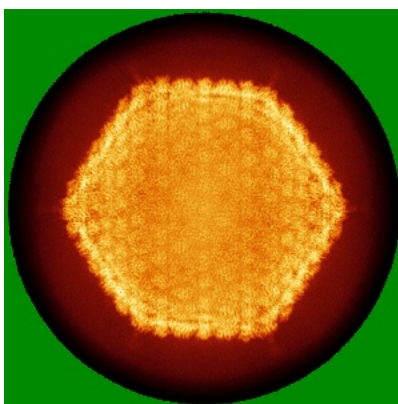
The images above show the largest variance slices of the map in three orthogonal directions.

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

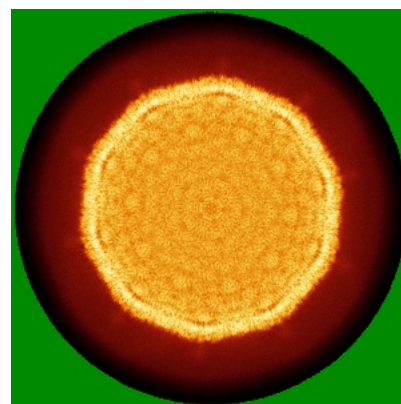
6.4.1 Primary map



X

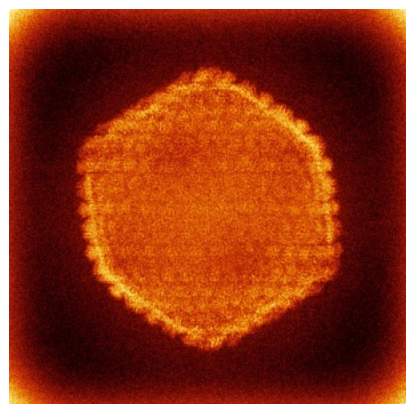


Y

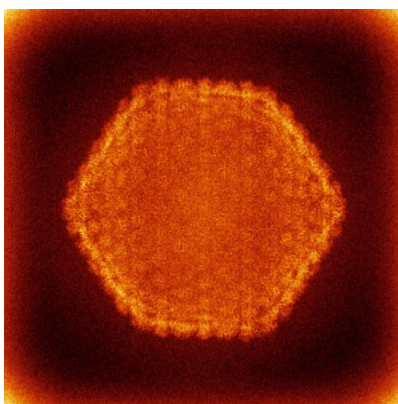


Z

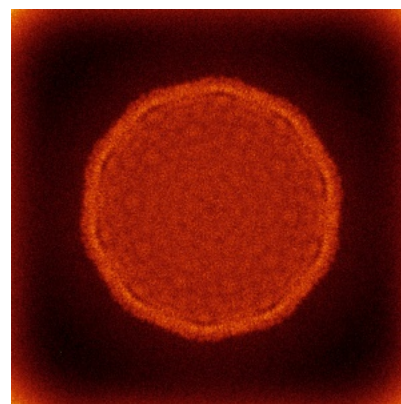
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



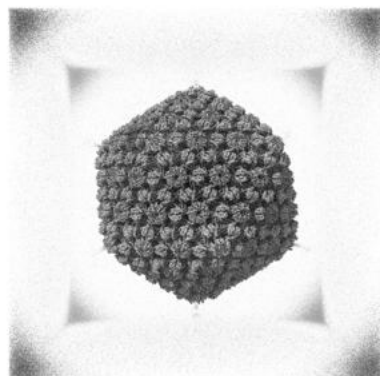
Y



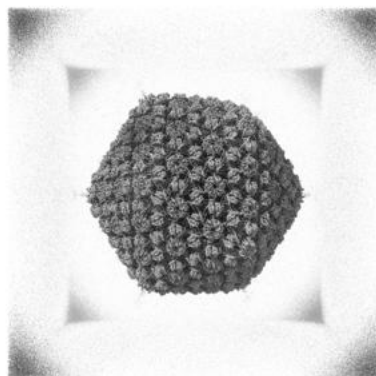
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

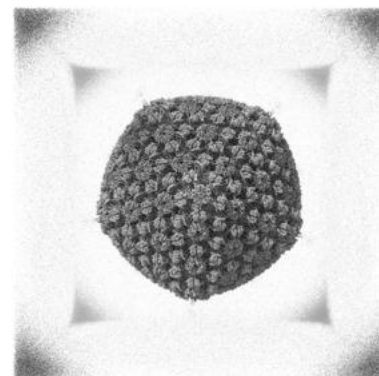
6.5.2 Raw map



X



Y



Z

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

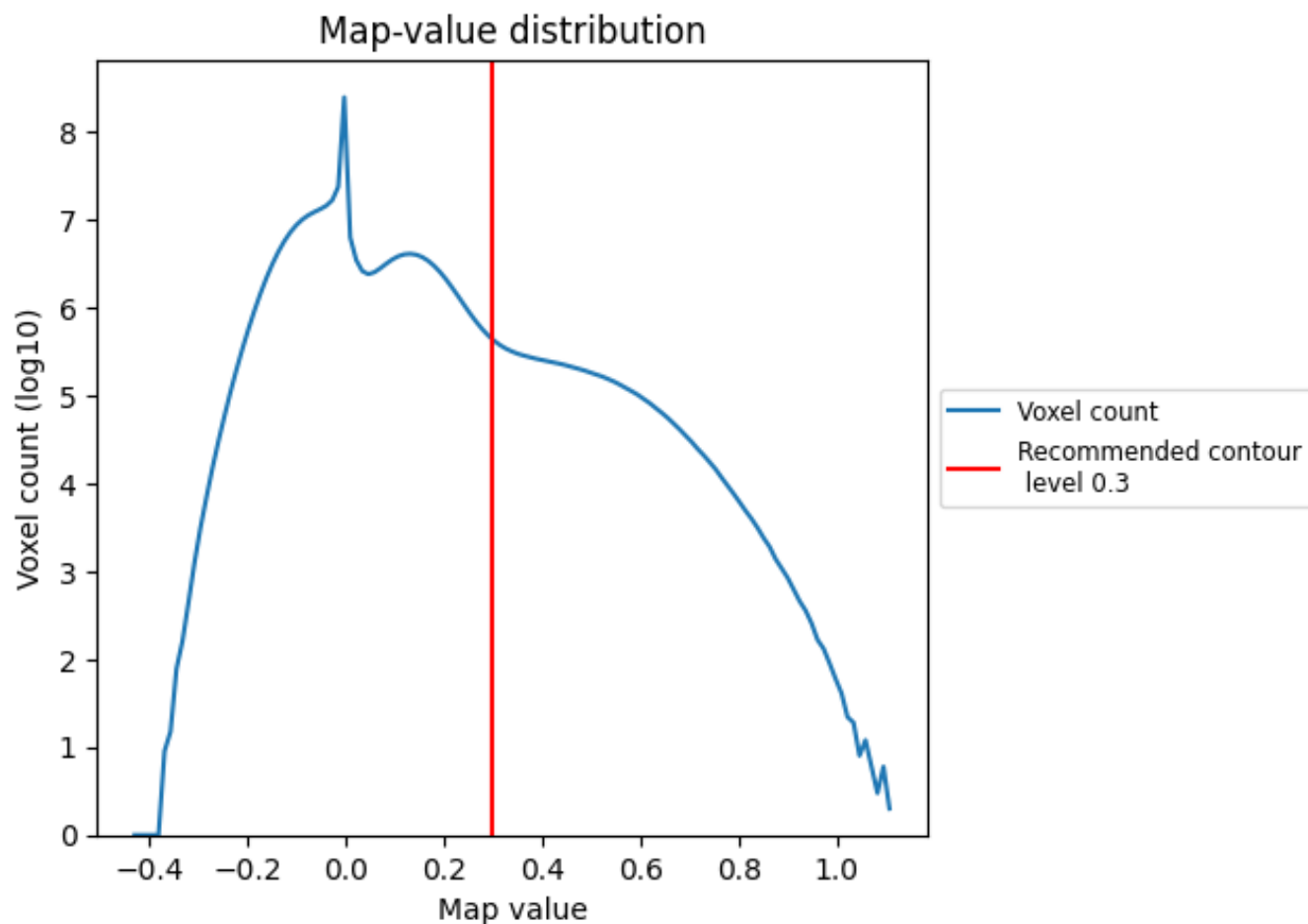
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

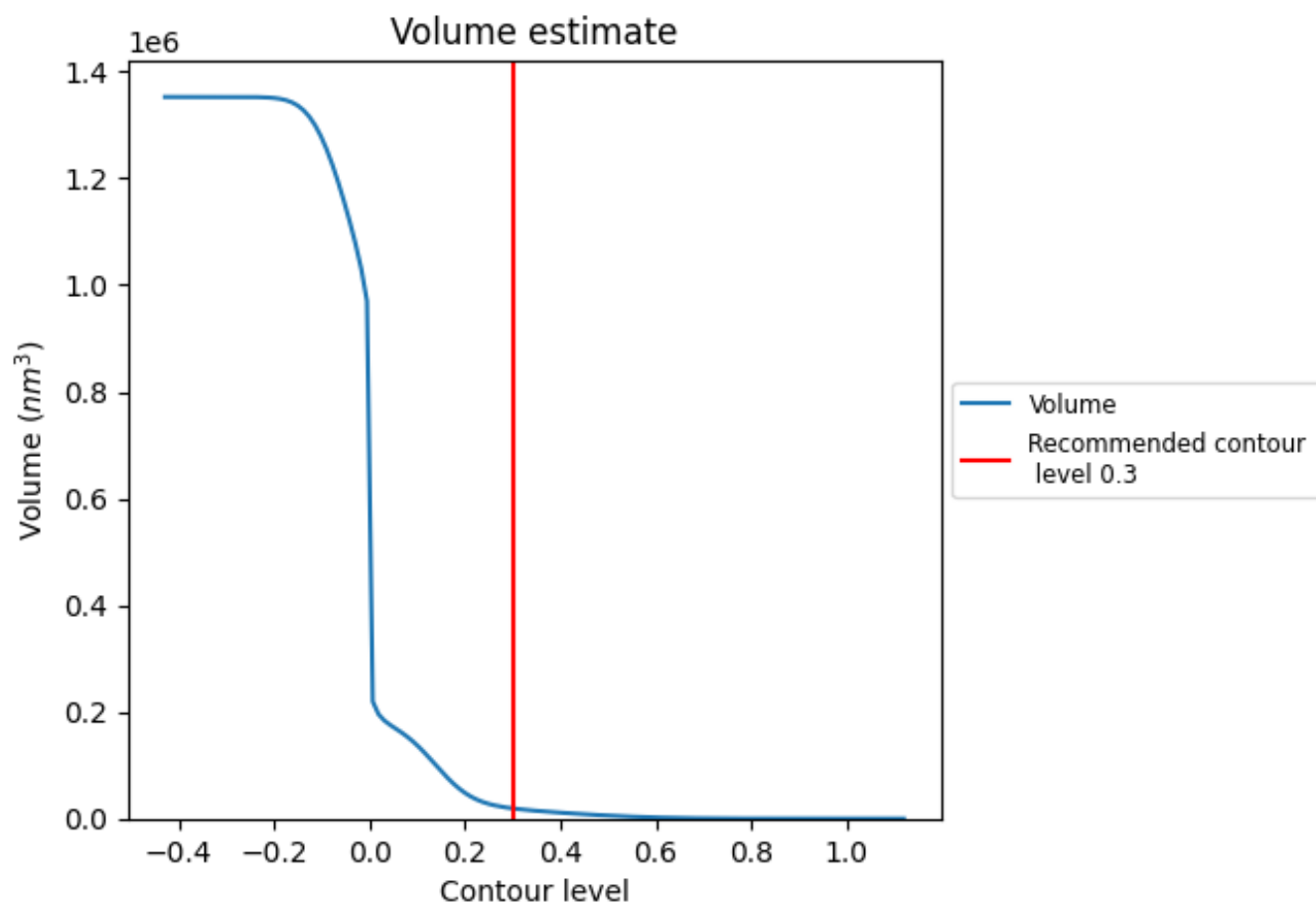
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

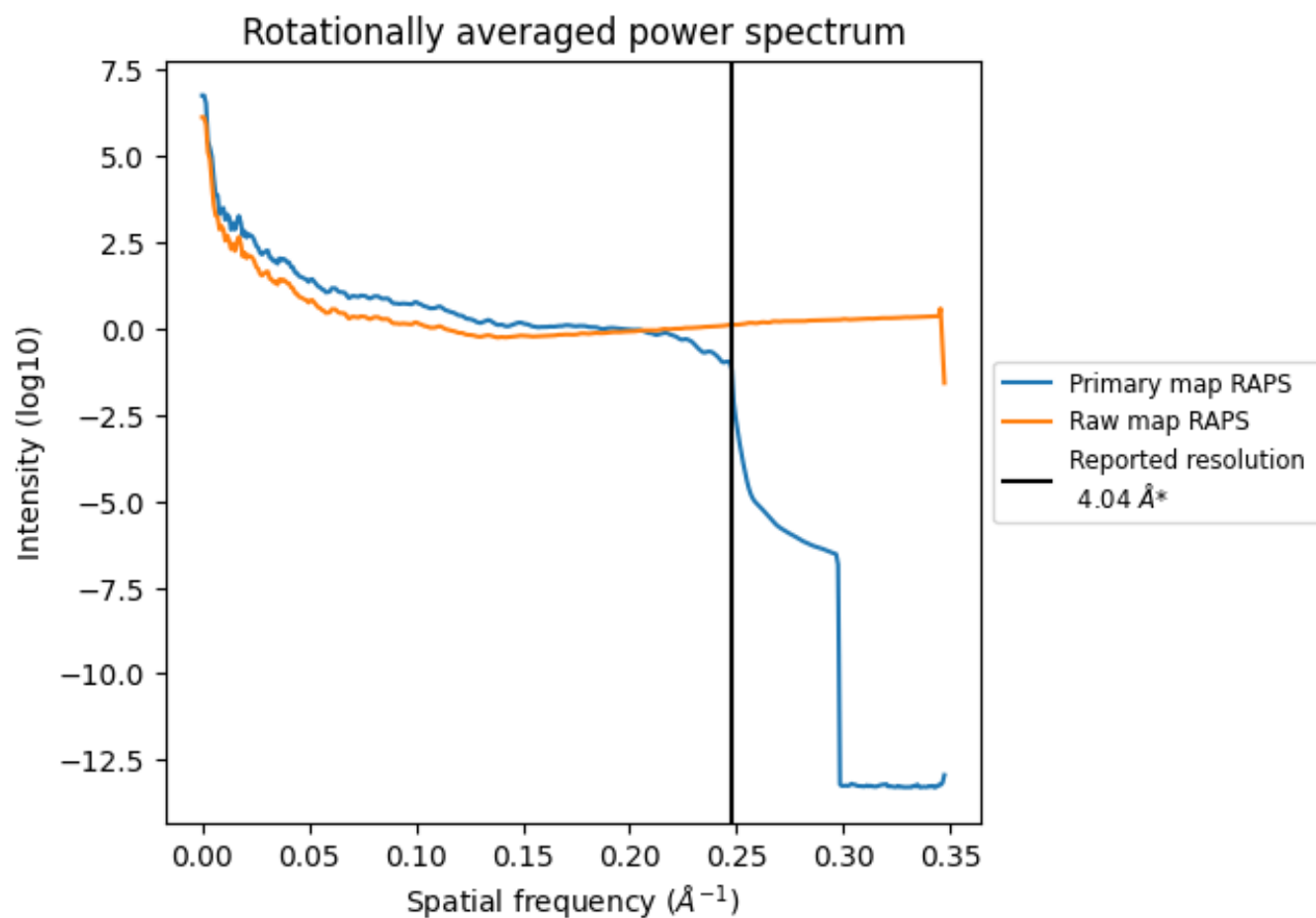
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 19132 nm³; this corresponds to an approximate mass of 17282 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

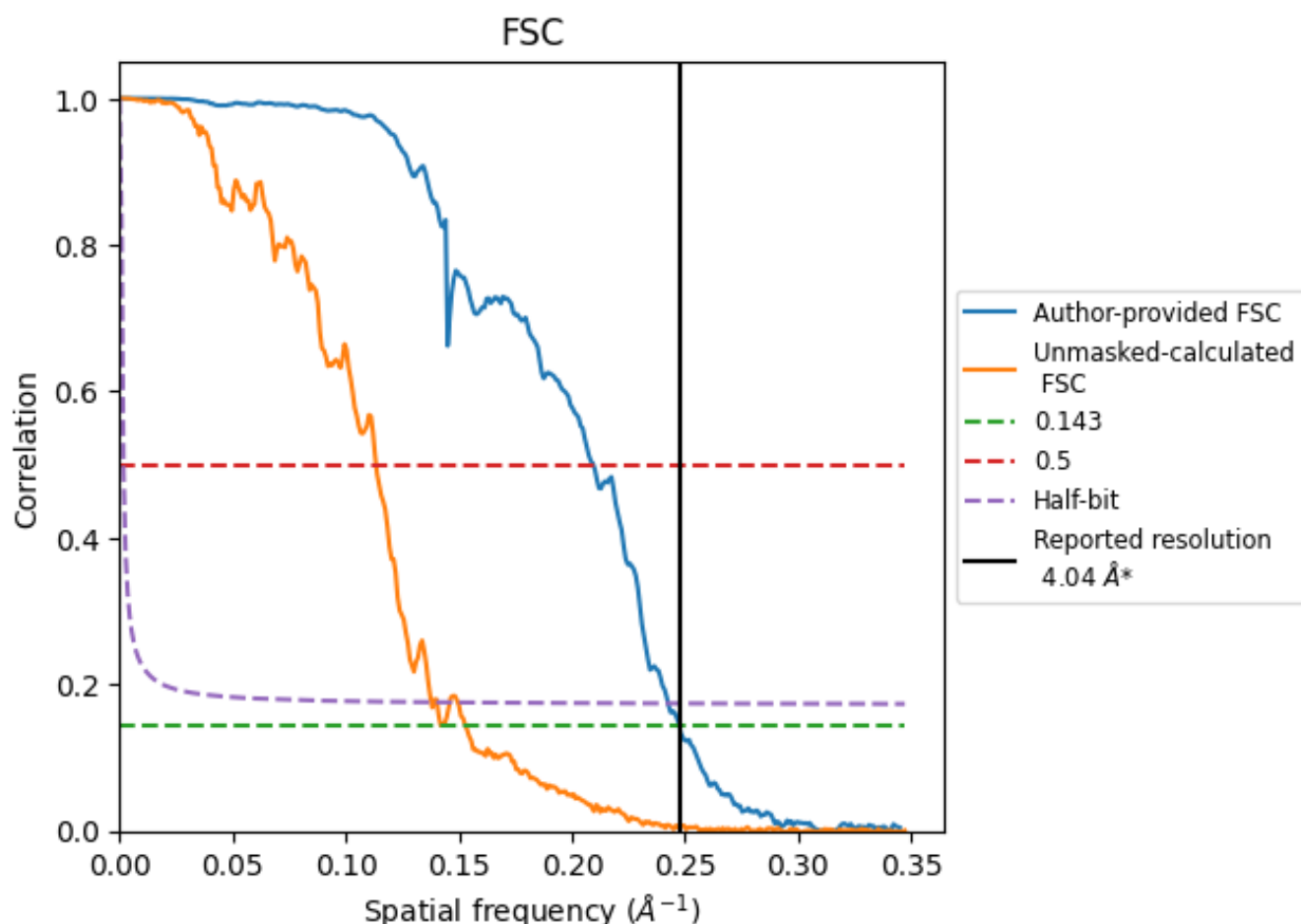


*Reported resolution corresponds to spatial frequency of 0.248 Å⁻¹

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 0.248 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.04	-	-
Author-provided FSC curve	4.04	4.77	4.12
Unmasked-calculated*	6.54	8.81	7.25

*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 6.54 differs from the reported value 4.04 by more than 10 %

9 Map-model fit [i](#)

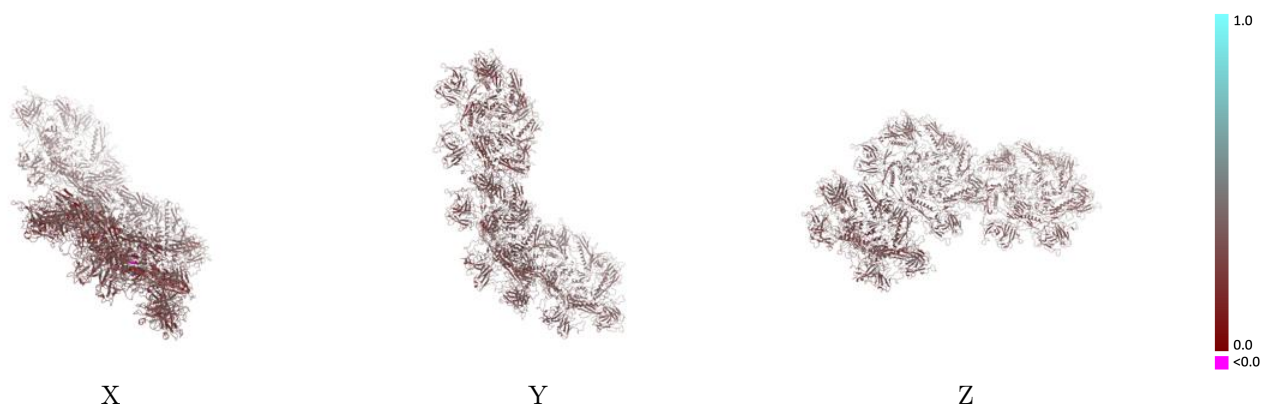
This section contains information regarding the fit between EMDB map EMD-29540 and PDB model 8FXP. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



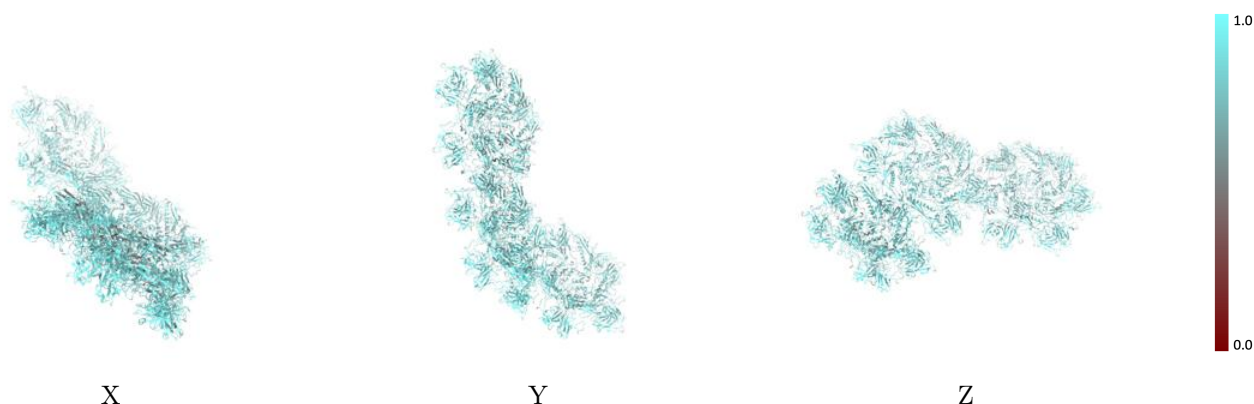
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



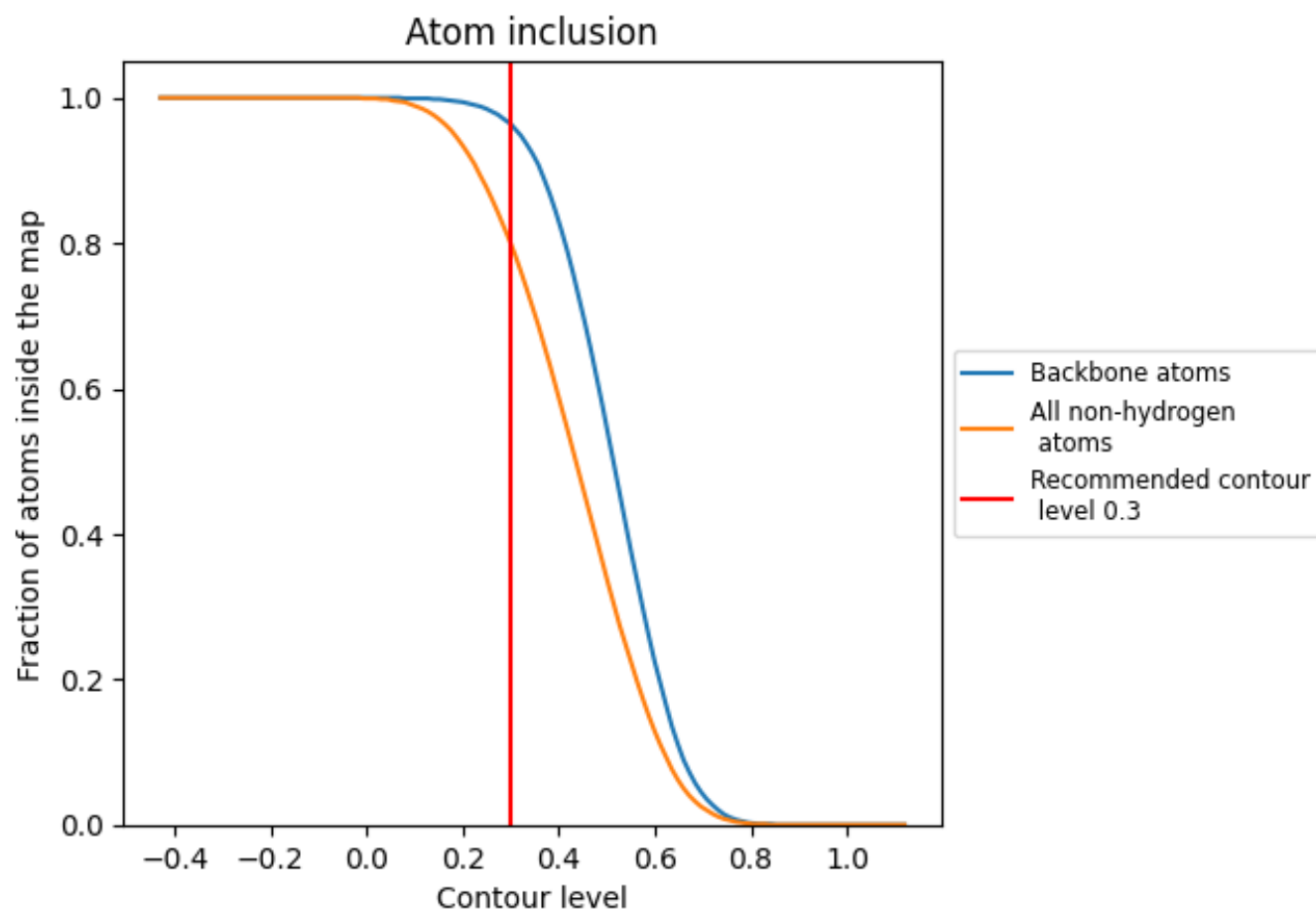
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





























































The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.3330
0	 0.8220	 0.3210
0A	 0.8140	 0.3180
0B	 0.8760	 0.3450
0C	 0.8060	 0.3320
0D	 0.8220	 0.3220
0E	 0.8590	 0.3500
0F	 0.8410	 0.3480
0G	 0.8220	 0.3250
0H	 0.8140	 0.3210
1	 0.8220	 0.3490
2	 0.8280	 0.3400
3	 0.7970	 0.3450
4	 0.8200	 0.3310
5	 0.8100	 0.3490
6	 0.8190	 0.3370
7	 0.7940	 0.3350
8	 0.8360	 0.3520
9	 0.8220	 0.3440
AA	 0.7480	 0.3060
AB	 0.7410	 0.2980
AC	 0.7390	 0.3090
AD	 0.7960	 0.3380
AE	 0.7970	 0.3300
AF	 0.7480	 0.3150
AG	 0.7530	 0.3130
AH	 0.8290	 0.3410
AI	 0.8020	 0.3200
AJ	 0.7660	 0.3120
AK	 0.8240	 0.3150
AL	 0.8200	 0.3150
AM	 0.8300	 0.3260
AN	 0.8340	 0.3340
AO	 0.7980	 0.3720
AP	 0.8080	 0.3620



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Chain	Atom inclusion	Q-score
AQ	 0.7980	 0.3630
AR	 0.7830	 0.3730
AS	 0.7090	 0.3360
AT	 0.8370	 0.3470
a	 0.7980	 0.3800
b	 0.8230	 0.3910
c	 0.8960	 0.3940
d	 0.8380	 0.3850
e	 0.8030	 0.3700
f	 0.8700	 0.3940
g	 0.7980	 0.3370
h	 0.8290	 0.3460
i	 0.7950	 0.3250
j	 0.7820	 0.3300
k	 0.8220	 0.3450
l	 0.8350	 0.3450
m	 0.8620	 0.3580
n	 0.8000	 0.3470
o	 0.7730	 0.3350
p	 0.8360	 0.3480
q	 0.8290	 0.3390
r	 0.7790	 0.3420
s	 0.8340	 0.3510
t	 0.8400	 0.3480
u	 0.8410	 0.3330
v	 0.8200	 0.3370
w	 0.7630	 0.3300
x	 0.7840	 0.3250
y	 0.8180	 0.3370
z	 0.8540	 0.3540