



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:18 AM UTC

PDB ID : 5A7X / pdb_00005a7x
EMDB ID : EMD-3086
Title : negative stain EM of BG505 SOSIP.664 in complex with sCD4, 17b, and 8ANC195
Authors : Scharf, L.; Wang, H.; Gao, H.; Chen, S.; McDowall, A.; Bjorkman, P.
Deposited on : 2015-07-10
Resolution : 17.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

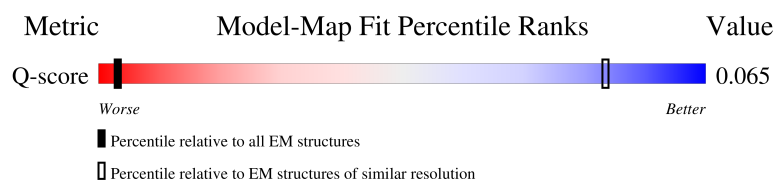
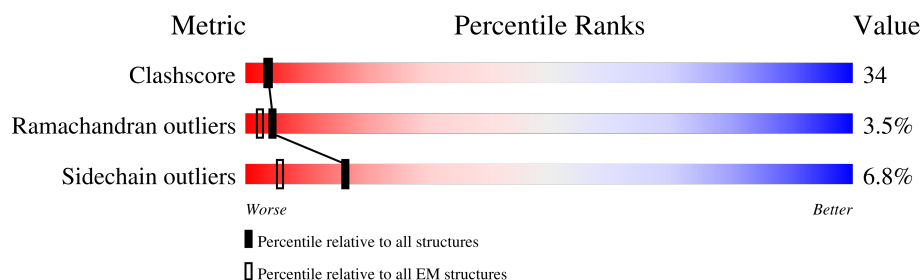
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	36 (16.30 - 17.30)

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	A	313	
1	E	313	
1	I	313	
2	B	181	

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Mol	Chain	Length	Quality of chain
2	F	181	
2	J	181	
3	C	214	
3	G	214	
3	K	214	
4	D	229	
4	H	229	
4	L	229	
5	M	215	
5	O	215	
5	Q	215	
6	N	244	
6	P	244	
6	R	244	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	A	588	X	-	-	-
7	NAG	A	741	X	-	-	-
7	NAG	E	588	X	-	-	-
7	NAG	E	741	X	-	-	-
7	NAG	I	588	X	-	-	-
7	NAG	I	741	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 31872 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 HIV-1 YU2 GP120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		
1	E	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		
1	I	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		

- Molecule 2 is a protein called T-CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		
2	F	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		
2	J	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		

- Molecule 3 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		
3	G	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		
3	K	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		

- Molecule 4 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		
4	L	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		

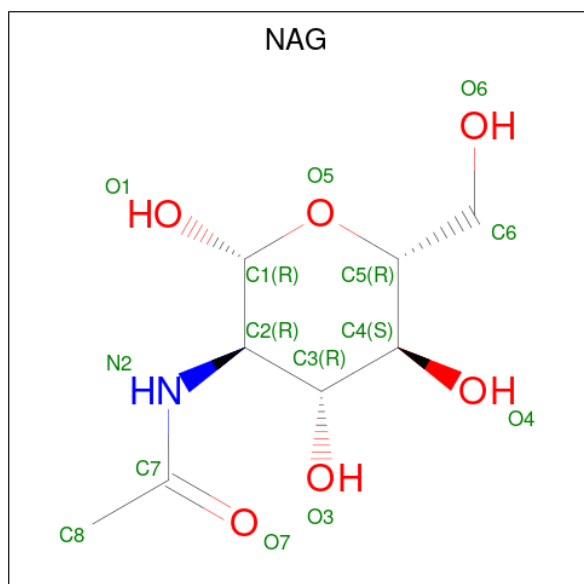
- Molecule 5 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		
5	O	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		
5	Q	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		

- Molecule 6 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		
6	P	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		
6	R	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
7	E	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	N	1	Total 14	C 8	N 1	O 5	0

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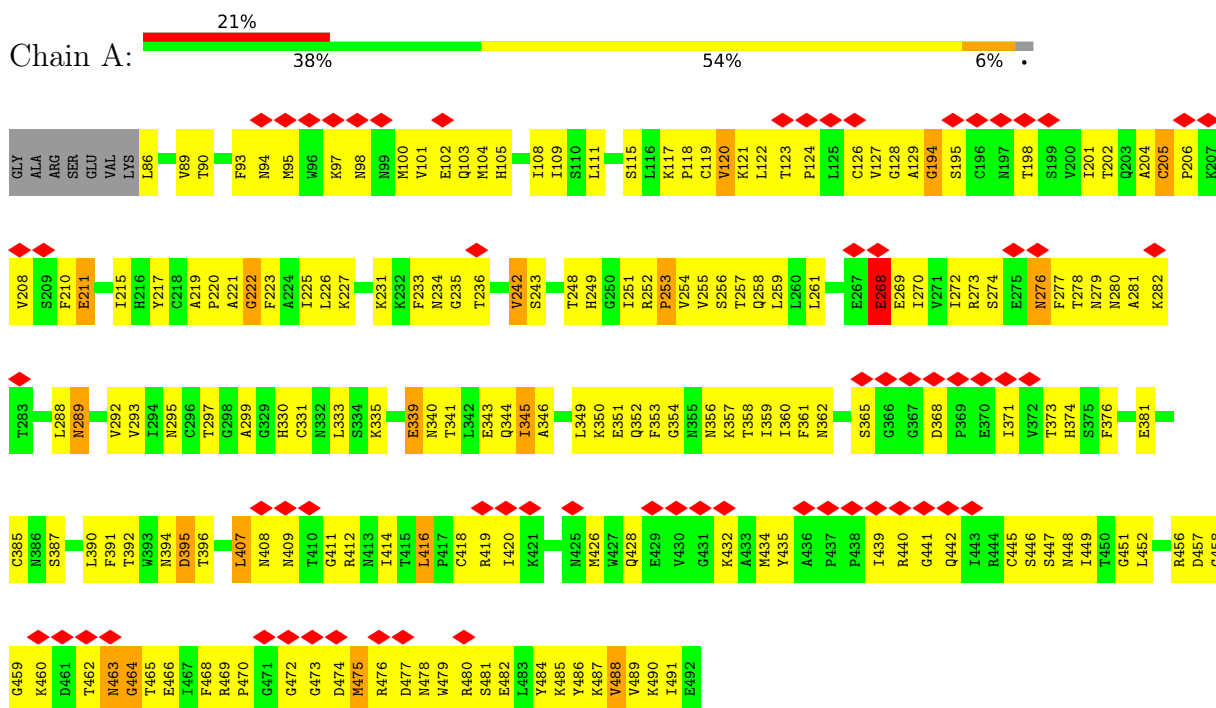
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Mol	Chain	Residues	Atoms				AltConf
7	P	1	Total	C	N	O	0
			14	8	1	5	
7	R	1	Total	C	N	O	0
			14	8	1	5	

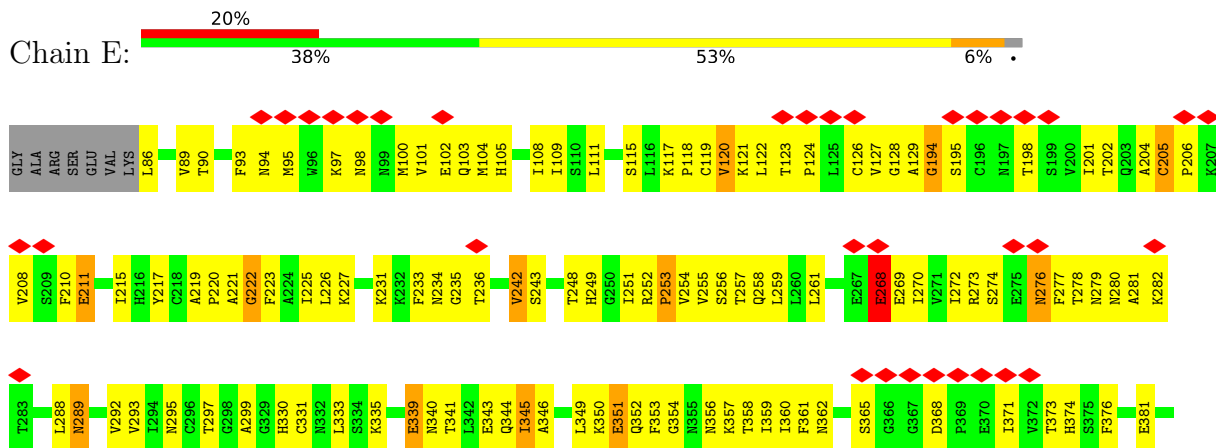
3 Residue-property plots

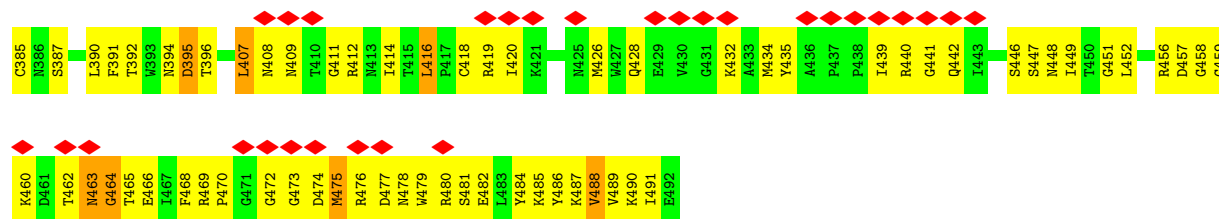
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: HIV-1 YU2 GP120

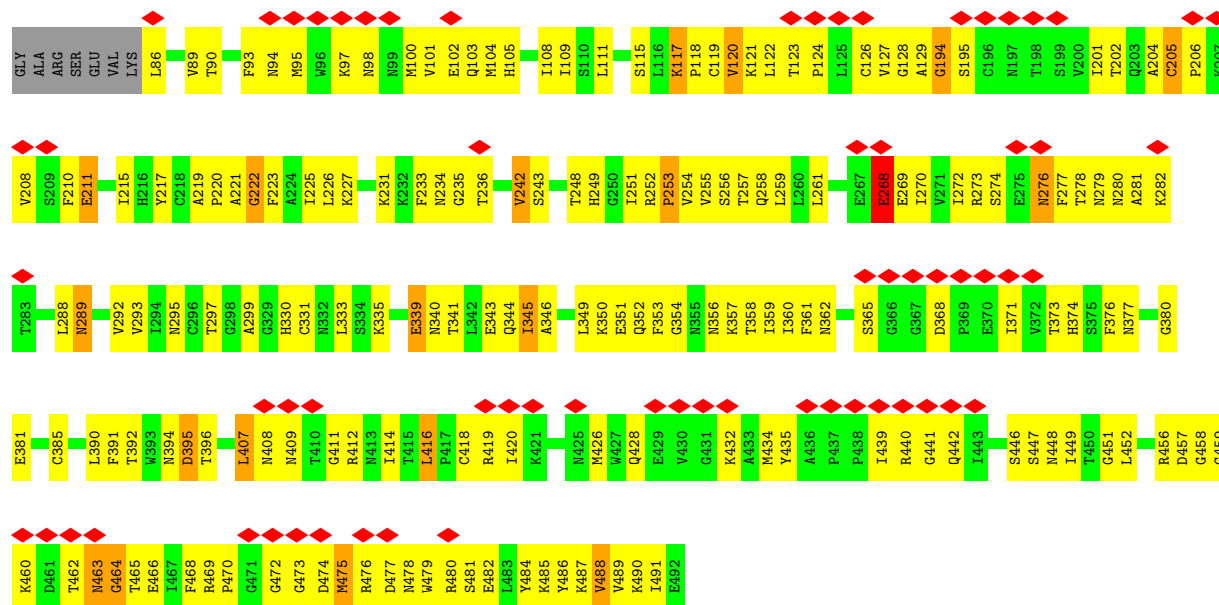


• Molecule 1: HIV-1 YU2 GP120

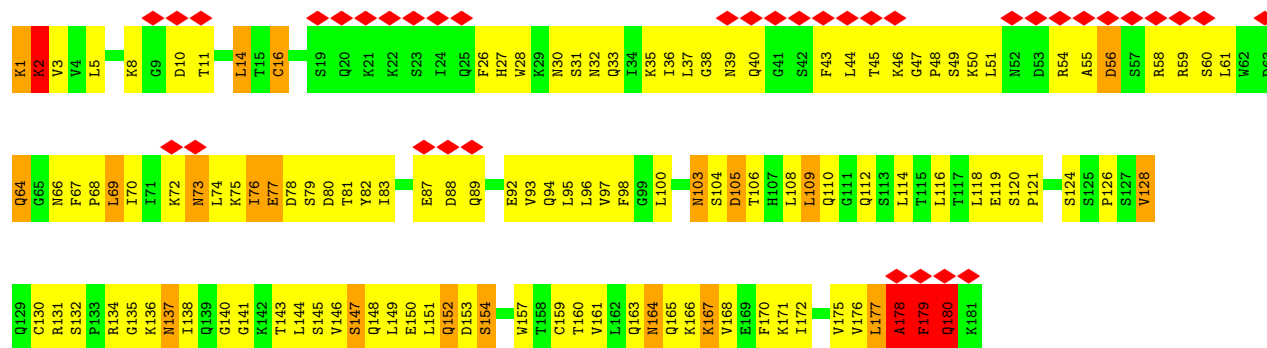




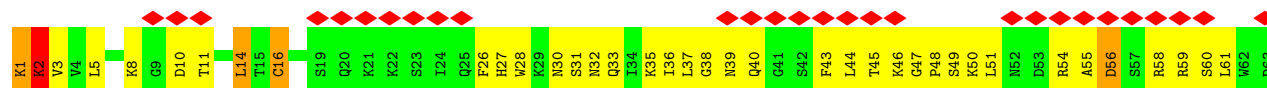
• Molecule 1: HIV-1 YU2 GP120

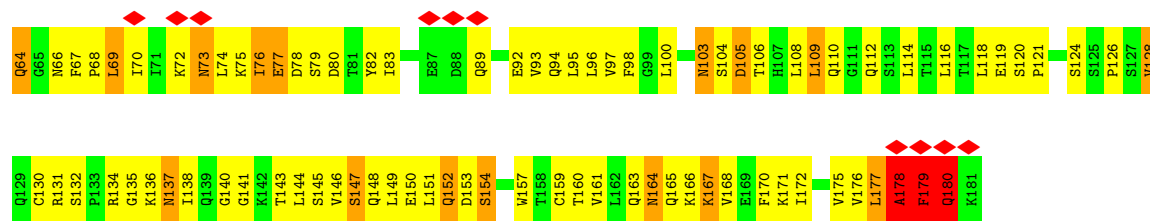


• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4



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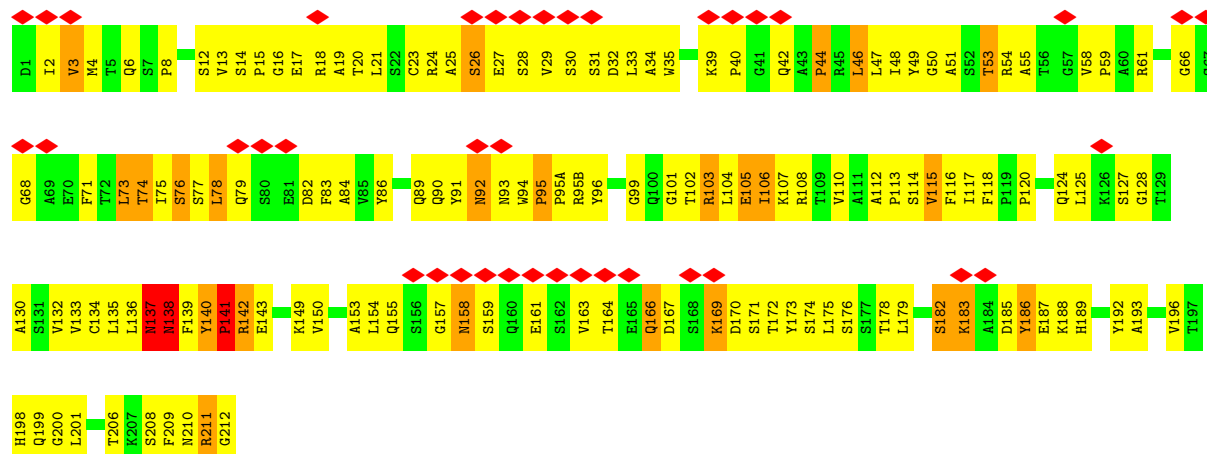




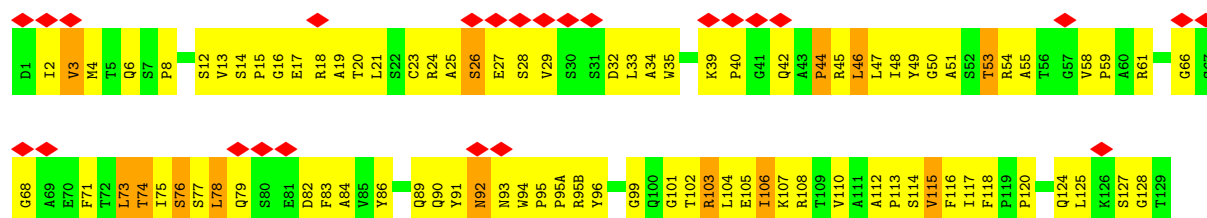
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

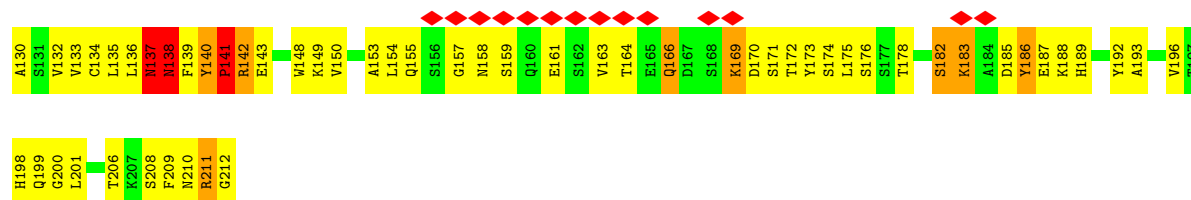


• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

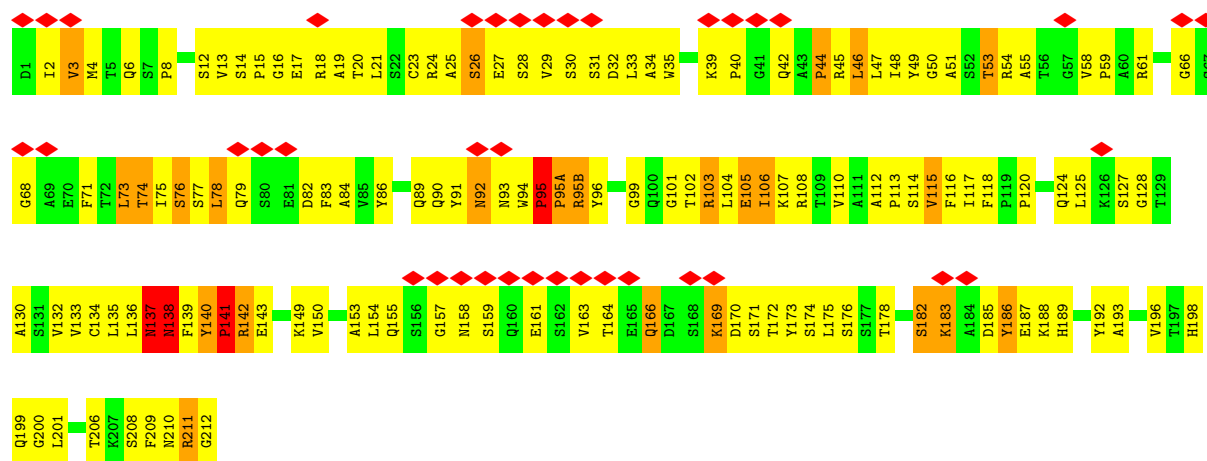


• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

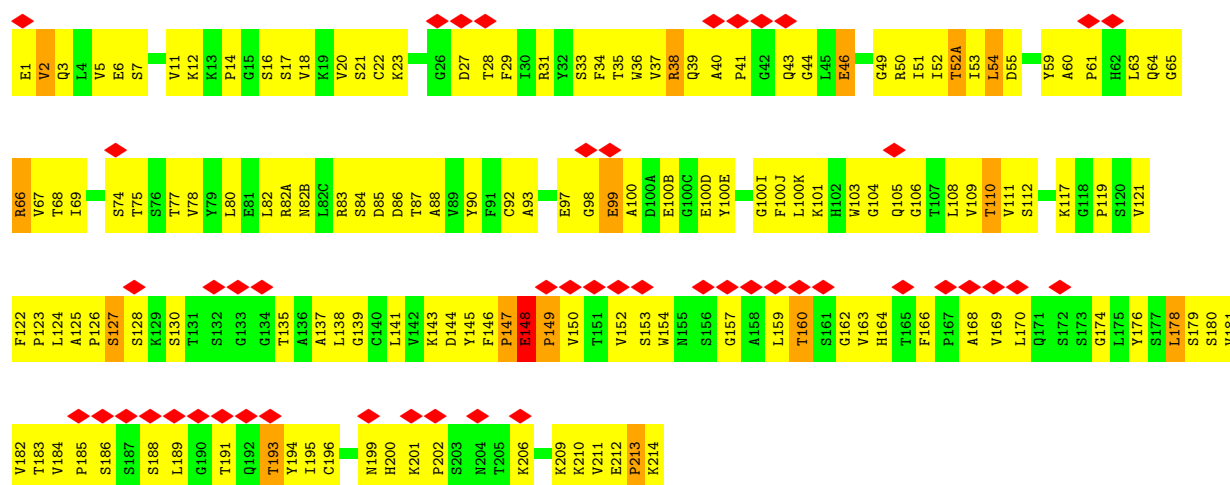




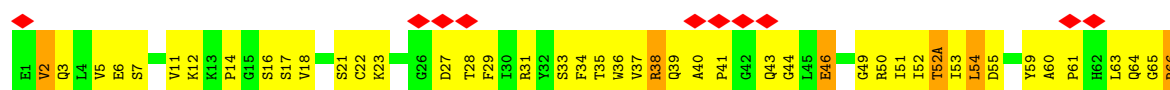
• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

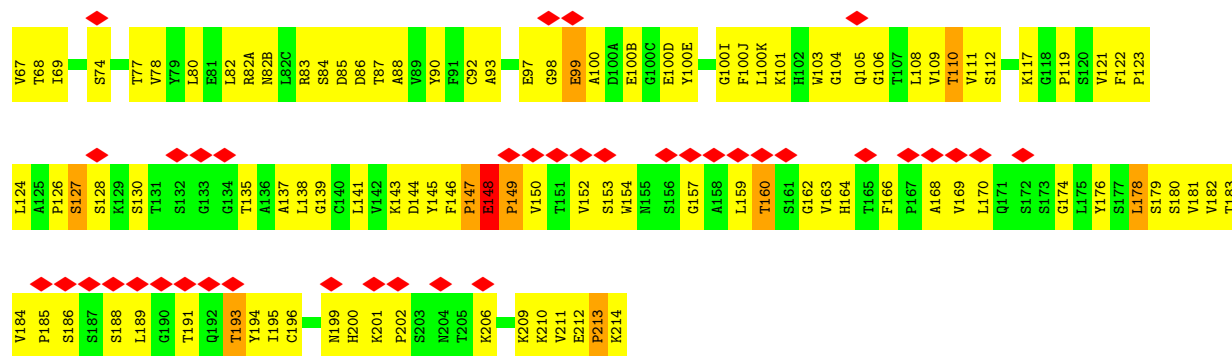


• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

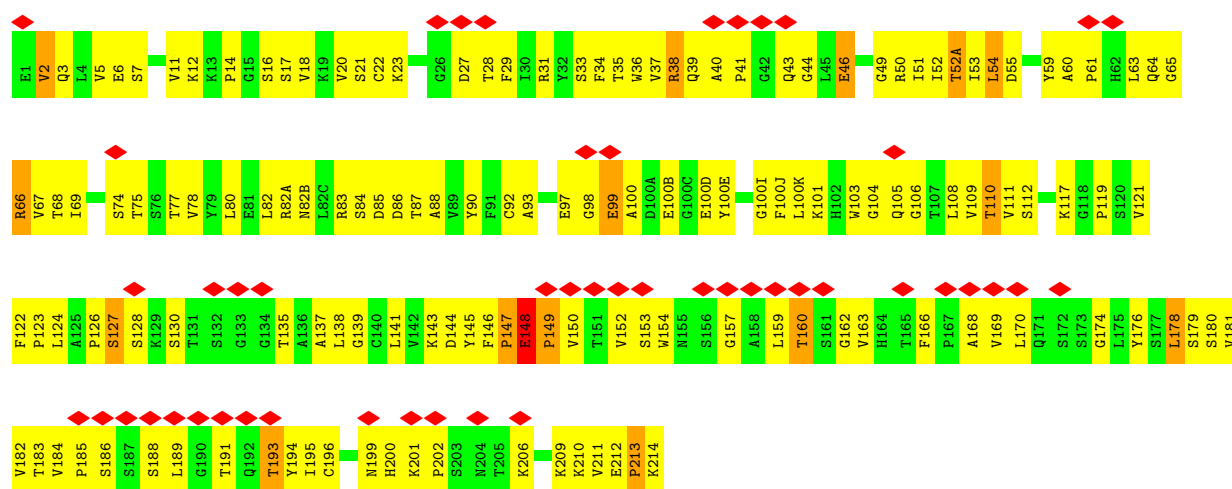


• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

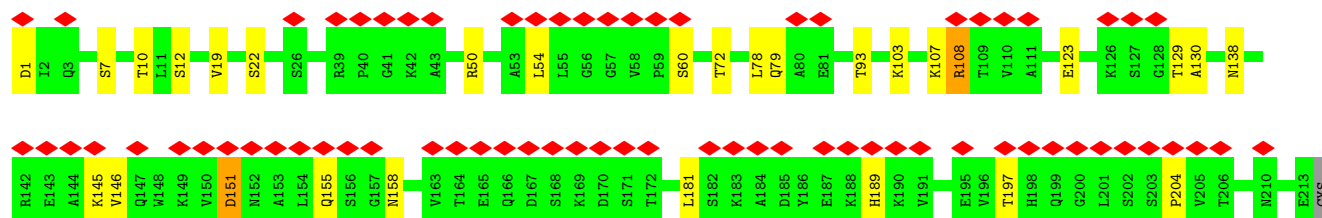
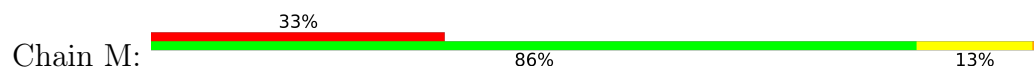




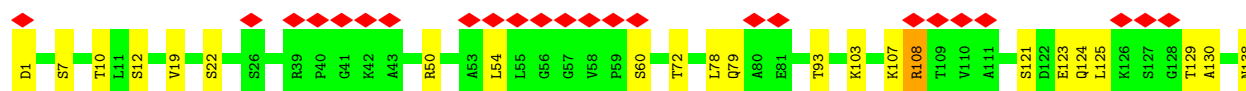
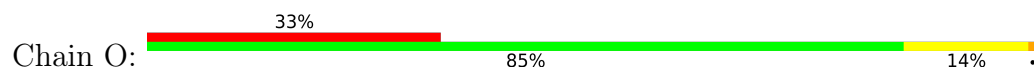
• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

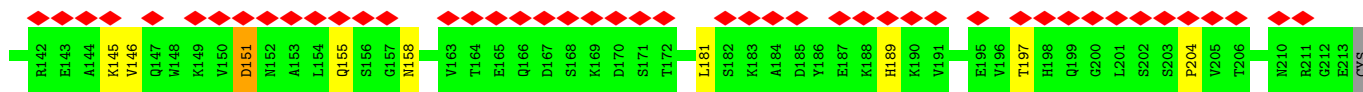


• Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195

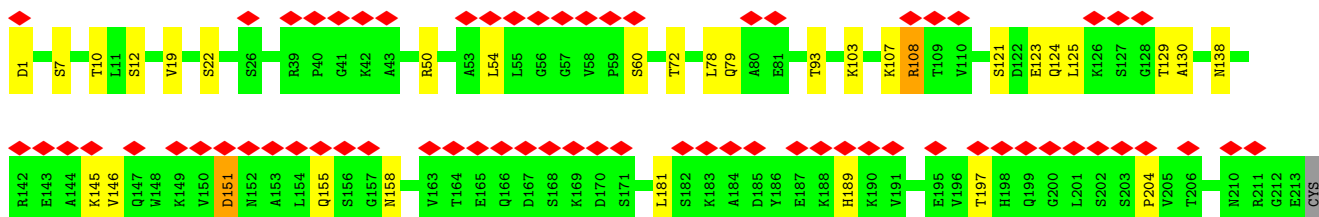
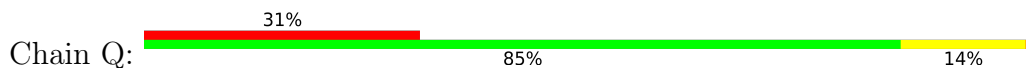


• Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195

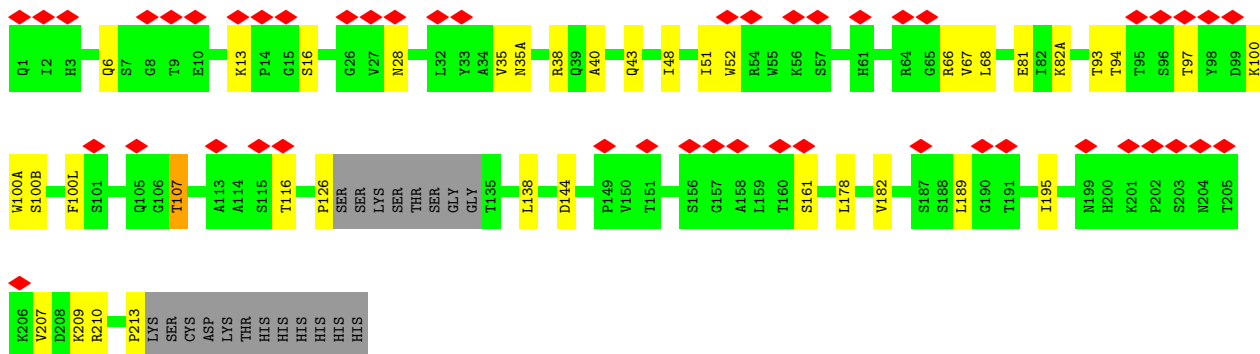
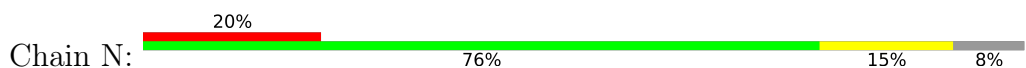




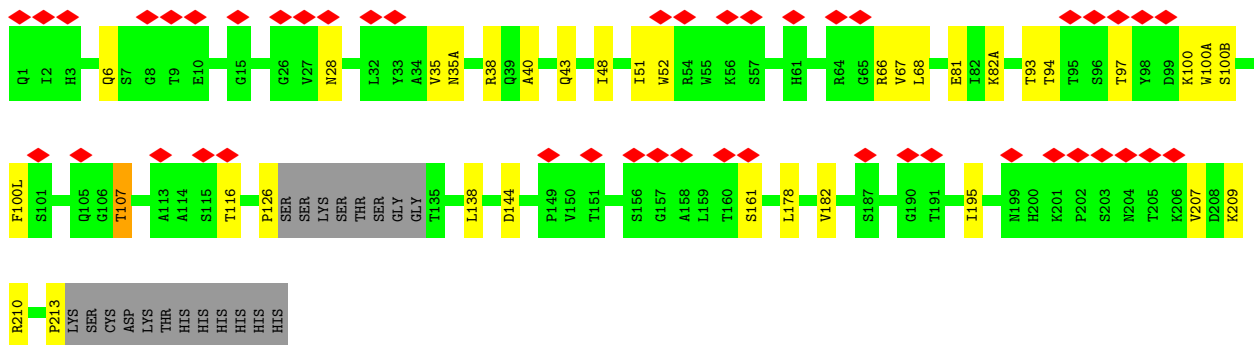
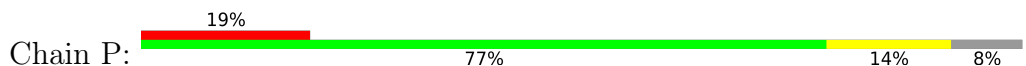
● Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195



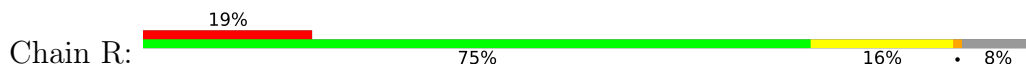
- Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195

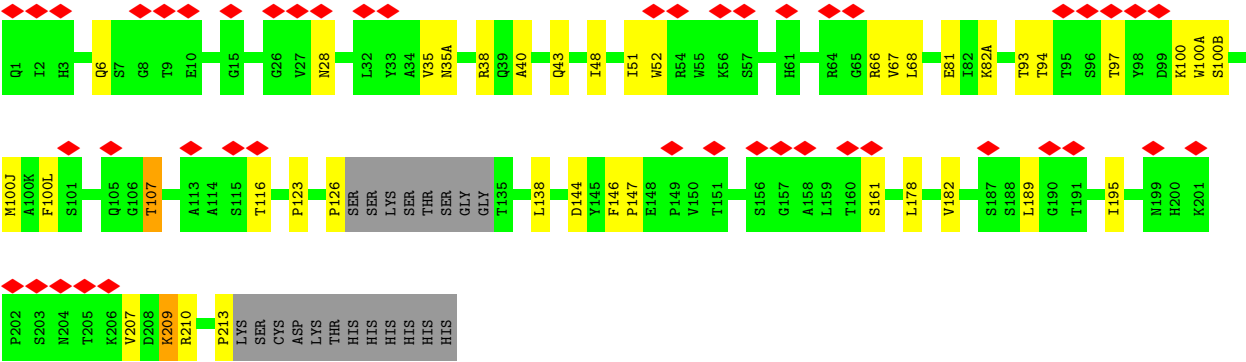


● Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195



- Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	7174	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	42000	Depositor
Image detector	GATAN ULTRASCAN 1000 (2k x 2k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.079	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0269	Depositor
Map size ($\text{\AA}$)	320.0, 320.0, 320.0	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.5, 2.5, 2.5	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/2432	0.98	11/3296 (0.3%)
1	E	0.58	0/2432	0.98	11/3296 (0.3%)
1	I	0.58	0/2432	0.97	11/3296 (0.3%)
2	B	0.52	0/1432	1.00	7/1930 (0.4%)
2	F	0.51	0/1432	1.00	7/1930 (0.4%)
2	J	0.51	0/1432	1.00	7/1930 (0.4%)
3	C	0.49	0/1684	1.27	10/2288 (0.4%)
3	G	0.49	0/1684	1.27	10/2288 (0.4%)
3	K	0.49	0/1684	1.27	10/2288 (0.4%)
4	D	0.51	0/1762	0.94	6/2399 (0.3%)
4	H	0.51	0/1762	0.94	6/2399 (0.3%)
4	L	0.51	0/1762	0.94	6/2399 (0.3%)
5	M	0.68	0/1640	0.86	2/2232 (0.1%)
5	O	0.68	0/1640	0.86	2/2232 (0.1%)
5	Q	0.68	0/1640	0.86	2/2232 (0.1%)
6	N	0.68	1/1687 (0.1%)	0.90	3/2310 (0.1%)
6	P	0.68	1/1687 (0.1%)	0.90	3/2310 (0.1%)
6	R	0.68	1/1687 (0.1%)	0.89	4/2310 (0.2%)
All	All	0.58	3/31911 (0.0%)	1.00	118/43365 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	213	PRO	N-CD	5.22	1.55	1.47
6	N	213	PRO	N-CD	5.22	1.55	1.47
6	R	213	PRO	N-CD	5.14	1.54	1.47

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	140	TYR	CA-C-N	21.96	179.70	127.00
3	K	140	TYR	C-N-CA	21.96	179.70	127.00
3	G	140	TYR	CA-C-N	21.93	179.63	127.00
3	G	140	TYR	C-N-CA	21.93	179.63	127.00
3	C	140	TYR	CA-C-N	21.93	179.62	127.00
3	C	140	TYR	C-N-CA	21.93	179.62	127.00
3	C	140	TYR	C-N-CD	-21.39	73.54	120.60
3	K	140	TYR	C-N-CD	-21.37	73.58	120.60
3	G	140	TYR	C-N-CD	-21.37	73.59	120.60
2	F	179	PHE	N-CA-C	-11.98	85.27	110.80
2	J	179	PHE	N-CA-C	-11.97	85.30	110.80
2	B	179	PHE	N-CA-C	-11.97	85.31	110.80
1	A	345	ILE	N-CA-C	-11.16	102.81	111.62
1	E	345	ILE	N-CA-C	-11.14	102.82	111.62
1	I	345	ILE	N-CA-C	-11.03	102.86	112.12
2	B	180	GLN	N-CA-C	10.42	132.99	110.80
2	F	180	GLN	N-CA-C	10.39	132.93	110.80
2	J	180	GLN	N-CA-C	10.39	132.92	110.80
2	J	47	GLY	CA-C-N	7.38	129.07	119.84
2	J	47	GLY	C-N-CA	7.38	129.07	119.84
3	G	183	LYS	N-CA-C	-7.38	103.12	112.93
3	C	183	LYS	N-CA-C	-7.34	103.17	112.93
2	B	47	GLY	CA-C-N	7.31	128.98	119.84
2	B	47	GLY	C-N-CA	7.31	128.98	119.84
2	F	47	GLY	CA-C-N	7.31	128.98	119.84
2	F	47	GLY	C-N-CA	7.31	128.98	119.84
3	K	183	LYS	N-CA-C	-7.31	103.21	112.93
1	I	222	GLY	N-CA-C	-6.95	106.37	115.47
1	E	222	GLY	N-CA-C	-6.94	106.38	115.47
1	A	222	GLY	N-CA-C	-6.92	106.41	115.47
5	Q	151	ASP	N-CA-C	-6.51	103.91	112.24
5	O	151	ASP	N-CA-C	-6.48	103.94	112.24
5	M	151	ASP	N-CA-C	-6.45	103.98	112.24
3	C	137	ASN	N-CA-C	6.43	119.56	110.50
3	K	137	ASN	N-CA-C	6.41	119.54	110.50
3	K	186	TYR	N-CA-C	-6.36	104.43	111.36
3	C	186	TYR	N-CA-C	-6.34	104.45	111.36
3	G	137	ASN	N-CA-C	6.34	119.44	110.50
3	G	186	TYR	N-CA-C	-6.33	104.46	111.36
6	P	144	ASP	N-CA-C	6.33	120.38	111.52
1	E	111	LEU	N-CA-C	-6.30	105.56	113.18
6	N	144	ASP	N-CA-C	6.30	120.33	111.52
6	R	144	ASP	N-CA-C	6.30	120.33	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	LEU	N-CA-C	-6.29	105.57	113.18
1	I	111	LEU	N-CA-C	-6.26	105.61	113.18
4	H	2	VAL	N-CA-C	6.25	117.27	110.21
4	L	2	VAL	N-CA-C	6.24	117.26	110.21
4	D	2	VAL	N-CA-C	6.19	117.21	110.21
6	P	28	ASN	N-CA-C	6.19	118.57	111.02
6	N	28	ASN	N-CA-C	6.14	118.51	111.02
6	R	28	ASN	N-CA-C	6.12	118.48	111.02
3	G	115	VAL	N-CA-C	6.01	117.05	108.93
3	K	115	VAL	N-CA-C	6.01	117.04	108.93
3	C	115	VAL	N-CA-C	5.98	117.00	108.93
3	G	166	GLN	N-CA-C	-5.84	101.64	110.28
3	K	166	GLN	N-CA-C	-5.83	101.66	110.28
3	C	101	GLY	N-CA-C	5.82	118.84	111.85
3	G	101	GLY	N-CA-C	5.82	118.83	111.85
3	C	166	GLN	N-CA-C	-5.81	101.68	110.28
3	K	101	GLY	N-CA-C	5.79	118.80	111.85
4	D	2	VAL	CB-CA-C	-5.79	104.97	111.45
4	H	2	VAL	CB-CA-C	-5.74	105.03	111.45
4	L	2	VAL	CB-CA-C	-5.71	105.05	111.45
1	A	128	GLY	N-CA-C	-5.67	107.74	114.48
1	I	128	GLY	N-CA-C	-5.64	107.76	114.48
2	F	178	ALA	CA-C-N	5.59	132.22	121.54
2	F	178	ALA	C-N-CA	5.59	132.22	121.54
2	J	178	ALA	CA-C-N	5.58	132.20	121.54
2	J	178	ALA	C-N-CA	5.58	132.20	121.54
1	E	128	GLY	N-CA-C	-5.58	107.84	114.48
2	B	178	ALA	CA-C-N	5.53	132.10	121.54
2	B	178	ALA	C-N-CA	5.53	132.10	121.54
1	I	330	HIS	N-CA-C	5.48	115.60	107.88
1	A	330	HIS	N-CA-C	5.47	115.59	107.88
3	C	141	PRO	N-CA-C	-5.45	97.93	112.10
1	E	330	HIS	N-CA-C	5.45	115.56	107.88
3	K	141	PRO	N-CA-C	-5.44	97.96	112.10
3	G	141	PRO	N-CA-C	-5.44	97.96	112.10
4	H	33	SER	N-CA-C	-5.40	100.38	109.07
5	O	138	ASN	N-CA-C	5.37	118.66	111.24
4	L	33	SER	N-CA-C	-5.37	100.43	109.07
4	D	33	SER	N-CA-C	-5.36	100.44	109.07
5	M	138	ASN	N-CA-C	5.36	118.64	111.24
5	Q	138	ASN	N-CA-C	5.32	118.57	111.24
1	E	289	ASN	N-CA-C	-5.31	106.85	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	100(B)	SER	N-CA-C	5.30	117.06	111.28
6	N	100(B)	SER	N-CA-C	5.29	117.04	111.28
1	E	211	GLU	CA-C-N	5.27	125.57	119.93
1	E	211	GLU	C-N-CA	5.27	125.57	119.93
1	I	211	GLU	CA-C-N	5.27	125.57	119.93
1	I	211	GLU	C-N-CA	5.27	125.57	119.93
1	I	289	ASN	N-CA-C	-5.27	106.90	113.38
2	F	64	GLN	N-CA-C	-5.27	105.56	112.72
1	A	211	GLU	CA-C-N	5.26	125.56	119.93
1	A	211	GLU	C-N-CA	5.26	125.56	119.93
2	B	64	GLN	N-CA-C	-5.26	105.57	112.72
6	R	100(B)	SER	N-CA-C	5.25	117.01	111.28
1	A	289	ASN	N-CA-C	-5.25	106.92	113.38
2	J	64	GLN	N-CA-C	-5.24	105.60	112.72
4	H	191	THR	N-CA-C	-5.23	108.66	114.62
1	A	117	LYS	CA-C-N	5.23	125.51	119.92
1	A	117	LYS	C-N-CA	5.23	125.51	119.92
4	D	191	THR	N-CA-C	-5.21	108.68	114.62
1	I	117	LYS	CA-C-N	5.21	125.49	119.92
1	I	117	LYS	C-N-CA	5.21	125.49	119.92
4	L	191	THR	N-CA-C	-5.19	108.70	114.62
1	E	117	LYS	CA-C-N	5.19	125.47	119.92
1	E	117	LYS	C-N-CA	5.19	125.47	119.92
4	D	174	GLY	N-CA-C	-5.18	107.64	114.95
4	L	160	THR	N-CA-C	-5.17	107.02	113.38
4	H	174	GLY	N-CA-C	-5.15	107.69	114.95
4	H	160	THR	N-CA-C	-5.15	107.05	113.38
4	D	160	THR	N-CA-C	-5.14	107.06	113.38
4	L	174	GLY	N-CA-C	-5.14	107.70	114.95
1	I	351	GLU	N-CA-C	-5.12	107.32	113.21
1	E	351	GLU	N-CA-C	-5.10	107.35	113.21
1	A	351	GLU	N-CA-C	-5.07	107.37	113.21
6	R	100(J)	MET	N-CA-C	5.02	116.70	109.07

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	A	2385	0	2327	220	0
1	E	2385	0	2327	220	0
1	I	2385	0	2327	216	0
2	B	1412	0	1444	160	0
2	F	1412	0	1444	157	0
2	J	1412	0	1444	157	0
3	C	1647	0	1593	177	0
3	G	1647	0	1593	178	0
3	K	1647	0	1593	177	0
4	D	1722	0	1691	162	0
4	H	1722	0	1691	160	0
4	L	1722	0	1691	158	0
5	M	1605	0	1521	12	0
5	O	1605	0	1521	14	0
5	Q	1605	0	1521	14	0
6	N	1643	0	1586	21	0
6	P	1643	0	1586	19	0
6	R	1643	0	1586	21	0
7	A	196	0	182	21	0
7	E	196	0	182	19	0
7	I	196	0	182	19	0
7	N	14	0	13	0	0
7	P	14	0	13	0	0
7	R	14	0	13	0	0
All	All	31872	0	31071	2143	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 34.

All (2143) 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)
2:B:176:VAL:C	2:B:177:LEU:HD12	1.62	1.24
2:J:176:VAL:C	2:J:177:LEU:HD12	1.62	1.23
2:F:176:VAL:C	2:F:177:LEU:HD12	1.62	1.21
2:J:108:LEU:HD21	2:J:112:GLN:HB3	1.28	1.15
2:B:108:LEU:HD21	2:B:112:GLN:HB3	1.28	1.13
6:P:93:THR:HG21	6:P:100(L):PHE:HB3	1.32	1.09
4:L:148:GLU:HG3	4:L:149:PRO:HA	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:GLU:HG3	4:D:149:PRO:HA	1.34	1.07
6:N:93:THR:HG21	6:N:100(L):PHE:HB3	1.32	1.06
2:F:108:LEU:HD21	2:F:112:GLN:HB3	1.28	1.06
6:R:93:THR:HG21	6:R:100(L):PHE:HB3	1.32	1.06
2:B:178:ALA:O	2:B:179:PHE:HD1	1.38	1.06
2:J:178:ALA:O	2:J:179:PHE:HD1	1.38	1.05
2:F:178:ALA:O	2:F:179:PHE:HD1	1.38	1.04
4:H:148:GLU:HG3	4:H:149:PRO:HA	1.34	1.04
6:P:93:THR:CG2	6:P:100(L):PHE:HB3	1.89	1.03
6:R:93:THR:CG2	6:R:100(L):PHE:HB3	1.89	1.02
6:N:93:THR:CG2	6:N:100(L):PHE:HB3	1.89	1.01
2:J:179:PHE:O	2:J:180:GLN:HB2	1.62	0.99
2:B:179:PHE:O	2:B:180:GLN:HB2	1.62	0.98
3:G:94:TRP:CZ3	3:G:95(A):PRO:HG3	1.99	0.98
3:K:94:TRP:CZ3	3:K:95(A):PRO:HG3	1.99	0.98
3:C:94:TRP:CZ3	3:C:95(A):PRO:HG3	1.99	0.97
4:L:127:SER:HB3	4:L:130:SER:HB2	1.48	0.95
2:F:179:PHE:O	2:F:180:GLN:HB2	1.62	0.95
2:F:150:GLU:HB3	2:F:152:GLN:HE22	1.33	0.94
2:J:130:CYS:HA	2:J:159:CYS:HA	1.50	0.94
4:H:127:SER:HB3	4:H:130:SER:HB2	1.49	0.93
4:D:127:SER:HB3	4:D:130:SER:HB2	1.49	0.93
3:K:46:LEU:HD12	4:L:101:LYS:HA	1.50	0.93
2:J:150:GLU:HB3	2:J:152:GLN:HE22	1.33	0.93
2:F:140:GLY:HA3	2:F:144:LEU:HG	1.51	0.93
2:B:150:GLU:HB3	2:B:152:GLN:HE22	1.33	0.92
2:J:140:GLY:HA3	2:J:144:LEU:HG	1.51	0.92
2:F:130:CYS:HA	2:F:159:CYS:HA	1.50	0.92
2:B:130:CYS:HA	2:B:159:CYS:HA	1.50	0.92
2:B:140:GLY:HA3	2:B:144:LEU:HG	1.51	0.91
3:G:46:LEU:HD12	4:H:101:LYS:HA	1.50	0.91
3:C:46:LEU:HD12	4:D:101:LYS:HA	1.50	0.91
1:I:95:MET:HE2	1:I:484:TYR:HB2	1.53	0.90
1:A:95:MET:HE2	1:A:484:TYR:HB2	1.53	0.89
1:E:95:MET:HE2	1:E:484:TYR:HB2	1.53	0.89
2:F:108:LEU:O	2:F:177:LEU:HD13	1.76	0.85
2:J:108:LEU:O	2:J:177:LEU:HD13	1.76	0.85
2:B:128:VAL:HB	2:B:144:LEU:HD11	1.59	0.85
2:J:128:VAL:HB	2:J:144:LEU:HD11	1.59	0.85
4:L:148:GLU:HG3	4:L:149:PRO:CA	2.07	0.85
4:H:148:GLU:HG3	4:H:149:PRO:CA	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:193:ALA:HA	3:K:208:SER:HB3	1.58	0.84
2:B:150:GLU:HB3	2:B:152:GLN:NE2	1.92	0.84
3:G:193:ALA:HA	3:G:208:SER:HB3	1.58	0.84
2:F:150:GLU:HB3	2:F:152:GLN:NE2	1.92	0.84
2:B:108:LEU:O	2:B:177:LEU:HD13	1.76	0.84
4:D:148:GLU:HG3	4:D:149:PRO:CA	2.07	0.84
2:J:150:GLU:HB3	2:J:152:GLN:NE2	1.92	0.84
3:K:46:LEU:HD22	3:K:55:ALA:HB2	1.60	0.83
4:D:195:ILE:HG12	4:D:210:LYS:HA	1.60	0.83
3:C:193:ALA:HA	3:C:208:SER:HB3	1.58	0.83
4:L:147:PRO:O	4:L:148:GLU:HB2	1.79	0.83
3:C:46:LEU:HD22	3:C:55:ALA:HB2	1.60	0.83
3:K:78:LEU:HD11	3:K:104:LEU:HD21	1.61	0.82
4:H:147:PRO:O	4:H:148:GLU:HB2	1.79	0.82
2:B:178:ALA:O	2:B:179:PHE:CD1	2.30	0.82
4:L:195:ILE:HG12	4:L:210:LYS:HA	1.60	0.82
3:C:29:VAL:HG13	3:C:92:ASN:HB3	1.62	0.82
3:G:29:VAL:HG13	3:G:92:ASN:HB3	1.62	0.82
4:H:195:ILE:HG12	4:H:210:LYS:HA	1.60	0.81
3:C:78:LEU:HD11	3:C:104:LEU:HD21	1.62	0.81
7:E:963:NAG:H3	7:E:963:NAG:H82	1.62	0.81
2:F:128:VAL:HB	2:F:144:LEU:HD11	1.59	0.81
3:G:46:LEU:HD22	3:G:55:ALA:HB2	1.60	0.81
7:I:963:NAG:H3	7:I:963:NAG:H82	1.62	0.81
3:C:140:TYR:CG	3:C:141:PRO:HD3	2.16	0.81
3:G:78:LEU:HD11	3:G:104:LEU:HD21	1.61	0.81
2:F:131:ARG:CZ	2:F:137:ASN:HB3	2.12	0.80
2:B:131:ARG:CZ	2:B:137:ASN:HB3	2.12	0.80
3:C:49:TYR:O	3:C:53:THR:HG23	1.82	0.80
2:J:131:ARG:CZ	2:J:137:ASN:HB3	2.12	0.80
3:G:140:TYR:CG	3:G:141:PRO:HD3	2.16	0.80
2:J:178:ALA:O	2:J:179:PHE:CD1	2.30	0.80
3:K:29:VAL:HG13	3:K:92:ASN:HB3	1.62	0.80
7:A:963:NAG:H3	7:A:963:NAG:H82	1.62	0.80
2:F:178:ALA:O	2:F:179:PHE:CD1	2.30	0.80
3:G:49:TYR:O	3:G:53:THR:HG23	1.82	0.79
3:K:140:TYR:CG	3:K:141:PRO:HD3	2.16	0.79
4:H:39:GLN:HE21	4:H:44:GLY:HA2	1.47	0.79
1:A:280:ASN:O	2:B:35:LYS:HD2	1.82	0.79
1:E:280:ASN:O	2:F:35:LYS:HD2	1.82	0.79
3:K:49:TYR:O	3:K:53:THR:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:PRO:O	4:D:148:GLU:HB2	1.79	0.79
4:D:39:GLN:HE21	4:D:44:GLY:HA2	1.48	0.79
1:I:412:ARG:HA	7:I:908:NAG:O6	1.83	0.78
1:A:412:ARG:HA	7:A:908:NAG:O6	1.83	0.78
1:E:412:ARG:HA	7:E:908:NAG:O6	1.83	0.78
6:P:52:TRP:HE1	6:P:97:THR:HG21	1.49	0.78
2:B:77:GLU:CD	2:B:77:GLU:H	1.91	0.78
4:D:163:VAL:HG12	4:D:182:VAL:HB	1.66	0.78
1:E:273:ARG:HG2	1:E:273:ARG:HH11	1.49	0.78
1:I:280:ASN:O	2:J:35:LYS:HD2	1.82	0.78
6:N:126:PRO:HG3	6:N:138:LEU:HB3	1.66	0.78
4:L:163:VAL:HG12	4:L:182:VAL:HB	1.66	0.78
6:P:126:PRO:HG3	6:P:138:LEU:HB3	1.66	0.78
4:H:163:VAL:HG12	4:H:182:VAL:HB	1.66	0.77
6:N:52:TRP:HE1	6:N:97:THR:HG21	1.49	0.77
4:L:39:GLN:HE21	4:L:44:GLY:HA2	1.47	0.77
1:E:95:MET:HE1	1:E:273:ARG:HH11	1.50	0.77
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.49	0.76
3:C:141:PRO:HB3	3:C:143:GLU:OE2	1.85	0.76
2:J:77:GLU:CD	2:J:77:GLU:H	1.91	0.76
6:R:126:PRO:HG3	6:R:138:LEU:HB3	1.66	0.76
2:F:77:GLU:H	2:F:77:GLU:CD	1.91	0.76
1:A:392:THR:HG22	7:A:894:NAG:HN2	1.50	0.76
1:E:269:GLU:HA	1:E:289:ASN:ND2	2.01	0.76
6:R:52:TRP:HE1	6:R:97:THR:HG21	1.49	0.76
3:G:141:PRO:HB3	3:G:143:GLU:OE2	1.85	0.76
2:F:176:VAL:C	2:F:177:LEU:CD1	2.53	0.76
1:A:95:MET:HE1	1:A:273:ARG:HH11	1.50	0.76
1:A:269:GLU:HA	1:A:289:ASN:ND2	2.01	0.76
3:C:94:TRP:HA	3:C:95:PRO:C	2.11	0.75
3:K:198:HIS:CD2	3:K:199:GLN:H	2.05	0.75
1:I:269:GLU:HA	1:I:289:ASN:ND2	2.01	0.75
3:K:94:TRP:HA	3:K:95:PRO:C	2.11	0.75
1:E:392:THR:HG22	7:E:894:NAG:HN2	1.50	0.75
3:C:198:HIS:CD2	3:C:199:GLN:H	2.04	0.75
3:K:141:PRO:HB3	3:K:143:GLU:OE2	1.85	0.75
1:I:95:MET:HE1	1:I:273:ARG:HH11	1.50	0.75
6:N:93:THR:HG21	6:N:100(L):PHE:CB	2.14	0.75
6:P:93:THR:HG21	6:P:100(L):PHE:CB	2.14	0.75
1:I:463:ASN:O	1:I:465:THR:HG22	1.87	0.75
1:A:460:LYS:HB2	2:B:32:ASN:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:94:TRP:HA	3:G:95:PRO:C	2.11	0.74
1:I:460:LYS:HB2	2:J:32:ASN:O	1.87	0.74
2:F:61:LEU:HB3	2:F:66:ASN:HB3	1.69	0.74
3:K:113:PRO:HD3	3:K:198:HIS:ND1	2.02	0.74
1:I:273:ARG:HH11	1:I:273:ARG:HG2	1.49	0.74
2:J:176:VAL:C	2:J:177:LEU:CD1	2.53	0.74
1:I:95:MET:CE	1:I:484:TYR:HB2	2.18	0.74
1:A:95:MET:CE	1:A:484:TYR:HB2	2.18	0.74
3:G:198:HIS:CD2	3:G:199:GLN:H	2.04	0.73
3:G:113:PRO:HD3	3:G:198:HIS:ND1	2.02	0.73
1:A:463:ASN:O	1:A:465:THR:HG22	1.87	0.73
2:B:178:ALA:HB1	2:B:180:GLN:H	1.53	0.73
1:E:95:MET:CE	1:E:484:TYR:HB2	2.18	0.73
2:J:76:ILE:H	2:J:76:ILE:HD12	1.54	0.73
1:E:463:ASN:O	1:E:465:THR:HG22	1.87	0.73
1:I:392:THR:HG22	7:I:894:NAG:HN2	1.50	0.73
1:E:460:LYS:HB2	2:F:32:ASN:O	1.87	0.73
3:K:198:HIS:H	3:K:201:LEU:HD12	1.54	0.73
2:B:76:ILE:H	2:B:76:ILE:HD12	1.54	0.73
3:C:113:PRO:HD3	3:C:198:HIS:ND1	2.02	0.73
4:H:135:THR:HA	4:H:185:PRO:HA	1.71	0.73
6:R:93:THR:HG21	6:R:100(L):PHE:CB	2.14	0.73
2:B:176:VAL:C	2:B:177:LEU:CD1	2.53	0.72
3:C:198:HIS:H	3:C:201:LEU:HD12	1.54	0.72
2:J:178:ALA:HB1	2:J:180:GLN:H	1.53	0.72
2:F:76:ILE:HD12	2:F:76:ILE:H	1.54	0.72
2:J:61:LEU:HB3	2:J:66:ASN:HB3	1.69	0.72
3:G:198:HIS:H	3:G:201:LEU:HD12	1.54	0.72
2:B:154:SER:HB2	2:B:176:VAL:H	1.55	0.72
3:K:175:LEU:HD12	3:K:176:SER:H	1.54	0.72
3:C:175:LEU:HD12	3:C:176:SER:H	1.54	0.72
3:G:32:ASP:HB2	3:G:92:ASN:HB2	1.72	0.72
3:G:175:LEU:HD12	3:G:176:SER:H	1.54	0.72
1:A:104:MET:HE2	1:A:215:ILE:HD11	1.71	0.71
2:B:61:LEU:HB3	2:B:66:ASN:HB3	1.69	0.71
4:D:135:THR:HA	4:D:185:PRO:HA	1.71	0.71
2:J:154:SER:HB2	2:J:176:VAL:H	1.55	0.71
2:F:178:ALA:HB1	2:F:180:GLN:H	1.53	0.71
4:L:135:THR:HA	4:L:185:PRO:HA	1.71	0.71
2:F:161:VAL:O	2:F:167:LYS:HA	1.90	0.71
3:G:93:ASN:ND2	3:G:95(B):ARG:HB2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:182:VAL:HG22	4:L:184:VAL:HG13	1.72	0.71
1:E:104:MET:HE2	1:E:215:ILE:HD11	1.71	0.71
4:H:182:VAL:HG22	4:H:184:VAL:HG13	1.72	0.71
2:F:154:SER:HB2	2:F:176:VAL:H	1.55	0.71
3:G:154:LEU:HD13	3:G:154:LEU:O	1.91	0.71
3:K:154:LEU:O	3:K:154:LEU:HD13	1.91	0.71
2:B:36:ILE:HG22	2:B:37:LEU:HD22	1.72	0.71
3:G:46:LEU:HD12	4:H:101:LYS:CA	2.21	0.71
4:H:146:PHE:CD1	4:H:147:PRO:HA	2.26	0.71
2:J:36:ILE:HG22	2:J:37:LEU:HD22	1.72	0.71
3:C:93:ASN:ND2	3:C:95(B):ARG:HB2	2.05	0.71
4:H:126:PRO:HG3	4:H:138:LEU:HD13	1.73	0.71
2:B:177:LEU:HD12	2:B:177:LEU:N	2.06	0.70
4:D:146:PHE:CD1	4:D:147:PRO:HA	2.26	0.70
4:L:126:PRO:HG3	4:L:138:LEU:HD13	1.73	0.70
3:K:93:ASN:ND2	3:K:95(B):ARG:HB2	2.05	0.70
4:L:99:GLU:N	4:L:100(D):GLU:OE1	2.25	0.70
2:F:177:LEU:HD12	2:F:177:LEU:N	2.06	0.70
4:L:146:PHE:CD1	4:L:147:PRO:HA	2.26	0.70
3:C:20:THR:HG23	3:C:74:THR:HG23	1.74	0.70
4:D:126:PRO:HG3	4:D:138:LEU:HD13	1.73	0.70
4:H:11:VAL:HG21	4:H:147:PRO:HG3	1.74	0.70
2:J:161:VAL:O	2:J:167:LYS:HA	1.90	0.70
3:C:154:LEU:O	3:C:154:LEU:HD13	1.91	0.70
2:F:36:ILE:HG22	2:F:37:LEU:HD22	1.72	0.70
4:H:82(B):ASN:HD22	4:H:82(B):ASN:N	1.90	0.70
4:D:82(B):ASN:HD22	4:D:82(B):ASN:N	1.90	0.70
1:E:440:ARG:HD2	1:E:442:GLN:O	1.92	0.70
1:I:440:ARG:HD2	1:I:442:GLN:O	1.92	0.70
2:J:3:VAL:HG22	2:J:94:GLN:HB3	1.74	0.70
2:B:161:VAL:O	2:B:167:LYS:HA	1.90	0.70
4:D:11:VAL:HG21	4:D:147:PRO:HG3	1.74	0.70
3:K:32:ASP:HB2	3:K:92:ASN:HB2	1.72	0.70
4:D:99:GLU:N	4:D:100(D):GLU:OE1	2.24	0.69
1:I:104:MET:HE2	1:I:215:ILE:HD11	1.71	0.69
2:J:177:LEU:HD12	2:J:177:LEU:N	2.06	0.69
4:D:182:VAL:HG22	4:D:184:VAL:HG13	1.72	0.69
3:C:182:SER:OG	3:C:185:ASP:HB3	1.93	0.69
1:A:95:MET:HE1	1:A:273:ARG:HG2	1.75	0.69
3:C:32:ASP:HB2	3:C:92:ASN:HB2	1.72	0.69
3:C:46:LEU:HD12	4:D:101:LYS:CA	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:VAL:HG12	1:E:434:MET:HE2	1.75	0.69
4:H:99:GLU:N	4:H:100(D):GLU:OE1	2.25	0.69
1:I:120:VAL:HG12	1:I:434:MET:HE2	1.75	0.69
3:K:20:THR:HG23	3:K:74:THR:HG23	1.74	0.69
3:C:149:LYS:HE2	3:C:154:LEU:HD23	1.74	0.69
2:F:3:VAL:HG22	2:F:94:GLN:HB3	1.74	0.69
2:B:3:VAL:HG22	2:B:94:GLN:HB3	1.74	0.69
3:G:182:SER:OG	3:G:185:ASP:HB3	1.93	0.69
2:J:128:VAL:HA	2:J:160:THR:O	1.93	0.69
4:L:11:VAL:HG21	4:L:147:PRO:HG3	1.74	0.69
3:K:46:LEU:HD12	4:L:101:LYS:CA	2.21	0.69
6:P:68:LEU:HD12	6:P:81:GLU:OE1	1.93	0.69
6:R:68:LEU:HD12	6:R:81:GLU:OE1	1.93	0.69
6:R:81:GLU:OE2	6:R:82(A):LYS:HE2	1.93	0.69
2:B:134:ARG:HE	2:B:152:GLN:HB2	1.58	0.69
2:F:134:ARG:HE	2:F:152:GLN:HB2	1.58	0.69
3:G:149:LYS:HE2	3:G:154:LEU:HD23	1.74	0.69
1:A:440:ARG:HD2	1:A:442:GLN:O	1.92	0.69
5:M:10:THR:HG22	5:M:103:LYS:HB3	1.75	0.69
4:H:124:LEU:HD11	4:H:141:LEU:HB2	1.75	0.68
5:Q:155:GLN:HE21	5:Q:158:ASN:HD21	1.40	0.68
1:A:120:VAL:HG12	1:A:434:MET:HE2	1.75	0.68
5:M:155:GLN:HE21	5:M:158:ASN:HD21	1.40	0.68
1:I:95:MET:HE1	1:I:273:ARG:HG2	1.75	0.68
4:L:82(B):ASN:HD22	4:L:82(B):ASN:N	1.90	0.68
6:P:81:GLU:OE2	6:P:82(A):LYS:HE2	1.93	0.68
2:B:128:VAL:HA	2:B:160:THR:O	1.93	0.68
2:F:154:SER:HB2	2:F:176:VAL:HG23	1.75	0.68
1:I:288:LEU:HD12	1:I:449:ILE:O	1.93	0.68
1:A:288:LEU:HD12	1:A:449:ILE:O	1.93	0.68
2:J:140:GLY:CA	2:J:144:LEU:HG	2.24	0.68
5:O:10:THR:HG22	5:O:103:LYS:HB3	1.75	0.68
3:K:149:LYS:HE2	3:K:154:LEU:HD23	1.74	0.68
6:N:68:LEU:HD12	6:N:81:GLU:OE1	1.93	0.68
1:E:439:ILE:HD12	1:E:440:ARG:N	2.09	0.68
1:E:95:MET:HE1	1:E:273:ARG:HG2	1.75	0.68
3:G:20:THR:HG23	3:G:74:THR:HG23	1.74	0.68
6:N:81:GLU:OE2	6:N:82(A):LYS:HE2	1.93	0.68
5:O:155:GLN:HE21	5:O:158:ASN:HD21	1.40	0.68
2:B:154:SER:HB2	2:B:176:VAL:HG23	1.75	0.68
3:K:133:VAL:HG21	4:L:141:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:10:THR:HG22	5:Q:103:LYS:HB3	1.75	0.68
3:C:133:VAL:HG21	4:D:141:LEU:HD13	1.76	0.67
2:J:103:ASN:HD22	2:J:103:ASN:N	1.90	0.67
2:J:134:ARG:HE	2:J:152:GLN:HB2	1.58	0.67
2:F:128:VAL:HA	2:F:160:THR:O	1.93	0.67
1:A:202:THR:HG22	3:C:95:PRO:HG3	1.76	0.67
4:D:119:PRO:HB3	4:D:145:TYR:HB3	1.77	0.67
1:E:288:LEU:HD12	1:E:449:ILE:O	1.93	0.67
3:K:182:SER:OG	3:K:185:ASP:HB3	1.93	0.67
2:B:103:ASN:HD22	2:B:103:ASN:N	1.90	0.67
3:C:12:SER:HB2	3:C:107:LYS:HB2	1.77	0.67
1:I:202:THR:HG22	3:K:95:PRO:HG3	1.76	0.67
4:D:7:SER:HB3	4:D:21:SER:OG	1.95	0.67
4:D:159:LEU:HD21	4:D:184:VAL:HG11	1.77	0.67
4:H:7:SER:HB3	4:H:21:SER:OG	1.95	0.67
4:H:159:LEU:HD21	4:H:184:VAL:HG11	1.77	0.67
1:A:439:ILE:HD12	1:A:440:ARG:N	2.09	0.67
2:F:176:VAL:O	2:F:177:LEU:HD12	1.95	0.67
2:B:140:GLY:CA	2:B:144:LEU:HG	2.24	0.67
3:K:140:TYR:CD2	3:K:141:PRO:HD3	2.29	0.67
4:L:7:SER:HB3	4:L:21:SER:OG	1.95	0.67
1:A:127:VAL:HG23	1:A:129:ALA:H	1.60	0.67
4:L:159:LEU:HD21	4:L:184:VAL:HG11	1.77	0.67
1:I:439:ILE:HD12	1:I:440:ARG:N	2.09	0.67
3:K:39:LYS:HB2	3:K:42:GLN:OE1	1.95	0.67
4:L:124:LEU:HD11	4:L:141:LEU:HB2	1.75	0.67
3:C:140:TYR:CD2	3:C:141:PRO:HD3	2.29	0.66
3:C:39:LYS:HB2	3:C:42:GLN:OE1	1.95	0.66
1:E:202:THR:HG22	3:G:95:PRO:HG3	1.76	0.66
2:F:140:GLY:CA	2:F:144:LEU:HG	2.24	0.66
3:G:133:VAL:HG21	4:H:141:LEU:HD13	1.76	0.66
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.77	0.66
1:I:121:LYS:NZ	1:I:426:MET:HE1	2.11	0.66
3:G:39:LYS:HB2	3:G:42:GLN:OE1	1.95	0.66
4:L:119:PRO:HB3	4:L:145:TYR:HB3	1.77	0.66
2:B:98:PHE:HB3	2:B:118:LEU:HD11	1.77	0.66
4:D:124:LEU:HD11	4:D:141:LEU:HB2	1.75	0.66
2:F:103:ASN:HD22	2:F:103:ASN:N	1.91	0.66
2:J:50:LYS:O	2:J:50:LYS:HG2	1.95	0.66
2:J:154:SER:HB2	2:J:176:VAL:HG23	1.75	0.66
4:D:100:ALA:HA	4:D:100(D):GLU:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:12:SER:HB2	3:G:107:LYS:HB2	1.77	0.66
3:G:140:TYR:CD2	3:G:141:PRO:HD3	2.29	0.66
3:K:12:SER:HB2	3:K:107:LYS:HB2	1.77	0.66
1:A:475:MET:O	1:A:478:ASN:HB2	1.95	0.66
3:C:159:SER:HA	3:C:178:THR:O	1.96	0.66
2:F:50:LYS:HG2	2:F:50:LYS:O	1.95	0.66
1:I:475:MET:O	1:I:478:ASN:HB2	1.95	0.66
4:L:36:TRP:CE2	4:L:80:LEU:HB2	2.31	0.66
1:A:121:LYS:NZ	1:A:426:MET:HE1	2.11	0.66
2:B:50:LYS:O	2:B:50:LYS:HG2	1.95	0.66
3:C:91:TYR:HA	3:C:96:TYR:CD1	2.31	0.66
1:E:475:MET:O	1:E:478:ASN:HB2	1.95	0.66
4:H:100:ALA:HA	4:H:100(D):GLU:O	1.96	0.66
1:I:127:VAL:HG23	1:I:129:ALA:H	1.60	0.66
1:I:419:ARG:NH2	4:L:99:GLU:OE1	2.29	0.66
2:J:154:SER:CB	2:J:176:VAL:H	2.09	0.66
2:B:154:SER:CB	2:B:176:VAL:H	2.09	0.66
5:Q:151:ASP:OD2	5:Q:189:HIS:ND1	2.26	0.66
2:F:75:LYS:HB3	2:F:77:GLU:OE2	1.96	0.65
3:K:159:SER:HA	3:K:178:THR:O	1.96	0.65
5:O:151:ASP:OD2	5:O:189:HIS:ND1	2.26	0.65
1:A:419:ARG:NH2	4:D:99:GLU:OE1	2.29	0.65
4:D:12:LYS:O	4:D:111:VAL:HA	1.96	0.65
1:A:459:GLY:O	1:A:462:THR:HG23	1.96	0.65
1:A:487:LYS:O	1:A:487:LYS:HG3	1.97	0.65
1:E:121:LYS:NZ	1:E:426:MET:HE1	2.11	0.65
2:F:98:PHE:HB3	2:F:118:LEU:HD11	1.77	0.65
3:K:91:TYR:HA	3:K:96:TYR:CD1	2.31	0.65
4:D:212:GLU:C	4:D:214:LYS:H	2.05	0.65
4:L:100:ALA:HA	4:L:100(D):GLU:O	1.96	0.65
4:L:212:GLU:C	4:L:214:LYS:H	2.05	0.65
2:B:176:VAL:O	2:B:177:LEU:HD12	1.95	0.65
1:E:419:ARG:NH2	4:H:99:GLU:OE1	2.29	0.65
2:J:75:LYS:HB3	2:J:77:GLU:OE2	1.96	0.65
1:E:127:VAL:HG23	1:E:129:ALA:H	1.60	0.65
3:G:91:TYR:HA	3:G:96:TYR:CD1	2.31	0.65
1:A:339:GLU:O	1:A:343:GLU:HG3	1.97	0.65
2:B:75:LYS:HB3	2:B:77:GLU:OE2	1.96	0.65
4:D:36:TRP:CE2	4:D:80:LEU:HB2	2.31	0.65
2:F:154:SER:CB	2:F:176:VAL:H	2.09	0.65
4:H:12:LYS:O	4:H:111:VAL:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:212:GLU:C	4:H:214:LYS:H	2.05	0.65
1:I:339:GLU:O	1:I:343:GLU:HG3	1.97	0.65
1:I:487:LYS:O	1:I:487:LYS:HG3	1.97	0.65
2:J:98:PHE:HB3	2:J:118:LEU:HD11	1.77	0.65
3:G:159:SER:HA	3:G:178:THR:O	1.96	0.65
4:H:36:TRP:CE2	4:H:80:LEU:HB2	2.31	0.65
1:I:459:GLY:O	1:I:462:THR:HG23	1.97	0.65
1:A:205:CYS:N	1:A:206:PRO:HD3	2.12	0.64
4:H:150:VAL:HG23	4:H:199:ASN:O	1.97	0.64
1:I:451:GLY:C	1:I:452:LEU:HD12	2.23	0.64
4:L:12:LYS:O	4:L:111:VAL:HA	1.96	0.64
1:E:487:LYS:HG3	1:E:487:LYS:O	1.97	0.64
3:G:18:ARG:HA	3:G:76:SER:O	1.97	0.64
1:I:205:CYS:N	1:I:206:PRO:HD3	2.12	0.64
3:K:18:ARG:HA	3:K:76:SER:O	1.97	0.64
1:A:451:GLY:C	1:A:452:LEU:HD12	2.23	0.64
1:E:339:GLU:O	1:E:343:GLU:HG3	1.97	0.64
3:G:193:ALA:CA	3:G:208:SER:HB3	2.27	0.64
2:J:176:VAL:O	2:J:177:LEU:HD12	1.94	0.64
1:E:205:CYS:N	1:E:206:PRO:HD3	2.13	0.64
1:E:459:GLY:O	1:E:462:THR:HG23	1.96	0.64
4:H:138:LEU:HD12	4:H:211:VAL:CG1	2.28	0.64
4:L:138:LEU:HD12	4:L:211:VAL:CG1	2.28	0.64
4:L:138:LEU:HD12	4:L:211:VAL:HG11	1.80	0.64
4:L:154:TRP:HB2	4:L:159:LEU:O	1.98	0.64
1:A:280:ASN:HD22	1:A:458:GLY:N	1.95	0.64
4:H:138:LEU:HD12	4:H:211:VAL:HG11	1.80	0.64
1:A:279:ASN:HD22	1:A:282:LYS:HG2	1.63	0.64
4:D:138:LEU:HD12	4:D:211:VAL:CG1	2.28	0.64
4:H:154:TRP:HB2	4:H:159:LEU:O	1.98	0.64
1:I:456:ARG:HB3	1:I:468:PHE:CE2	2.33	0.64
3:C:86:TYR:HE2	3:C:104:LEU:HD22	1.63	0.64
6:P:100:LYS:HB2	6:P:100(A):TRP:CE3	2.33	0.63
1:E:280:ASN:HD22	1:E:458:GLY:N	1.95	0.63
4:L:40:ALA:HB3	4:L:43:GLN:HG3	1.81	0.63
1:A:335:LYS:HD3	1:A:407:LEU:O	1.98	0.63
1:A:456:ARG:HB3	1:A:468:PHE:CE2	2.33	0.63
1:E:456:ARG:HB3	1:E:468:PHE:CE2	2.33	0.63
1:I:280:ASN:HD22	1:I:458:GLY:N	1.95	0.63
6:R:100:LYS:HB2	6:R:100(A):TRP:CE3	2.33	0.63
4:D:138:LEU:HD12	4:D:211:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:VAL:HG23	4:D:199:ASN:O	1.97	0.63
1:E:368:ASP:CG	2:F:59:ARG:HH22	2.07	0.63
1:E:391:PHE:CD2	1:E:470:PRO:HG3	2.34	0.63
2:F:163:GLN:HG3	2:F:164:ASN:OD1	1.99	0.63
3:G:185:ASP:OD1	3:G:185:ASP:O	2.16	0.63
1:I:272:ILE:HG13	1:I:272:ILE:O	1.99	0.63
3:K:86:TYR:HE2	3:K:104:LEU:HD22	1.63	0.63
1:E:335:LYS:HD3	1:E:407:LEU:O	1.98	0.63
1:E:353:PHE:CE1	1:E:456:ARG:HD3	2.34	0.63
1:E:451:GLY:C	1:E:452:LEU:HD12	2.23	0.63
1:A:272:ILE:HG13	1:A:272:ILE:O	1.99	0.62
2:B:114:LEU:O	2:B:145:SER:HA	1.99	0.62
2:F:114:LEU:O	2:F:145:SER:HA	1.99	0.62
1:I:368:ASP:CG	2:J:59:ARG:HH22	2.06	0.62
2:B:163:GLN:HG3	2:B:164:ASN:OD1	1.99	0.62
1:E:279:ASN:HD22	1:E:282:LYS:HG2	1.63	0.62
2:F:131:ARG:NH1	2:F:137:ASN:HB3	2.14	0.62
1:I:391:PHE:CD2	1:I:470:PRO:HG3	2.34	0.62
1:A:215:ILE:HG12	1:A:251:ILE:O	1.99	0.62
3:G:46:LEU:CD1	4:H:101:LYS:HA	2.27	0.62
3:K:46:LEU:CD1	4:L:101:LYS:HA	2.28	0.62
3:K:185:ASP:OD1	3:K:185:ASP:O	2.17	0.62
2:B:131:ARG:NH1	2:B:137:ASN:HB3	2.14	0.62
3:C:18:ARG:HA	3:C:76:SER:O	1.98	0.62
1:E:215:ILE:HG12	1:E:251:ILE:O	1.99	0.62
1:I:335:LYS:HD3	1:I:407:LEU:O	1.98	0.62
3:K:187:GLU:HA	3:K:211:ARG:NH1	2.15	0.62
4:L:150:VAL:HG23	4:L:199:ASN:O	1.97	0.62
6:N:100:LYS:HB2	6:N:100(A):TRP:CE3	2.33	0.62
1:I:215:ILE:HG12	1:I:251:ILE:O	1.99	0.62
1:I:353:PHE:CE1	1:I:456:ARG:HD3	2.34	0.62
2:J:163:GLN:HG3	2:J:164:ASN:OD1	1.99	0.62
3:C:93:ASN:HD21	3:C:95(B):ARG:HB2	1.65	0.62
3:C:185:ASP:OD1	3:C:185:ASP:O	2.16	0.62
4:D:98:GLY:O	4:D:100:ALA:N	2.32	0.62
1:A:391:PHE:CD2	1:A:470:PRO:HG3	2.34	0.62
4:D:154:TRP:HB2	4:D:159:LEU:O	1.98	0.62
1:A:353:PHE:CE1	1:A:456:ARG:HD3	2.34	0.62
1:I:279:ASN:HD22	1:I:282:LYS:HG2	1.63	0.62
5:M:151:ASP:OD2	5:M:189:HIS:ND1	2.26	0.62
3:G:86:TYR:HE2	3:G:104:LEU:HD22	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:108:LEU:HD12	4:H:109:VAL:H	1.65	0.62
2:J:170:PHE:O	2:J:172:ILE:HG12	2.00	0.62
2:B:170:PHE:O	2:B:172:ILE:HG12	2.00	0.61
4:H:98:GLY:O	4:H:100:ALA:N	2.32	0.61
3:G:187:GLU:HA	3:G:211:ARG:NH1	2.15	0.61
4:H:40:ALA:HB3	4:H:43:GLN:HG3	1.80	0.61
2:J:114:LEU:O	2:J:145:SER:HA	1.99	0.61
2:J:177:LEU:CD1	2:J:177:LEU:N	2.64	0.61
3:C:141:PRO:C	3:C:143:GLU:H	2.08	0.61
1:E:272:ILE:O	1:E:272:ILE:HG13	1.99	0.61
1:A:365:SER:HB2	2:B:46:LYS:O	2.00	0.61
2:B:58:ARG:HG2	2:B:61:LEU:HG	1.82	0.61
4:D:40:ALA:HB3	4:D:43:GLN:HG3	1.81	0.61
4:D:50:ARG:NH2	4:D:97:GLU:OE2	2.33	0.61
1:E:279:ASN:HB3	1:E:282:LYS:HG2	1.82	0.61
1:E:280:ASN:HD22	1:E:458:GLY:CA	2.14	0.61
4:L:50:ARG:NH2	4:L:97:GLU:OE2	2.33	0.61
1:A:368:ASP:CG	2:B:59:ARG:HH22	2.07	0.61
4:D:126:PRO:HG3	4:D:138:LEU:CD1	2.30	0.61
1:I:115:SER:O	1:I:208:VAL:HG11	2.00	0.61
4:L:126:PRO:HG3	4:L:138:LEU:CD1	2.31	0.61
3:C:193:ALA:CA	3:C:208:SER:HB3	2.27	0.61
1:E:204:ALA:C	1:E:206:PRO:HD3	2.26	0.61
2:F:177:LEU:CD1	2:F:177:LEU:N	2.64	0.61
1:I:204:ALA:C	1:I:206:PRO:HD3	2.26	0.61
1:A:204:ALA:C	1:A:206:PRO:HD3	2.26	0.61
3:K:2:ILE:HG12	3:K:27:GLU:OE1	2.01	0.61
2:B:26:PHE:CE1	2:B:39:ASN:HB3	2.36	0.61
3:C:187:GLU:HA	3:C:211:ARG:NH1	2.15	0.61
4:D:108:LEU:HD12	4:D:109:VAL:H	1.65	0.61
1:E:115:SER:O	1:E:208:VAL:HG11	2.00	0.61
3:G:93:ASN:HD21	3:G:95(B):ARG:HB2	1.65	0.61
3:G:141:PRO:C	3:G:143:GLU:H	2.08	0.61
2:J:131:ARG:NH1	2:J:137:ASN:HB3	2.14	0.61
3:K:193:ALA:CA	3:K:208:SER:HB3	2.27	0.61
1:A:280:ASN:HD22	1:A:458:GLY:CA	2.14	0.61
1:A:456:ARG:HB3	1:A:468:PHE:CD2	2.36	0.61
3:C:135:LEU:HD23	3:C:136:LEU:N	2.16	0.61
1:E:100:MET:HE1	1:E:486:TYR:CB	2.31	0.61
1:E:456:ARG:HB3	1:E:468:PHE:CD2	2.36	0.61
2:F:58:ARG:HG2	2:F:61:LEU:HG	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:189:HIS:O	3:K:211:ARG:NE	2.34	0.61
1:A:373:THR:HB	1:A:385:CYS:O	2.01	0.60
3:G:78:LEU:HD11	3:G:104:LEU:CD2	2.31	0.60
1:A:100:MET:HE1	1:A:486:TYR:CB	2.31	0.60
1:A:115:SER:O	1:A:208:VAL:HG11	2.00	0.60
1:A:394:ASN:C	1:A:396:THR:H	2.09	0.60
1:E:255:VAL:HG13	1:E:475:MET:SD	2.41	0.60
3:K:48:ILE:HD13	3:K:54:ARG:HA	1.84	0.60
3:C:136:LEU:HD22	3:C:175:LEU:HD23	1.82	0.60
4:L:108:LEU:HD12	4:L:109:VAL:H	1.65	0.60
1:A:255:VAL:HG13	1:A:475:MET:SD	2.41	0.60
1:A:279:ASN:HB3	1:A:282:LYS:HG2	1.82	0.60
2:B:177:LEU:CD1	2:B:177:LEU:N	2.64	0.60
3:C:48:ILE:HD13	3:C:54:ARG:HA	1.84	0.60
2:F:170:PHE:O	2:F:172:ILE:HG12	2.00	0.60
3:G:2:ILE:HG12	3:G:27:GLU:OE1	2.01	0.60
1:I:279:ASN:HB3	1:I:282:LYS:HG2	1.82	0.60
2:J:120:SER:OG	2:J:121:PRO:HD2	2.01	0.60
2:F:26:PHE:CE1	2:F:39:ASN:HB3	2.36	0.60
4:H:38:ARG:HD2	4:H:46:GLU:OE1	2.01	0.60
4:H:126:PRO:HG3	4:H:138:LEU:CD1	2.30	0.60
1:I:255:VAL:HG13	1:I:475:MET:SD	2.41	0.60
2:J:58:ARG:HG2	2:J:61:LEU:HG	1.82	0.60
1:A:280:ASN:HD22	1:A:458:GLY:H	1.49	0.60
4:D:38:ARG:HD2	4:D:46:GLU:OE1	2.01	0.60
4:H:50:ARG:NH2	4:H:97:GLU:OE2	2.33	0.60
1:I:100:MET:HE1	1:I:486:TYR:CB	2.31	0.60
4:L:38:ARG:HD2	4:L:46:GLU:OE1	2.01	0.60
4:L:108:LEU:HD12	4:L:109:VAL:N	2.17	0.60
1:E:365:SER:HB2	2:F:46:LYS:O	2.00	0.60
1:I:121:LYS:HZ1	1:I:426:MET:HE1	1.66	0.60
1:I:280:ASN:HD22	1:I:458:GLY:CA	2.14	0.60
2:J:26:PHE:CE1	2:J:39:ASN:HB3	2.36	0.60
3:K:135:LEU:HD23	3:K:136:LEU:N	2.16	0.60
3:K:136:LEU:HD22	3:K:175:LEU:HD23	1.82	0.60
3:G:135:LEU:HD23	3:G:136:LEU:N	2.16	0.60
3:G:136:LEU:HD22	3:G:175:LEU:HD23	1.82	0.60
1:I:365:SER:HB2	2:J:46:LYS:O	2.00	0.60
1:I:391:PHE:CG	1:I:470:PRO:HG3	2.37	0.60
3:K:78:LEU:HD11	3:K:104:LEU:CD2	2.31	0.60
3:C:78:LEU:HD11	3:C:104:LEU:CD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ASN:HD22	1:E:458:GLY:H	1.49	0.60
1:E:391:PHE:CG	1:E:470:PRO:HG3	2.37	0.60
3:G:48:ILE:HD13	3:G:54:ARG:HA	1.84	0.60
3:C:2:ILE:HG12	3:C:27:GLU:OE1	2.01	0.60
1:E:373:THR:HB	1:E:385:CYS:O	2.01	0.60
3:G:189:HIS:O	3:G:211:ARG:NE	2.34	0.60
3:K:139:PHE:HE1	3:K:175:LEU:H	1.50	0.60
1:A:86:LEU:HA	1:A:243:SER:CB	2.32	0.59
3:C:189:HIS:O	3:C:211:ARG:NE	2.34	0.59
4:H:108:LEU:HD12	4:H:109:VAL:N	2.17	0.59
3:C:78:LEU:CD1	3:C:104:LEU:HD21	2.33	0.59
1:E:394:ASN:C	1:E:396:THR:H	2.09	0.59
3:G:135:LEU:HD23	3:G:135:LEU:C	2.28	0.59
1:I:280:ASN:HD22	1:I:458:GLY:H	1.49	0.59
1:I:456:ARG:HB3	1:I:468:PHE:CD2	2.36	0.59
6:N:100:LYS:HB2	6:N:100(A):TRP:CZ3	2.37	0.59
3:C:135:LEU:HD23	3:C:135:LEU:C	2.28	0.59
2:B:120:SER:OG	2:B:121:PRO:HD2	2.01	0.59
2:F:55:ALA:O	2:F:56:ASP:HB2	2.02	0.59
4:H:141:LEU:HD12	4:H:179:SER:OG	2.03	0.59
1:I:86:LEU:HA	1:I:243:SER:CB	2.32	0.59
3:K:93:ASN:HD21	3:K:95(B):ARG:HB2	1.65	0.59
4:L:141:LEU:HD12	4:L:179:SER:OG	2.03	0.59
1:A:391:PHE:CG	1:A:470:PRO:HG3	2.37	0.59
2:B:8:LYS:HD2	2:B:76:ILE:HG13	1.85	0.59
1:E:86:LEU:HA	1:E:243:SER:CB	2.32	0.59
2:J:2:LYS:HD3	2:J:3:VAL:H	1.67	0.59
1:A:448:ASN:ND2	7:A:948:NAG:H82	2.18	0.59
4:D:108:LEU:HD12	4:D:109:VAL:N	2.17	0.59
2:J:55:ALA:O	2:J:56:ASP:HB2	2.02	0.59
6:R:100:LYS:HB2	6:R:100(A):TRP:CZ3	2.37	0.59
3:K:141:PRO:C	3:K:143:GLU:H	2.08	0.59
2:F:120:SER:OG	2:F:121:PRO:HD2	2.01	0.59
3:G:139:PHE:HE1	3:G:175:LEU:H	1.50	0.59
1:I:94:ASN:ND2	1:I:97:LYS:HB3	2.18	0.59
3:K:44:PRO:HD2	4:L:103:TRP:CE3	2.38	0.59
2:B:2:LYS:HD3	2:B:3:VAL:H	1.67	0.59
2:F:2:LYS:HD3	2:F:3:VAL:H	1.67	0.59
3:G:116:PHE:CD2	4:H:137:ALA:HB3	2.38	0.59
1:A:242:VAL:HG22	1:A:243:SER:N	2.18	0.58
1:I:124:PRO:CG	2:J:60:SER:HA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:100:LYS:HB2	6:P:100(A):TRP:CZ3	2.38	0.58
1:A:278:THR:HG22	7:A:776:NAG:O6	2.03	0.58
3:C:46:LEU:CD1	4:D:101:LYS:HA	2.28	0.58
2:F:164:ASN:O	2:F:166:LYS:N	2.36	0.58
1:I:242:VAL:HG22	1:I:243:SER:N	2.18	0.58
3:K:116:PHE:CD2	4:L:137:ALA:HB3	2.38	0.58
3:K:135:LEU:HD23	3:K:135:LEU:C	2.28	0.58
1:A:371:ILE:HD12	1:A:472:GLY:O	2.04	0.58
1:E:94:ASN:ND2	1:E:97:LYS:HB3	2.18	0.58
1:E:371:ILE:HD12	1:E:472:GLY:O	2.04	0.58
1:I:276:ASN:OD1	1:I:278:THR:HB	2.03	0.58
1:I:373:THR:HB	1:I:385:CYS:O	2.01	0.58
4:L:60:ALA:HB3	4:L:63:LEU:HD12	1.85	0.58
1:A:124:PRO:CG	2:B:60:SER:HA	2.33	0.58
3:C:139:PHE:HE1	3:C:175:LEU:H	1.50	0.58
3:G:29:VAL:HG11	3:G:90:GLN:HG2	1.85	0.58
3:G:78:LEU:CD1	3:G:104:LEU:HD21	2.33	0.58
1:I:448:ASN:ND2	7:I:948:NAG:H82	2.18	0.58
3:K:193:ALA:HA	3:K:208:SER:CB	2.32	0.58
1:E:448:ASN:ND2	7:E:948:NAG:H82	2.18	0.58
1:I:394:ASN:C	1:I:396:THR:H	2.09	0.58
1:A:94:ASN:ND2	1:A:97:LYS:HB3	2.18	0.58
2:B:164:ASN:O	2:B:166:LYS:N	2.37	0.58
3:C:198:HIS:HB3	3:C:201:LEU:HG	1.86	0.58
1:E:124:PRO:CG	2:F:60:SER:HA	2.33	0.58
3:G:193:ALA:HA	3:G:208:SER:CB	2.32	0.58
3:C:29:VAL:HG11	3:C:90:GLN:HG2	1.85	0.58
1:E:104:MET:O	1:E:108:ILE:HG12	2.04	0.58
1:E:242:VAL:HG22	1:E:243:SER:N	2.18	0.58
2:F:8:LYS:HD2	2:F:76:ILE:HG13	1.85	0.58
3:G:44:PRO:HD2	4:H:103:TRP:CE3	2.38	0.58
1:I:278:THR:HG22	7:I:776:NAG:O6	2.03	0.58
3:K:29:VAL:HG12	3:K:29:VAL:O	2.04	0.58
4:D:141:LEU:HD12	4:D:179:SER:OG	2.03	0.58
3:G:59:PRO:HB3	3:G:61:ARG:NH1	2.19	0.58
1:I:279:ASN:HD22	1:I:282:LYS:CG	2.17	0.58
3:K:59:PRO:HB3	3:K:61:ARG:NH1	2.19	0.58
3:K:78:LEU:CD1	3:K:104:LEU:HD21	2.32	0.58
3:K:141:PRO:C	3:K:143:GLU:N	2.61	0.58
4:D:214:LYS:O	4:D:214:LYS:HD3	2.04	0.58
1:E:279:ASN:HD22	1:E:282:LYS:HD3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:O	1:A:108:ILE:HG12	2.04	0.57
3:G:29:VAL:O	3:G:29:VAL:HG12	2.04	0.57
2:J:8:LYS:HD2	2:J:76:ILE:HG13	1.85	0.57
3:K:29:VAL:HG11	3:K:90:GLN:HG2	1.85	0.57
1:A:279:ASN:HD22	1:A:282:LYS:HD3	1.68	0.57
4:D:51:ILE:O	4:D:51:ILE:HG23	2.04	0.57
1:E:276:ASN:OD1	1:E:278:THR:HB	2.03	0.57
3:G:94:TRP:HA	3:G:95:PRO:O	2.05	0.57
1:I:104:MET:HA	1:I:217:TYR:OH	2.04	0.57
4:L:6:GLU:OE2	4:L:106:GLY:N	2.36	0.57
1:A:233:PHE:CE2	1:A:235:GLY:HA2	2.39	0.57
1:A:276:ASN:OD1	1:A:278:THR:HB	2.03	0.57
2:B:55:ALA:O	2:B:56:ASP:HB2	2.02	0.57
3:C:18:ARG:HG3	3:C:75:ILE:O	2.04	0.57
1:I:273:ARG:HG2	1:I:273:ARG:NH1	2.20	0.57
5:Q:22:SER:CB	5:Q:72:THR:HG22	2.34	0.57
1:A:104:MET:HA	1:A:217:TYR:OH	2.04	0.57
3:C:116:PHE:CD2	4:D:137:ALA:HB3	2.38	0.57
1:E:278:THR:HG22	7:E:776:NAG:O6	2.03	0.57
1:E:279:ASN:HD22	1:E:282:LYS:CG	2.17	0.57
2:F:76:ILE:HD12	2:F:76:ILE:N	2.19	0.57
1:I:104:MET:O	1:I:108:ILE:HG12	2.04	0.57
1:I:371:ILE:HD12	1:I:472:GLY:O	2.04	0.57
2:J:76:ILE:H	2:J:76:ILE:CD1	2.13	0.57
3:K:18:ARG:HG3	3:K:75:ILE:O	2.04	0.57
3:K:94:TRP:HA	3:K:95:PRO:O	2.05	0.57
3:C:44:PRO:HD2	4:D:103:TRP:CE3	2.38	0.57
3:C:59:PRO:HB3	3:C:61:ARG:NH1	2.19	0.57
2:F:83:ILE:HG23	2:F:92:GLU:HG3	1.87	0.57
2:F:178:ALA:CB	2:F:180:GLN:H	2.18	0.57
3:G:135:LEU:C	3:G:136:LEU:HD12	2.29	0.57
4:L:193:THR:HB	4:L:210:LYS:HE2	1.86	0.57
2:B:83:ILE:HG23	2:B:92:GLU:HG3	1.87	0.57
3:C:143:GLU:OE1	3:C:143:GLU:N	2.37	0.57
4:D:60:ALA:HB3	4:D:63:LEU:HD12	1.85	0.57
3:G:18:ARG:HG3	3:G:75:ILE:O	2.04	0.57
3:G:141:PRO:C	3:G:143:GLU:N	2.61	0.57
4:H:60:ALA:HB3	4:H:63:LEU:HD12	1.85	0.57
4:L:98:GLY:O	4:L:100:ALA:N	2.32	0.57
4:L:214:LYS:O	4:L:214:LYS:HD3	2.04	0.57
1:A:466:GLU:HB3	1:A:468:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:PHE:CE2	1:E:235:GLY:HA2	2.39	0.57
1:E:466:GLU:HB3	1:E:468:PHE:CE1	2.39	0.57
3:G:198:HIS:CD2	3:G:199:GLN:N	2.72	0.57
3:K:189:HIS:HB2	3:K:192:TYR:OH	2.05	0.57
5:O:22:SER:CB	5:O:72:THR:HG22	2.35	0.57
2:B:178:ALA:CB	2:B:180:GLN:H	2.18	0.57
3:C:29:VAL:HG12	3:C:29:VAL:O	2.04	0.57
4:H:51:ILE:HG23	4:H:51:ILE:O	2.04	0.57
2:J:178:ALA:CB	2:J:180:GLN:H	2.18	0.57
3:C:141:PRO:C	3:C:143:GLU:N	2.61	0.57
4:D:126:PRO:HG3	4:D:138:LEU:CB	2.35	0.57
4:D:193:THR:HB	4:D:210:LYS:HE2	1.86	0.57
3:K:8:PRO:O	3:K:102:THR:HG23	2.05	0.57
4:L:126:PRO:HG3	4:L:138:LEU:CB	2.35	0.57
3:C:189:HIS:HB2	3:C:192:TYR:OH	2.05	0.57
1:E:108:ILE:HD12	1:E:253:PRO:CB	2.35	0.57
4:H:214:LYS:O	4:H:214:LYS:HD3	2.04	0.57
5:M:22:SER:CB	5:M:72:THR:HG22	2.34	0.57
3:G:189:HIS:HB2	3:G:192:TYR:OH	2.05	0.56
2:J:83:ILE:HG23	2:J:92:GLU:HG3	1.87	0.56
2:J:164:ASN:O	2:J:166:LYS:N	2.37	0.56
3:K:198:HIS:HB3	3:K:201:LEU:HG	1.86	0.56
3:C:193:ALA:HA	3:C:208:SER:CB	2.32	0.56
3:G:198:HIS:HB3	3:G:201:LEU:HG	1.86	0.56
1:I:233:PHE:CE2	1:I:235:GLY:HA2	2.39	0.56
1:I:466:GLU:HB3	1:I:468:PHE:CE1	2.40	0.56
1:A:108:ILE:HD12	1:A:253:PRO:CB	2.35	0.56
1:A:122:LEU:HD11	4:D:54:LEU:HG	1.86	0.56
1:A:279:ASN:HD22	1:A:282:LYS:CG	2.17	0.56
2:B:16:CYS:HB2	2:B:28:TRP:CZ2	2.41	0.56
3:C:8:PRO:O	3:C:102:THR:HG23	2.05	0.56
3:C:135:LEU:HD12	4:D:181:VAL:HG11	1.86	0.56
3:C:136:LEU:HD22	3:C:175:LEU:HB3	1.87	0.56
4:D:6:GLU:OE2	4:D:106:GLY:N	2.36	0.56
4:D:12:LYS:HE2	4:D:17:SER:O	2.05	0.56
2:F:16:CYS:HB2	2:F:28:TRP:CZ2	2.41	0.56
2:F:44:LEU:HD12	2:F:45:THR:N	2.21	0.56
1:I:122:LEU:HD11	4:L:54:LEU:HG	1.86	0.56
2:J:108:LEU:C	2:J:108:LEU:HD23	2.31	0.56
3:K:135:LEU:HD12	4:L:181:VAL:HG11	1.86	0.56
3:K:136:LEU:HD22	3:K:175:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:22:SER:HB2	5:Q:72:THR:HG22	1.87	0.56
2:B:69:LEU:HD22	2:B:69:LEU:C	2.31	0.56
1:E:104:MET:HA	1:E:217:TYR:OH	2.04	0.56
3:G:136:LEU:HD22	3:G:175:LEU:HB3	1.87	0.56
4:H:12:LYS:HE2	4:H:17:SER:O	2.05	0.56
1:I:279:ASN:HD22	1:I:282:LYS:HD3	1.69	0.56
4:L:51:ILE:O	4:L:51:ILE:HG23	2.04	0.56
2:B:108:LEU:C	2:B:108:LEU:HD23	2.31	0.56
4:H:92:CYS:O	4:H:104:GLY:N	2.38	0.56
3:C:94:TRP:HA	3:C:95:PRO:O	2.05	0.56
3:C:135:LEU:C	3:C:136:LEU:HD12	2.29	0.56
3:G:135:LEU:HD12	4:H:181:VAL:HG11	1.86	0.56
2:J:26:PHE:CE2	2:J:67:PHE:HB3	2.41	0.56
2:J:76:ILE:HD12	2:J:76:ILE:N	2.19	0.56
2:B:76:ILE:HD12	2:B:76:ILE:N	2.19	0.56
4:H:193:THR:HB	4:H:210:LYS:HE2	1.86	0.56
1:I:279:ASN:HD22	1:I:282:LYS:CD	2.19	0.56
2:J:70:ILE:HD12	2:J:70:ILE:N	2.21	0.56
1:A:273:ARG:HG2	1:A:273:ARG:NH1	2.20	0.56
2:B:44:LEU:HD12	2:B:45:THR:N	2.21	0.56
2:B:70:ILE:HD12	2:B:70:ILE:N	2.21	0.56
1:E:279:ASN:HD22	1:E:282:LYS:CD	2.19	0.56
2:F:26:PHE:CE2	2:F:67:PHE:HB3	2.41	0.56
2:F:108:LEU:HD23	2:F:108:LEU:C	2.31	0.56
1:I:108:ILE:HD12	1:I:253:PRO:CB	2.35	0.56
3:K:135:LEU:C	3:K:136:LEU:HD12	2.29	0.56
4:L:52:ILE:HG23	4:L:100(E):TYR:CZ	2.41	0.56
1:A:394:ASN:O	1:A:396:THR:N	2.37	0.56
3:C:15:PRO:HD3	3:C:106:ILE:HG22	1.88	0.56
4:H:41:PRO:C	4:H:43:GLN:H	2.14	0.56
4:H:52:ILE:HG23	4:H:100(E):TYR:CZ	2.41	0.56
4:H:126:PRO:HG3	4:H:138:LEU:CB	2.35	0.56
4:L:168:ALA:HA	4:L:178:LEU:HB3	1.88	0.56
2:B:26:PHE:CE2	2:B:67:PHE:HB3	2.41	0.56
1:E:122:LEU:HD11	4:H:54:LEU:HG	1.86	0.56
3:K:198:HIS:CD2	3:K:199:GLN:N	2.72	0.56
4:L:41:PRO:C	4:L:43:GLN:H	2.14	0.56
4:D:52:ILE:HG23	4:D:100(E):TYR:CZ	2.41	0.55
4:H:27:ASP:CG	4:H:28:THR:H	2.14	0.55
2:J:16:CYS:HB2	2:J:28:TRP:CZ2	2.41	0.55
1:E:100:MET:HE2	1:E:487:LYS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:8:PRO:O	3:G:102:THR:HG23	2.05	0.55
2:J:44:LEU:HD12	2:J:45:THR:N	2.21	0.55
3:C:135:LEU:HD11	4:D:181:VAL:HG21	1.88	0.55
3:C:198:HIS:CD2	3:C:199:GLN:N	2.72	0.55
1:E:254:VAL:HG11	1:E:261:LEU:HB2	1.89	0.55
2:F:69:LEU:C	2:F:69:LEU:HD22	2.31	0.55
1:I:371:ILE:HD11	1:I:473:GLY:HA3	1.89	0.55
3:K:135:LEU:HD11	4:L:181:VAL:HG21	1.89	0.55
4:L:12:LYS:HE2	4:L:17:SER:O	2.05	0.55
2:B:76:ILE:H	2:B:76:ILE:CD1	2.14	0.55
4:D:168:ALA:HA	4:D:178:LEU:HB3	1.88	0.55
2:F:76:ILE:HA	2:F:97:VAL:HB	1.89	0.55
2:J:69:LEU:C	2:J:69:LEU:HD22	2.31	0.55
4:L:27:ASP:CG	4:L:28:THR:H	2.14	0.55
1:A:100:MET:HE2	1:A:487:LYS:HA	1.88	0.55
2:B:103:ASN:N	2:B:103:ASN:ND2	2.55	0.55
2:J:76:ILE:HA	2:J:97:VAL:HB	1.89	0.55
3:K:176:SER:HB2	4:L:166:PHE:CE2	2.42	0.55
2:F:70:ILE:N	2:F:70:ILE:HD12	2.21	0.55
4:H:146:PHE:CG	4:H:147:PRO:HA	2.42	0.55
1:I:254:VAL:HG11	1:I:261:LEU:HB2	1.89	0.55
2:J:138:ILE:HD13	2:J:146:VAL:HG22	1.88	0.55
4:L:146:PHE:CG	4:L:147:PRO:HA	2.42	0.55
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.89	0.55
1:A:279:ASN:HD22	1:A:282:LYS:CD	2.19	0.55
2:B:138:ILE:HD13	2:B:146:VAL:HG22	1.88	0.55
4:D:41:PRO:C	4:D:43:GLN:H	2.14	0.55
4:H:97:GLU:OE1	4:H:97:GLU:HA	2.07	0.55
5:O:22:SER:HB2	5:O:72:THR:HG22	1.88	0.55
1:A:371:ILE:HD11	1:A:473:GLY:HA3	1.88	0.55
4:D:5:VAL:O	4:D:22:CYS:HA	2.07	0.55
4:D:67:VAL:HG22	4:D:68:THR:N	2.22	0.55
3:G:135:LEU:HD11	4:H:181:VAL:HG21	1.89	0.55
3:G:176:SER:HB2	4:H:166:PHE:CE2	2.42	0.55
1:I:394:ASN:O	1:I:396:THR:N	2.37	0.55
2:F:36:ILE:HD13	2:F:49:SER:CB	2.37	0.55
4:H:82(B):ASN:N	4:H:82(B):ASN:ND2	2.55	0.55
2:J:108:LEU:HD23	2:J:109:LEU:N	2.22	0.55
1:I:129:ALA:O	1:I:195:SER:N	2.40	0.55
3:K:192:TYR:HB2	3:K:209:PHE:CE1	2.42	0.55
5:M:22:SER:HB2	5:M:72:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:ALA:O	1:E:195:SER:N	2.40	0.54
4:H:154:TRP:CZ2	4:H:196:CYS:HB3	2.42	0.54
2:J:132:SER:HB3	2:J:136:LYS:HB2	1.89	0.54
4:H:5:VAL:O	4:H:22:CYS:HA	2.07	0.54
1:I:100:MET:HE2	1:I:487:LYS:HA	1.88	0.54
2:B:164:ASN:C	2:B:166:LYS:H	2.15	0.54
4:D:146:PHE:CG	4:D:147:PRO:HA	2.42	0.54
1:A:129:ALA:O	1:A:195:SER:N	2.40	0.54
2:B:76:ILE:HA	2:B:97:VAL:HB	1.89	0.54
3:C:116:PHE:CE2	4:D:137:ALA:HB3	2.43	0.54
2:F:138:ILE:HD13	2:F:146:VAL:HG22	1.88	0.54
3:G:192:TYR:HB2	3:G:209:PHE:CE1	2.42	0.54
1:A:105:HIS:O	1:A:109:ILE:HG13	2.08	0.54
2:B:36:ILE:HD13	2:B:49:SER:CB	2.37	0.54
2:B:108:LEU:HD23	2:B:109:LEU:N	2.22	0.54
3:C:176:SER:HB2	4:D:166:PHE:CE2	2.42	0.54
3:C:192:TYR:HB2	3:C:209:PHE:CE1	2.42	0.54
1:E:100:MET:HE1	1:E:486:TYR:C	2.33	0.54
2:F:132:SER:HB3	2:F:136:LYS:HB2	1.89	0.54
3:K:15:PRO:HD3	3:K:106:ILE:HG22	1.88	0.54
3:K:163:VAL:HG12	3:K:164:THR:N	2.23	0.54
4:L:5:VAL:O	4:L:22:CYS:HA	2.07	0.54
4:L:16:SER:OG	4:L:17:SER:N	2.40	0.54
4:L:82(B):ASN:N	4:L:82(B):ASN:ND2	2.55	0.54
4:L:93:ALA:HB3	4:L:100(K):LEU:HD13	1.90	0.54
1:A:118:PRO:HG3	1:A:435:TYR:CZ	2.42	0.54
3:C:135:LEU:CD1	4:D:181:VAL:HG21	2.37	0.54
2:F:103:ASN:N	2:F:103:ASN:ND2	2.55	0.54
3:G:21:LEU:HD12	3:G:21:LEU:N	2.23	0.54
4:L:154:TRP:CZ2	4:L:196:CYS:HB3	2.42	0.54
1:E:105:HIS:O	1:E:109:ILE:HG13	2.08	0.54
1:E:273:ARG:HG2	1:E:273:ARG:NH1	2.20	0.54
1:I:118:PRO:HG3	1:I:435:TYR:CZ	2.42	0.54
2:B:178:ALA:CB	2:B:180:GLN:HA	2.38	0.54
4:D:27:ASP:CG	4:D:28:THR:H	2.15	0.54
1:E:371:ILE:HD11	1:E:473:GLY:HA3	1.88	0.54
3:G:116:PHE:CE2	4:H:137:ALA:HB3	2.43	0.54
3:G:135:LEU:CD1	4:H:181:VAL:HG21	2.37	0.54
4:H:212:GLU:O	4:H:214:LYS:N	2.41	0.54
3:K:116:PHE:CE2	4:L:137:ALA:HB3	2.43	0.54
3:K:135:LEU:CD1	4:L:181:VAL:HG21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MET:HE1	1:A:486:TYR:C	2.33	0.54
4:D:154:TRP:CZ2	4:D:196:CYS:HB3	2.42	0.54
1:E:361:PHE:C	1:E:362:ASN:HD22	2.16	0.54
3:G:149:LYS:HA	3:G:153:ALA:O	2.08	0.54
1:I:361:PHE:C	1:I:362:ASN:HD22	2.16	0.54
2:J:178:ALA:CB	2:J:180:GLN:HA	2.38	0.54
3:K:3:VAL:N	3:K:26:SER:OG	2.35	0.54
1:A:452:LEU:HD12	1:A:452:LEU:N	2.23	0.54
2:B:54:ARG:O	2:B:72:LYS:NZ	2.40	0.54
2:F:108:LEU:HD23	2:F:109:LEU:N	2.22	0.54
2:F:176:VAL:CA	2:F:177:LEU:HD12	2.36	0.54
3:G:4:MET:HE3	3:G:23:CYS:SG	2.48	0.54
4:H:67:VAL:HG22	4:H:68:THR:N	2.22	0.54
2:J:36:ILE:HD13	2:J:49:SER:CB	2.37	0.54
2:J:103:ASN:N	2:J:103:ASN:ND2	2.55	0.54
3:K:29:VAL:CG1	3:K:90:GLN:HG2	2.38	0.54
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.90	0.53
1:E:118:PRO:HG3	1:E:435:TYR:CZ	2.42	0.53
7:E:894:NAG:H83	7:E:894:NAG:O3	2.08	0.53
3:G:15:PRO:HD3	3:G:106:ILE:HG22	1.88	0.53
1:I:349:LEU:HD22	1:I:468:PHE:CE2	2.44	0.53
3:K:106:ILE:HG13	3:K:166:GLN:HE21	1.73	0.53
1:A:349:LEU:HD22	1:A:468:PHE:CE2	2.44	0.53
7:A:894:NAG:H83	7:A:894:NAG:O3	2.08	0.53
3:C:21:LEU:N	3:C:21:LEU:HD12	2.22	0.53
3:G:106:ILE:HG13	3:G:166:GLN:HE21	1.73	0.53
1:I:105:HIS:O	1:I:109:ILE:HG13	2.08	0.53
1:I:452:LEU:HD12	1:I:452:LEU:N	2.23	0.53
2:J:164:ASN:C	2:J:166:LYS:H	2.15	0.53
3:C:163:VAL:HG12	3:C:164:THR:N	2.23	0.53
1:E:101:VAL:HG13	1:E:479:TRP:HB2	1.90	0.53
4:H:168:ALA:HA	4:H:178:LEU:HB3	1.89	0.53
2:J:54:ARG:O	2:J:72:LYS:NZ	2.40	0.53
3:K:149:LYS:HA	3:K:153:ALA:O	2.08	0.53
1:A:86:LEU:HA	1:A:243:SER:HB2	1.91	0.53
1:A:361:PHE:C	1:A:362:ASN:HD22	2.16	0.53
4:D:66:ARG:O	4:D:82:LEU:HD23	2.09	0.53
1:E:349:LEU:HD22	1:E:468:PHE:CE2	2.44	0.53
4:H:214:LYS:HD3	4:H:214:LYS:C	2.34	0.53
1:I:100:MET:HE1	1:I:486:TYR:C	2.33	0.53
3:K:21:LEU:N	3:K:21:LEU:HD12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.91	0.53
3:C:113:PRO:HD2	3:C:201:LEU:HG	1.91	0.53
4:D:93:ALA:HB3	4:D:100(K):LEU:HD13	1.90	0.53
2:F:164:ASN:C	2:F:166:LYS:H	2.15	0.53
2:F:178:ALA:CB	2:F:180:GLN:HA	2.38	0.53
3:G:29:VAL:CG1	3:G:90:GLN:HG2	2.39	0.53
3:K:113:PRO:HD2	3:K:201:LEU:HG	1.91	0.53
4:L:67:VAL:HG22	4:L:68:THR:N	2.22	0.53
4:L:97:GLU:OE1	4:L:97:GLU:HA	2.07	0.53
1:A:280:ASN:ND2	1:A:458:GLY:HA3	2.24	0.53
2:B:132:SER:HB3	2:B:136:LYS:HB2	1.89	0.53
1:E:371:ILE:CD1	1:E:473:GLY:HA3	2.39	0.53
1:E:452:LEU:HD12	1:E:452:LEU:N	2.23	0.53
1:E:474:ASP:O	1:E:476:ARG:N	2.42	0.53
3:G:150:VAL:O	3:G:153:ALA:HB3	2.09	0.53
3:G:150:VAL:HG13	3:G:192:TYR:CE1	2.44	0.53
1:A:242:VAL:CG2	1:A:243:SER:N	2.72	0.53
3:C:117:ILE:HD11	3:C:132:VAL:CG1	2.39	0.53
3:C:150:VAL:HG13	3:C:192:TYR:CE1	2.44	0.53
2:F:98:PHE:CD2	2:F:161:VAL:HG11	2.44	0.53
1:I:407:LEU:HB3	7:I:894:NAG:H81	1.91	0.53
7:I:894:NAG:H83	7:I:894:NAG:O3	2.08	0.53
3:K:4:MET:HE3	3:K:23:CYS:SG	2.48	0.53
3:K:150:VAL:HG13	3:K:192:TYR:CE1	2.44	0.53
1:A:395:ASP:OD1	1:A:395:ASP:O	2.27	0.53
3:C:124:GLN:HG3	4:D:122:PHE:CD2	2.44	0.53
3:C:149:LYS:HA	3:C:153:ALA:O	2.08	0.53
3:G:113:PRO:HD2	3:G:201:LEU:HG	1.91	0.53
4:H:66:ARG:O	4:H:82:LEU:HD23	2.09	0.53
1:I:474:ASP:O	1:I:476:ARG:N	2.42	0.53
2:J:98:PHE:CD2	2:J:161:VAL:HG11	2.44	0.53
3:K:117:ILE:HD11	3:K:132:VAL:CG1	2.39	0.53
4:L:214:LYS:HD3	4:L:214:LYS:C	2.34	0.53
1:A:474:ASP:O	1:A:476:ARG:N	2.42	0.53
4:D:82(B):ASN:N	4:D:82(B):ASN:ND2	2.55	0.53
4:D:214:LYS:HD3	4:D:214:LYS:C	2.34	0.53
1:E:120:VAL:HA	1:E:201:ILE:O	2.09	0.53
1:E:124:PRO:CB	2:F:60:SER:HA	2.39	0.53
1:E:395:ASP:OD1	1:E:395:ASP:O	2.27	0.53
1:I:219:ALA:HB2	1:I:225:ILE:HG13	1.91	0.53
1:I:395:ASP:OD1	1:I:395:ASP:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:66:ARG:O	4:L:82:LEU:HD23	2.09	0.53
6:R:6:GLN:HB3	6:R:107:THR:HG22	1.91	0.53
3:C:106:ILE:HG13	3:C:166:GLN:HE21	1.73	0.52
3:C:150:VAL:O	3:C:153:ALA:HB3	2.09	0.52
2:J:10:ASP:O	2:J:74:LEU:HB2	2.09	0.52
4:L:29:PHE:CE2	4:L:52(A):THR:HG21	2.44	0.52
1:A:120:VAL:HA	1:A:201:ILE:O	2.09	0.52
2:B:176:VAL:CA	2:B:177:LEU:HD12	2.36	0.52
4:D:97:GLU:OE1	4:D:97:GLU:HA	2.07	0.52
3:G:117:ILE:HD11	3:G:132:VAL:CG1	2.39	0.52
1:I:242:VAL:CG2	1:I:243:SER:N	2.72	0.52
4:L:35:THR:HG23	4:L:49:GLY:O	2.09	0.52
1:A:124:PRO:CB	2:B:60:SER:HA	2.39	0.52
4:D:85:ASP:OD1	4:D:85:ASP:N	2.41	0.52
3:G:115:VAL:HG22	3:G:196:VAL:HG21	1.90	0.52
4:H:139:GLY:HA2	4:H:154:TRP:CH2	2.44	0.52
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.90	0.52
1:I:120:VAL:HA	1:I:201:ILE:O	2.09	0.52
3:K:124:GLN:HG3	4:L:122:PHE:CD2	2.44	0.52
3:K:143:GLU:N	3:K:143:GLU:OE1	2.38	0.52
4:L:212:GLU:O	4:L:214:LYS:N	2.41	0.52
1:A:257:THR:HG22	1:A:475:MET:HE1	1.90	0.52
1:A:457:ASP:OD2	1:A:469:ARG:NE	2.39	0.52
2:B:98:PHE:CD2	2:B:161:VAL:HG11	2.44	0.52
4:D:139:GLY:HA2	4:D:154:TRP:CH2	2.45	0.52
1:E:100:MET:HE1	1:E:486:TYR:HB3	1.92	0.52
1:E:221:ALA:C	1:E:223:PHE:H	2.17	0.52
1:E:257:THR:HG22	1:E:475:MET:HE1	1.90	0.52
1:E:269:GLU:HA	7:E:789:NAG:C1	2.40	0.52
4:H:93:ALA:HB3	4:H:100(K):LEU:HD13	1.90	0.52
4:D:35:THR:HG23	4:D:49:GLY:O	2.09	0.52
1:E:120:VAL:CG1	1:E:434:MET:HB3	2.40	0.52
1:E:407:LEU:HB3	7:E:894:NAG:H81	1.91	0.52
2:F:154:SER:HB2	2:F:176:VAL:CG2	2.39	0.52
3:G:163:VAL:HG12	3:G:164:THR:N	2.23	0.52
4:H:2:VAL:HG13	4:H:27:ASP:HB3	1.91	0.52
1:I:257:THR:HG22	1:I:475:MET:HE1	1.90	0.52
1:I:269:GLU:HA	7:I:789:NAG:C1	2.39	0.52
1:I:280:ASN:ND2	1:I:458:GLY:HA3	2.24	0.52
2:J:176:VAL:CA	2:J:177:LEU:HD12	2.36	0.52
3:K:150:VAL:O	3:K:153:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:ND2	1:A:458:GLY:CA	2.73	0.52
2:B:10:ASP:O	2:B:74:LEU:HB2	2.09	0.52
3:C:29:VAL:CG1	3:C:90:GLN:HG2	2.38	0.52
4:D:29:PHE:CE2	4:D:52(A):THR:HG21	2.44	0.52
1:E:394:ASN:O	1:E:396:THR:N	2.37	0.52
2:F:10:ASP:O	2:F:74:LEU:HB2	2.09	0.52
3:G:124:GLN:HG3	4:H:122:PHE:CD2	2.44	0.52
4:H:16:SER:OG	4:H:17:SER:N	2.40	0.52
1:I:86:LEU:HA	1:I:243:SER:HB2	1.91	0.52
1:I:120:VAL:CG1	1:I:434:MET:HB3	2.40	0.52
3:K:136:LEU:HB2	3:K:175:LEU:HB3	1.92	0.52
1:A:269:GLU:HA	7:A:789:NAG:C1	2.40	0.52
1:A:407:LEU:HB3	7:A:894:NAG:H81	1.90	0.52
3:C:4:MET:HE3	3:C:23:CYS:SG	2.48	0.52
3:C:33:LEU:HD22	3:C:89:GLN:O	2.10	0.52
1:E:242:VAL:CG2	1:E:243:SER:N	2.72	0.52
3:G:3:VAL:N	3:G:26:SER:OG	2.35	0.52
3:G:48:ILE:CD1	3:G:54:ARG:HG2	2.40	0.52
1:I:124:PRO:CB	2:J:60:SER:HA	2.39	0.52
1:A:95:MET:HE3	1:A:234:ASN:O	2.10	0.52
4:D:189:LEU:HD23	4:D:194:TYR:HE2	1.75	0.52
1:E:95:MET:HE3	1:E:234:ASN:O	2.10	0.52
1:E:219:ALA:HB2	1:E:225:ILE:HG13	1.91	0.52
1:E:353:PHE:CZ	1:E:456:ARG:HD3	2.45	0.52
1:I:95:MET:HE3	1:I:234:ASN:O	2.10	0.52
1:I:353:PHE:CZ	1:I:456:ARG:HD3	2.45	0.52
1:I:371:ILE:CD1	1:I:473:GLY:HA3	2.39	0.52
4:D:92:CYS:O	4:D:104:GLY:N	2.38	0.52
3:G:118:PHE:CD2	4:H:124:LEU:HD23	2.45	0.52
3:G:142:ARG:CG	3:G:163:VAL:HG11	2.40	0.52
4:H:35:THR:HG23	4:H:49:GLY:O	2.10	0.52
3:C:115:VAL:HG22	3:C:196:VAL:HG21	1.90	0.52
3:C:142:ARG:CG	3:C:163:VAL:HG11	2.40	0.52
1:E:280:ASN:ND2	1:E:458:GLY:HA3	2.24	0.52
1:I:385:CYS:HA	1:I:418:CYS:HA	1.92	0.52
3:K:48:ILE:CD1	3:K:54:ARG:HG2	2.40	0.52
3:K:115:VAL:HG22	3:K:196:VAL:HG21	1.90	0.52
3:K:118:PHE:CD2	4:L:124:LEU:HD23	2.45	0.52
3:C:48:ILE:CD1	3:C:54:ARG:HG2	2.40	0.51
3:C:118:PHE:CD2	4:D:124:LEU:HD23	2.45	0.51
2:J:154:SER:HB2	2:J:176:VAL:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MET:HE1	1:A:486:TYR:HB3	1.92	0.51
1:A:353:PHE:CZ	1:A:456:ARG:HD3	2.45	0.51
1:A:371:ILE:CD1	1:A:473:GLY:HA3	2.39	0.51
4:D:2:VAL:HG13	4:D:27:ASP:HB3	1.91	0.51
3:G:33:LEU:HD22	3:G:89:GLN:O	2.10	0.51
3:G:183:LYS:HD3	3:G:183:LYS:C	2.35	0.51
1:I:280:ASN:ND2	1:I:458:GLY:CA	2.73	0.51
1:A:86:LEU:HA	1:A:243:SER:HB3	1.92	0.51
1:A:221:ALA:C	1:A:223:PHE:H	2.17	0.51
3:C:183:LYS:C	3:C:183:LYS:HD3	2.35	0.51
1:E:346:ALA:O	1:E:350:LYS:HG2	2.10	0.51
3:G:143:GLU:N	3:G:143:GLU:OE1	2.38	0.51
4:H:29:PHE:CE2	4:H:52(A):THR:HG21	2.44	0.51
3:K:33:LEU:HD22	3:K:89:GLN:O	2.10	0.51
6:R:35:VAL:HB	6:R:51:ILE:HG22	1.93	0.51
1:A:346:ALA:O	1:A:350:LYS:HG2	2.10	0.51
1:E:295:ASN:O	1:E:331:CYS:HA	2.10	0.51
3:G:186:TYR:O	3:G:192:TYR:OH	2.29	0.51
4:H:135:THR:HG22	4:H:185:PRO:CA	2.41	0.51
1:I:295:ASN:O	1:I:331:CYS:HA	2.10	0.51
3:K:175:LEU:CD1	3:K:176:SER:H	2.23	0.51
3:K:183:LYS:C	3:K:183:LYS:HD3	2.35	0.51
2:F:100:LEU:HD12	2:F:170:PHE:CB	2.41	0.51
3:G:78:LEU:HD23	3:G:79:GLN:N	2.26	0.51
3:G:136:LEU:HB2	3:G:175:LEU:HB3	1.92	0.51
2:J:26:PHE:CZ	2:J:67:PHE:HB3	2.46	0.51
2:J:76:ILE:HG12	2:J:119:GLU:OE2	2.11	0.51
4:L:5:VAL:O	4:L:23:LYS:N	2.43	0.51
4:L:139:GLY:HA2	4:L:154:TRP:CH2	2.44	0.51
4:L:189:LEU:HD23	4:L:194:TYR:HE2	1.75	0.51
1:A:95:MET:HA	1:A:98:ASN:HB2	1.93	0.51
1:A:120:VAL:CG1	1:A:434:MET:HB3	2.40	0.51
3:C:175:LEU:CD1	3:C:176:SER:H	2.23	0.51
4:D:16:SER:OG	4:D:17:SER:N	2.39	0.51
1:I:457:ASP:HB3	2:J:48:PRO:HG2	1.93	0.51
3:K:142:ARG:CG	3:K:163:VAL:HG11	2.40	0.51
4:D:66:ARG:HH11	4:D:66:ARG:HB2	1.76	0.51
1:E:86:LEU:HA	1:E:243:SER:HB3	1.92	0.51
4:H:12:LYS:HG3	4:H:18:VAL:HB	1.93	0.51
4:L:12:LYS:HG3	4:L:18:VAL:HB	1.93	0.51
2:B:76:ILE:HG12	2:B:119:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:135:THR:HG22	4:D:185:PRO:CA	2.41	0.51
4:D:141:LEU:HD12	4:D:179:SER:HG	1.75	0.51
1:E:86:LEU:HA	1:E:243:SER:HB2	1.91	0.51
1:E:457:ASP:HB3	2:F:48:PRO:HG2	1.93	0.51
2:J:79:SER:O	2:J:80:ASP:HB2	2.10	0.51
4:L:2:VAL:HG13	4:L:27:ASP:HB3	1.91	0.51
4:L:40:ALA:O	4:L:43:GLN:HB2	2.11	0.51
4:L:92:CYS:O	4:L:104:GLY:N	2.38	0.51
2:B:154:SER:HB2	2:B:176:VAL:N	2.25	0.51
3:C:136:LEU:HB2	3:C:175:LEU:HB3	1.92	0.51
4:H:40:ALA:O	4:H:43:GLN:HB2	2.11	0.51
1:I:95:MET:HA	1:I:98:ASN:HB2	1.93	0.51
1:I:100:MET:HE1	1:I:486:TYR:HB3	1.92	0.51
1:I:346:ALA:O	1:I:350:LYS:HG2	2.10	0.51
1:A:252:ARG:O	1:A:254:VAL:N	2.44	0.51
1:A:357:LYS:HG3	1:A:464:GLY:CA	2.41	0.51
4:D:212:GLU:O	4:D:214:LYS:N	2.41	0.51
4:H:189:LEU:HD23	4:H:194:TYR:HE2	1.75	0.51
4:L:77:THR:HG22	4:L:78:VAL:N	2.26	0.51
2:B:100:LEU:HD12	2:B:170:PHE:CB	2.41	0.50
3:C:3:VAL:N	3:C:26:SER:OG	2.34	0.50
4:D:36:TRP:CD2	4:D:80:LEU:HB2	2.46	0.50
4:H:66:ARG:HB2	4:H:66:ARG:HH11	1.76	0.50
4:H:77:THR:HG22	4:H:78:VAL:N	2.26	0.50
1:I:357:LYS:HG3	1:I:464:GLY:CA	2.41	0.50
1:I:222:GLY:HA2	1:I:491:ILE:CG2	2.42	0.50
6:N:35:VAL:HB	6:N:51:ILE:HG22	1.92	0.50
6:N:195:ILE:HG12	6:N:210:ARG:CA	2.41	0.50
6:P:6:GLN:HB3	6:P:107:THR:HG22	1.91	0.50
1:A:295:ASN:O	1:A:331:CYS:HA	2.10	0.50
1:E:249:HIS:O	1:E:251:ILE:HG13	2.12	0.50
1:E:280:ASN:ND2	1:E:458:GLY:CA	2.73	0.50
1:E:343:GLU:C	1:E:345:ILE:H	2.19	0.50
3:G:175:LEU:CD1	3:G:176:SER:H	2.23	0.50
1:I:86:LEU:HA	1:I:243:SER:HB3	1.92	0.50
6:N:6:GLN:HB3	6:N:107:THR:HG22	1.91	0.50
6:P:35:VAL:HB	6:P:51:ILE:HG22	1.92	0.50
6:P:195:ILE:HG12	6:P:210:ARG:CA	2.41	0.50
5:Q:22:SER:HA	5:Q:72:THR:HG22	1.94	0.50
6:R:195:ILE:HG12	6:R:210:ARG:CA	2.41	0.50
3:C:115:VAL:CG2	3:C:196:VAL:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:138:ASN:OD1	3:K:138:ASN:N	2.44	0.50
5:M:22:SER:HA	5:M:72:THR:HG22	1.94	0.50
3:K:169:LYS:HA	3:K:169:LYS:HE3	1.94	0.50
3:K:186:TYR:O	3:K:192:TYR:OH	2.29	0.50
4:L:135:THR:HG22	4:L:185:PRO:CA	2.41	0.50
1:A:86:LEU:HD11	7:A:741:NAG:O7	2.12	0.50
2:B:154:SER:HB2	2:B:176:VAL:CG2	2.39	0.50
2:B:161:VAL:HB	2:B:168:VAL:HG22	1.94	0.50
4:D:40:ALA:O	4:D:43:GLN:HB2	2.11	0.50
1:E:357:LYS:HG3	1:E:464:GLY:CA	2.41	0.50
1:E:385:CYS:HA	1:E:418:CYS:HA	1.92	0.50
1:I:360:ILE:HG22	1:I:361:PHE:N	2.27	0.50
1:E:121:LYS:HZ1	1:E:426:MET:HE1	1.76	0.50
1:E:457:ASP:OD2	1:E:469:ARG:NE	2.39	0.50
3:G:115:VAL:CG2	3:G:196:VAL:HG21	2.42	0.50
4:H:6:GLU:OE2	4:H:106:GLY:N	2.36	0.50
1:I:100:MET:CG	1:I:488:VAL:HG12	2.42	0.50
1:I:249:HIS:O	1:I:251:ILE:HG13	2.12	0.50
1:I:252:ARG:O	1:I:254:VAL:N	2.44	0.50
3:K:115:VAL:CG2	3:K:196:VAL:HG21	2.42	0.50
3:C:78:LEU:HD23	3:C:79:GLN:N	2.26	0.50
3:C:169:LYS:HA	3:C:169:LYS:HE3	1.94	0.50
4:D:39:GLN:NE2	4:D:44:GLY:HA2	2.23	0.50
2:F:5:LEU:HD22	2:F:96:LEU:HB2	1.94	0.50
2:F:26:PHE:CZ	2:F:67:PHE:HB3	2.46	0.50
3:G:46:LEU:HD13	4:H:101:LYS:HD2	1.94	0.50
4:H:36:TRP:CD2	4:H:80:LEU:HB2	2.47	0.50
4:H:52:ILE:HG23	4:H:100(E):TYR:OH	2.12	0.50
4:H:85:ASP:OD1	4:H:85:ASP:N	2.41	0.50
4:L:36:TRP:CD2	4:L:80:LEU:HB2	2.46	0.50
6:R:40:ALA:O	6:R:43:GLN:HB2	2.12	0.50
2:B:26:PHE:CZ	2:B:67:PHE:HB3	2.46	0.50
3:C:33:LEU:HD13	3:C:33:LEU:C	2.37	0.50
4:D:52:ILE:HG23	4:D:100(E):TYR:OH	2.12	0.50
4:D:147:PRO:HG2	4:D:148:GLU:H	1.77	0.50
1:E:95:MET:HA	1:E:98:ASN:HB2	1.93	0.50
1:E:222:GLY:HA2	1:E:491:ILE:CG2	2.42	0.50
1:E:252:ARG:O	1:E:254:VAL:N	2.44	0.50
2:J:161:VAL:HB	2:J:168:VAL:HG22	1.94	0.50
3:K:33:LEU:HD13	3:K:33:LEU:C	2.37	0.50
4:L:66:ARG:HH11	4:L:66:ARG:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:22:SER:HA	5:O:72:THR:HG22	1.94	0.50
1:A:222:GLY:HA2	1:A:491:ILE:CG2	2.42	0.49
1:A:385:CYS:HA	1:A:418:CYS:HA	1.92	0.49
4:D:12:LYS:HG3	4:D:18:VAL:HB	1.93	0.49
2:F:79:SER:O	2:F:80:ASP:HB2	2.11	0.49
2:F:108:LEU:C	2:F:177:LEU:HD13	2.36	0.49
1:I:86:LEU:HD11	7:I:741:NAG:O7	2.12	0.49
1:I:360:ILE:CG2	1:I:361:PHE:N	2.75	0.49
1:I:411:GLY:O	7:I:908:NAG:O6	2.30	0.49
3:K:78:LEU:HD23	3:K:79:GLN:N	2.26	0.49
4:L:147:PRO:HG2	4:L:148:GLU:H	1.77	0.49
2:B:114:LEU:C	2:B:114:LEU:HD13	2.38	0.49
4:D:77:THR:HG22	4:D:78:VAL:N	2.26	0.49
6:P:40:ALA:O	6:P:43:GLN:HB2	2.12	0.49
5:Q:54:LEU:HD21	5:Q:60:SER:HA	1.94	0.49
2:B:5:LEU:HD22	2:B:96:LEU:HB2	1.94	0.49
3:C:19:ALA:HB1	3:C:104:LEU:HD11	1.95	0.49
1:E:360:ILE:CG2	1:E:361:PHE:N	2.75	0.49
2:F:76:ILE:HG12	2:F:119:GLU:OE2	2.11	0.49
2:J:5:LEU:HD22	2:J:96:LEU:HB2	1.94	0.49
2:J:100:LEU:HD12	2:J:170:PHE:CB	2.41	0.49
2:J:146:VAL:O	2:J:147:SER:C	2.56	0.49
2:B:79:SER:O	2:B:80:ASP:HB2	2.10	0.49
2:B:166:LYS:C	2:B:167:LYS:HD3	2.38	0.49
1:E:360:ILE:HG22	1:E:361:PHE:N	2.27	0.49
4:H:182:VAL:O	4:H:182:VAL:HG13	2.12	0.49
1:I:221:ALA:C	1:I:223:PHE:H	2.17	0.49
1:I:343:GLU:C	1:I:345:ILE:H	2.20	0.49
4:L:52:ILE:HG23	4:L:100(E):TYR:OH	2.12	0.49
1:A:457:ASP:HB3	2:B:48:PRO:HG2	1.93	0.49
2:B:146:VAL:O	2:B:147:SER:C	2.56	0.49
2:F:54:ARG:O	2:F:72:LYS:NZ	2.40	0.49
2:F:166:LYS:C	2:F:167:LYS:HD3	2.38	0.49
3:G:47:LEU:HD11	3:G:86:TYR:CE1	2.48	0.49
2:J:154:SER:HB2	2:J:176:VAL:N	2.25	0.49
3:K:47:LEU:HD11	3:K:86:TYR:CE1	2.48	0.49
1:A:100:MET:CG	1:A:488:VAL:HG12	2.42	0.49
1:A:343:GLU:C	1:A:345:ILE:H	2.19	0.49
1:A:344:GLN:HG2	7:A:789:NAG:C8	2.43	0.49
4:H:147:PRO:HG2	4:H:148:GLU:H	1.78	0.49
1:I:344:GLN:HG2	7:I:789:NAG:C8	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:193:ALA:HB1	3:K:206:THR:HG23	1.94	0.49
3:C:186:TYR:O	3:C:192:TYR:OH	2.29	0.49
2:F:161:VAL:HB	2:F:168:VAL:HG22	1.93	0.49
3:G:19:ALA:HB1	3:G:104:LEU:HD11	1.95	0.49
3:G:33:LEU:C	3:G:33:LEU:HD13	2.37	0.49
1:I:221:ALA:C	1:I:223:PHE:N	2.71	0.49
1:I:292:VAL:HG12	1:I:333:LEU:HD11	1.95	0.49
1:I:457:ASP:OD2	1:I:469:ARG:NE	2.38	0.49
2:J:2:LYS:CD	2:J:3:VAL:H	2.26	0.49
2:J:108:LEU:C	2:J:177:LEU:HD13	2.36	0.49
2:J:114:LEU:C	2:J:114:LEU:HD13	2.38	0.49
1:A:95:MET:CE	1:A:235:GLY:HA3	2.43	0.49
1:A:360:ILE:CG2	1:A:361:PHE:N	2.75	0.49
1:A:360:ILE:HG22	1:A:361:PHE:N	2.27	0.49
2:B:2:LYS:CD	2:B:3:VAL:H	2.26	0.49
3:C:46:LEU:HD13	4:D:101:LYS:HD2	1.94	0.49
3:C:138:ASN:OD1	3:C:138:ASN:N	2.45	0.49
1:E:292:VAL:HG12	1:E:333:LEU:HD11	1.95	0.49
2:F:77:GLU:OE1	2:F:77:GLU:N	2.45	0.49
2:F:146:VAL:O	2:F:147:SER:C	2.56	0.49
3:G:66:GLY:HA3	3:G:71:PHE:HA	1.95	0.49
1:A:344:GLN:HG2	7:A:789:NAG:H83	1.95	0.49
2:B:178:ALA:HB3	2:B:180:GLN:HA	1.95	0.49
3:C:47:LEU:HD11	3:C:86:TYR:CE1	2.48	0.49
4:D:5:VAL:O	4:D:23:LYS:N	2.43	0.49
1:E:95:MET:CE	1:E:235:GLY:HA3	2.43	0.49
1:E:109:ILE:HG23	1:E:428:GLN:HG2	1.95	0.49
1:E:344:GLN:HG2	7:E:789:NAG:H83	1.95	0.49
4:H:66:ARG:HH11	4:H:66:ARG:CB	2.26	0.49
3:K:117:ILE:HD11	3:K:132:VAL:HG12	1.95	0.49
6:N:40:ALA:O	6:N:43:GLN:HB2	2.12	0.49
1:A:249:HIS:O	1:A:251:ILE:HG13	2.12	0.49
1:E:86:LEU:HD11	7:E:741:NAG:O7	2.12	0.49
1:E:414:ILE:HG22	1:E:416:LEU:HD13	1.95	0.49
3:G:169:LYS:HA	3:G:169:LYS:HE3	1.94	0.49
1:I:414:ILE:HG22	1:I:416:LEU:HD13	1.95	0.49
2:J:77:GLU:OE1	2:J:77:GLU:N	2.45	0.49
5:M:54:LEU:HD21	5:M:60:SER:HA	1.94	0.49
2:B:77:GLU:OE1	2:B:77:GLU:N	2.45	0.48
3:C:174:SER:O	4:D:166:PHE:HE2	1.96	0.48
4:D:66:ARG:HH11	4:D:66:ARG:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:VAL:HG13	4:D:182:VAL:O	2.12	0.48
1:E:104:MET:HE2	1:E:215:ILE:CD1	2.42	0.48
2:F:114:LEU:HD13	2:F:114:LEU:C	2.38	0.48
3:G:174:SER:O	4:H:166:PHE:HE2	1.96	0.48
1:A:279:ASN:C	1:A:281:ALA:H	2.22	0.48
1:A:292:VAL:HG12	1:A:333:LEU:HD11	1.95	0.48
1:E:100:MET:CG	1:E:488:VAL:HG12	2.42	0.48
2:F:178:ALA:HB3	2:F:180:GLN:HA	1.95	0.48
3:G:47:LEU:HD11	3:G:86:TYR:HE1	1.78	0.48
3:K:186:TYR:CE1	3:K:192:TYR:CE2	3.01	0.48
5:O:54:LEU:HD21	5:O:60:SER:HA	1.94	0.48
1:A:456:ARG:HD2	1:A:468:PHE:CZ	2.48	0.48
3:G:138:ASN:N	3:G:138:ASN:OD1	2.44	0.48
3:K:19:ALA:HB1	3:K:104:LEU:HD11	1.95	0.48
4:L:162:GLY:O	4:L:182:VAL:HG23	2.13	0.48
4:D:126:PRO:CG	4:D:138:LEU:HD13	2.43	0.48
4:D:162:GLY:O	4:D:182:VAL:HG23	2.13	0.48
1:E:344:GLN:HG2	7:E:789:NAG:C8	2.43	0.48
4:H:84:SER:HA	4:H:111:VAL:O	2.13	0.48
1:I:95:MET:CE	1:I:235:GLY:HA3	2.43	0.48
3:K:66:GLY:HA3	3:K:71:PHE:HA	1.95	0.48
3:K:105:GLU:HG2	3:K:106:ILE:N	2.27	0.48
4:L:84:SER:HA	4:L:111:VAL:O	2.14	0.48
3:C:193:ALA:HB1	3:C:206:THR:HG23	1.94	0.48
3:G:193:ALA:HB1	3:G:206:THR:HG23	1.94	0.48
4:H:5:VAL:O	4:H:23:LYS:N	2.43	0.48
2:J:150:GLU:HB3	2:J:152:GLN:CD	2.38	0.48
3:K:142:ARG:N	3:K:143:GLU:OE1	2.47	0.48
1:A:124:PRO:HB3	2:B:60:SER:HA	1.96	0.48
3:C:143:GLU:H	3:C:143:GLU:CD	2.21	0.48
2:F:154:SER:HB2	2:F:176:VAL:N	2.25	0.48
3:G:90:GLN:C	3:G:90:GLN:CD	2.82	0.48
3:G:142:ARG:N	3:G:143:GLU:OE1	2.47	0.48
4:H:162:GLY:O	4:H:182:VAL:HG23	2.13	0.48
1:I:344:GLN:HG2	7:I:789:NAG:H83	1.95	0.48
3:K:47:LEU:HD11	3:K:86:TYR:HE1	1.78	0.48
4:L:121:VAL:HG11	4:L:196:CYS:SG	2.54	0.48
1:A:121:LYS:HZ1	1:A:426:MET:HE1	1.74	0.48
3:C:66:GLY:HA3	3:C:71:PHE:HA	1.95	0.48
3:C:142:ARG:N	3:C:143:GLU:OE1	2.47	0.48
3:C:186:TYR:CE1	3:C:192:TYR:CE2	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:GLU:HG2	7:E:789:NAG:HN2	1.79	0.48
1:E:272:ILE:O	1:E:272:ILE:CG1	2.62	0.48
3:G:186:TYR:CE1	3:G:192:TYR:CE2	3.01	0.48
4:L:126:PRO:CG	4:L:138:LEU:HD13	2.43	0.48
4:L:182:VAL:HG13	4:L:182:VAL:O	2.12	0.48
1:A:414:ILE:HG22	1:A:416:LEU:HD13	1.95	0.48
2:B:10:ASP:OD1	2:B:11:THR:N	2.41	0.48
3:G:33:LEU:HG	3:G:71:PHE:CG	2.49	0.48
3:G:120:PRO:HD3	3:G:132:VAL:HG22	1.96	0.48
3:G:187:GLU:O	3:G:211:ARG:NH1	2.47	0.48
4:H:117:LYS:HG3	4:H:117:LYS:O	2.14	0.48
4:H:145:TYR:CD1	4:H:145:TYR:C	2.92	0.48
1:I:119:CYS:N	1:I:205:CYS:SG	2.87	0.48
2:J:166:LYS:C	2:J:167:LYS:HD3	2.38	0.48
4:L:65:GLY:O	4:L:82(A):ARG:NH1	2.47	0.48
3:C:24:ARG:HG3	3:C:24:ARG:HH11	1.78	0.48
3:C:33:LEU:HG	3:C:71:PHE:CG	2.49	0.48
4:D:66:ARG:HA	4:D:82(A):ARG:HH11	1.79	0.48
4:D:121:VAL:HG11	4:D:196:CYS:SG	2.54	0.48
2:F:151:LEU:HA	2:F:176:VAL:HG11	1.96	0.48
1:I:279:ASN:C	1:I:281:ALA:H	2.22	0.48
2:J:83:ILE:HG23	2:J:92:GLU:CG	2.44	0.48
2:J:160:THR:HG23	2:J:167:LYS:HB2	1.96	0.48
2:J:178:ALA:HB3	2:J:180:GLN:HA	1.95	0.48
3:K:24:ARG:HG3	3:K:24:ARG:HH11	1.78	0.48
3:K:33:LEU:HG	3:K:71:PHE:CG	2.49	0.48
3:K:141:PRO:HB3	3:K:143:GLU:CD	2.39	0.48
3:K:174:SER:O	4:L:166:PHE:HE2	1.96	0.48
3:K:187:GLU:O	3:K:211:ARG:NH1	2.47	0.48
6:N:35(A):ASN:O	6:N:93:THR:HB	2.13	0.48
1:A:411:GLY:O	7:A:908:NAG:O6	2.30	0.48
1:E:411:GLY:O	7:E:908:NAG:O6	2.30	0.48
1:E:456:ARG:HD2	1:E:468:PHE:CZ	2.48	0.48
4:H:121:VAL:HG11	4:H:196:CYS:SG	2.54	0.48
3:K:143:GLU:H	3:K:143:GLU:CD	2.21	0.48
4:L:23:LYS:NZ	4:L:75:THR:O	2.43	0.48
6:N:13:LYS:O	6:N:16:SER:OG	2.27	0.48
6:P:35(A):ASN:O	6:P:93:THR:HB	2.13	0.48
6:R:35(A):ASN:O	6:R:93:THR:HB	2.13	0.48
3:C:47:LEU:HD11	3:C:86:TYR:HE1	1.78	0.47
3:C:117:ILE:HD11	3:C:132:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:456:ARG:HD2	1:I:468:PHE:CZ	2.48	0.47
3:K:105:GLU:HG3	3:K:166:GLN:NE2	2.29	0.47
4:L:66:ARG:HA	4:L:82(A):ARG:HH11	1.79	0.47
1:A:102:GLU:OE1	1:A:476:ARG:NE	2.43	0.47
3:C:90:GLN:CD	3:C:90:GLN:C	2.82	0.47
3:C:105:GLU:HG3	3:C:166:GLN:NE2	2.29	0.47
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.96	0.47
1:E:119:CYS:N	1:E:205:CYS:SG	2.87	0.47
1:E:335:LYS:HD3	1:E:408:ASN:HA	1.96	0.47
3:G:91:TYR:O	3:G:91:TYR:CD1	2.67	0.47
3:G:137:ASN:ND2	3:G:138:ASN:OD1	2.48	0.47
3:G:141:PRO:HB3	3:G:143:GLU:CD	2.39	0.47
3:G:143:GLU:H	3:G:143:GLU:CD	2.21	0.47
3:K:46:LEU:HD13	4:L:101:LYS:HD2	1.94	0.47
1:A:119:CYS:N	1:A:205:CYS:SG	2.87	0.47
2:B:83:ILE:HA	2:B:92:GLU:HA	1.97	0.47
4:D:65:GLY:O	4:D:82(A):ARG:NH1	2.47	0.47
1:E:279:ASN:C	1:E:281:ALA:H	2.22	0.47
2:F:2:LYS:CD	2:F:3:VAL:H	2.26	0.47
2:F:83:ILE:HA	2:F:92:GLU:HA	1.97	0.47
4:H:65:GLY:O	4:H:82(A):ARG:NH1	2.47	0.47
4:H:66:ARG:HB2	4:H:66:ARG:NH1	2.29	0.47
4:L:38:ARG:HB3	4:L:90:TYR:CD2	2.49	0.47
4:L:66:ARG:HB2	4:L:66:ARG:NH1	2.29	0.47
4:L:117:LYS:HG3	4:L:117:LYS:O	2.14	0.47
4:L:145:TYR:CD1	4:L:145:TYR:C	2.92	0.47
3:C:137:ASN:ND2	3:C:138:ASN:OD1	2.47	0.47
3:C:187:GLU:O	3:C:211:ARG:NH1	2.47	0.47
1:E:105:HIS:HB2	1:E:479:TRP:CD1	2.49	0.47
2:F:178:ALA:C	2:F:179:PHE:HD1	2.17	0.47
3:G:117:ILE:HD11	3:G:132:VAL:HG12	1.95	0.47
1:I:269:GLU:HG2	7:I:789:NAG:HN2	1.79	0.47
2:J:151:LEU:HA	2:J:176:VAL:HG11	1.96	0.47
3:K:48:ILE:HG22	3:K:49:TYR:N	2.29	0.47
3:K:90:GLN:CD	3:K:90:GLN:C	2.82	0.47
4:L:66:ARG:HH11	4:L:66:ARG:CB	2.26	0.47
1:A:124:PRO:HG2	2:B:60:SER:HA	1.96	0.47
2:B:3:VAL:HG22	2:B:94:GLN:CB	2.44	0.47
2:B:178:ALA:HB1	2:B:180:GLN:N	2.26	0.47
3:C:83:PHE:O	3:C:84:ALA:HB2	2.15	0.47
1:E:100:MET:HG3	1:E:488:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ALA:C	1:E:223:PHE:N	2.71	0.47
2:F:130:CYS:CA	2:F:159:CYS:HA	2.34	0.47
2:F:150:GLU:HB3	2:F:152:GLN:CD	2.38	0.47
4:H:38:ARG:HB3	4:H:90:TYR:CD2	2.49	0.47
1:A:109:ILE:HG23	1:A:428:GLN:HG2	1.95	0.47
1:A:215:ILE:HG13	1:A:215:ILE:O	2.15	0.47
1:A:371:ILE:HD11	2:B:43:PHE:CD2	2.50	0.47
3:C:91:TYR:O	3:C:91:TYR:CD1	2.67	0.47
4:D:66:ARG:HB2	4:D:66:ARG:NH1	2.29	0.47
4:D:145:TYR:CD1	4:D:145:TYR:C	2.92	0.47
4:D:178:LEU:HD12	4:D:178:LEU:C	2.40	0.47
1:E:371:ILE:HD11	2:F:43:PHE:CD2	2.49	0.47
3:G:24:ARG:HH11	3:G:24:ARG:HG3	1.78	0.47
3:G:105:GLU:HG2	3:G:106:ILE:N	2.27	0.47
1:I:124:PRO:HG2	2:J:60:SER:HA	1.97	0.47
1:I:231:LYS:HB2	1:I:268:GLU:HB2	1.96	0.47
1:I:272:ILE:O	1:I:272:ILE:CG1	2.62	0.47
3:K:120:PRO:HD3	3:K:132:VAL:HG22	1.96	0.47
3:K:198:HIS:HD2	3:K:199:GLN:H	1.59	0.47
1:A:105:HIS:HB2	1:A:479:TRP:CD1	2.49	0.47
1:A:227:LYS:HE3	1:A:485:LYS:HE3	1.96	0.47
2:B:83:ILE:HG23	2:B:92:GLU:CG	2.44	0.47
3:C:141:PRO:HB3	3:C:143:GLU:CD	2.39	0.47
3:C:198:HIS:HD2	3:C:199:GLN:H	1.59	0.47
4:D:38:ARG:HB3	4:D:90:TYR:CD2	2.49	0.47
4:D:84:SER:HA	4:D:111:VAL:O	2.13	0.47
4:D:117:LYS:HG3	4:D:117:LYS:O	2.14	0.47
4:D:137:ALA:HA	4:D:183:THR:HA	1.97	0.47
1:E:227:LYS:HE3	1:E:485:LYS:HE3	1.96	0.47
1:E:381:GLU:HB3	1:E:420:ILE:HD13	1.96	0.47
2:F:28:TRP:HB2	2:F:37:LEU:HD23	1.97	0.47
3:G:48:ILE:HG22	3:G:49:TYR:N	2.29	0.47
3:G:91:TYR:HB2	4:H:100(I):GLY:HA3	1.97	0.47
3:G:105:GLU:HG3	3:G:166:GLN:NE2	2.29	0.47
3:G:133:VAL:CG2	4:H:141:LEU:HD13	2.45	0.47
4:H:178:LEU:C	4:H:178:LEU:HD12	2.40	0.47
1:I:109:ILE:HG23	1:I:428:GLN:HG2	1.95	0.47
1:I:119:CYS:HB3	3:K:94:TRP:NE1	2.30	0.47
1:I:256:SER:HB2	1:I:376:PHE:HB3	1.96	0.47
2:B:108:LEU:C	2:B:177:LEU:HD13	2.36	0.47
4:D:7:SER:HB3	4:D:21:SER:HG	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:GLU:HB3	1:E:269:GLU:H	1.51	0.47
1:E:350:LYS:C	1:E:352:GLN:H	2.23	0.47
2:F:178:ALA:HB1	2:F:180:GLN:N	2.25	0.47
4:H:66:ARG:HA	4:H:82(A):ARG:HH11	1.79	0.47
1:I:350:LYS:C	1:I:352:GLN:H	2.23	0.47
3:K:137:ASN:ND2	3:K:138:ASN:OD1	2.48	0.47
4:L:189:LEU:HB3	4:L:213:PRO:CG	2.45	0.47
6:P:81:GLU:CD	6:P:82(A):LYS:HE2	2.40	0.47
6:R:38:ARG:HB3	6:R:48:ILE:HD11	1.97	0.47
6:R:81:GLU:CD	6:R:82(A):LYS:HE2	2.40	0.47
1:A:104:MET:HE2	1:A:215:ILE:CD1	2.42	0.47
1:A:272:ILE:O	1:A:272:ILE:CG1	2.62	0.47
1:A:335:LYS:HD3	1:A:408:ASN:HA	1.96	0.47
3:C:114:SER:O	3:C:116:PHE:CD1	2.68	0.47
4:D:189:LEU:HB3	4:D:213:PRO:CG	2.45	0.47
1:E:119:CYS:HB3	3:G:94:TRP:NE1	2.30	0.47
2:F:100:LEU:HB2	2:F:170:PHE:CD1	2.50	0.47
2:F:108:LEU:O	2:F:109:LEU:O	2.33	0.47
3:G:114:SER:O	3:G:116:PHE:CD1	2.68	0.47
1:I:102:GLU:OE1	1:I:476:ARG:NE	2.43	0.47
1:I:105:HIS:HB2	1:I:479:TRP:CD1	2.49	0.47
1:I:227:LYS:HE3	1:I:485:LYS:HE3	1.96	0.47
1:I:259:LEU:HB2	1:I:374:HIS:CE1	2.50	0.47
1:I:279:ASN:ND2	1:I:282:LYS:HG2	2.30	0.47
2:J:114:LEU:HD11	2:J:116:LEU:HD21	1.97	0.47
3:K:28:SER:HA	3:K:68:GLY:O	2.15	0.47
1:A:231:LYS:HB2	1:A:268:GLU:HB2	1.96	0.47
1:A:256:SER:HB2	1:A:376:PHE:HB3	1.96	0.47
3:K:91:TYR:O	3:K:91:TYR:CD1	2.67	0.47
3:K:94:TRP:CE3	3:K:95(A):PRO:HG3	2.49	0.47
4:L:7:SER:HB3	4:L:21:SER:H	1.80	0.47
5:M:145:LYS:HB3	5:M:197:THR:OG1	2.15	0.47
1:A:269:GLU:HG2	7:A:789:NAG:HN2	1.79	0.46
2:B:108:LEU:O	2:B:109:LEU:O	2.33	0.46
2:B:151:LEU:HA	2:B:176:VAL:HG11	1.96	0.46
3:C:105:GLU:HG2	3:C:106:ILE:N	2.27	0.46
1:E:124:PRO:HB3	2:F:60:SER:HA	1.96	0.46
2:F:83:ILE:HG23	2:F:92:GLU:CG	2.44	0.46
2:F:160:THR:HG23	2:F:167:LYS:HB2	1.96	0.46
6:P:38:ARG:HB3	6:P:48:ILE:HD11	1.97	0.46
1:A:350:LYS:C	1:A:352:GLN:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:SER:OG	2:B:175:VAL:HA	2.15	0.46
1:E:297:THR:C	1:E:299:ALA:H	2.23	0.46
3:G:83:PHE:O	3:G:84:ALA:HB2	2.15	0.46
3:G:193:ALA:CB	3:G:208:SER:HB3	2.45	0.46
4:H:7:SER:HB3	4:H:21:SER:H	1.80	0.46
2:J:37:LEU:N	2:J:37:LEU:HD23	2.31	0.46
2:J:100:LEU:HB2	2:J:170:PHE:CD1	2.50	0.46
4:L:163:VAL:HG12	4:L:182:VAL:CB	2.42	0.46
1:A:100:MET:HG3	1:A:488:VAL:HG12	1.97	0.46
1:A:273:ARG:NH1	1:A:484:TYR:CD1	2.84	0.46
3:C:28:SER:HA	3:C:68:GLY:O	2.15	0.46
3:C:133:VAL:CG2	4:D:141:LEU:HD13	2.44	0.46
4:D:126:PRO:O	4:D:128:SER:N	2.48	0.46
4:D:160:THR:O	4:D:163:VAL:HG22	2.15	0.46
4:D:170:LEU:HD13	4:D:176:TYR:CZ	2.50	0.46
1:E:390:LEU:HG	1:E:416:LEU:HD21	1.98	0.46
3:K:114:SER:O	3:K:116:PHE:CD1	2.68	0.46
3:K:193:ALA:CB	3:K:208:SER:HB3	2.45	0.46
6:N:81:GLU:CD	6:N:82(A):LYS:HE2	2.40	0.46
3:C:48:ILE:HG22	3:C:49:TYR:N	2.29	0.46
3:C:91:TYR:HB2	4:D:100(I):GLY:HA3	1.97	0.46
3:C:193:ALA:CB	3:C:208:SER:HB3	2.45	0.46
1:E:280:ASN:O	2:F:35:LYS:CD	2.60	0.46
1:E:465:THR:HG23	1:E:465:THR:O	2.16	0.46
2:F:76:ILE:H	2:F:76:ILE:CD1	2.14	0.46
1:I:93:PHE:CE2	1:I:487:LYS:HG2	2.51	0.46
2:J:108:LEU:HD22	2:J:149:LEU:HD23	1.98	0.46
3:K:83:PHE:O	3:K:84:ALA:HB2	2.15	0.46
4:L:39:GLN:NE2	4:L:44:GLY:HA2	2.23	0.46
4:L:126:PRO:HG3	4:L:138:LEU:HB3	1.98	0.46
4:L:137:ALA:HA	4:L:183:THR:HA	1.96	0.46
4:L:170:LEU:HD13	4:L:176:TYR:CZ	2.50	0.46
1:A:119:CYS:HB3	3:C:94:TRP:NE1	2.30	0.46
2:B:100:LEU:HB2	2:B:170:PHE:CD1	2.50	0.46
1:E:124:PRO:HG2	2:F:60:SER:HA	1.96	0.46
3:G:25:ALA:O	3:G:26:SER:O	2.33	0.46
1:I:124:PRO:HB3	2:J:60:SER:HA	1.96	0.46
1:I:335:LYS:HD3	1:I:408:ASN:HA	1.96	0.46
1:I:371:ILE:HD11	2:J:43:PHE:CD2	2.50	0.46
4:L:178:LEU:HD12	4:L:178:LEU:C	2.40	0.46
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:CYS:CA	2:B:159:CYS:HA	2.34	0.46
2:B:150:GLU:HB3	2:B:152:GLN:CD	2.38	0.46
3:C:25:ALA:O	3:C:26:SER:O	2.33	0.46
1:E:93:PHE:CE2	1:E:487:LYS:HG2	2.51	0.46
2:F:110:GLN:HA	2:F:176:VAL:HG13	1.98	0.46
1:I:273:ARG:NH1	1:I:484:TYR:CD1	2.84	0.46
3:K:91:TYR:HB2	4:L:100(I):GLY:HA3	1.97	0.46
1:A:280:ASN:O	2:B:35:LYS:CD	2.60	0.46
1:A:381:GLU:HB3	1:A:420:ILE:HD13	1.96	0.46
2:B:37:LEU:N	2:B:37:LEU:HD23	2.30	0.46
2:B:108:LEU:HD22	2:B:149:LEU:HD23	1.97	0.46
1:E:236:THR:O	1:E:236:THR:HG23	2.16	0.46
1:E:259:LEU:HB2	1:E:374:HIS:CE1	2.50	0.46
1:E:354:GLY:O	1:E:357:LYS:HB2	2.16	0.46
3:G:28:SER:HA	3:G:68:GLY:O	2.15	0.46
4:H:11:VAL:CG2	4:H:147:PRO:HG3	2.46	0.46
4:H:126:PRO:CG	4:H:138:LEU:HD13	2.43	0.46
1:I:100:MET:HG3	1:I:488:VAL:HG12	1.96	0.46
3:K:134:CYS:O	3:K:136:LEU:HD12	2.15	0.46
1:A:236:THR:HG23	1:A:236:THR:O	2.16	0.46
1:A:412:ARG:HA	7:A:908:NAG:C6	2.46	0.46
1:E:231:LYS:HB2	1:E:268:GLU:HB2	1.96	0.46
1:E:256:SER:HB2	1:E:376:PHE:HB3	1.96	0.46
1:I:215:ILE:HG13	1:I:215:ILE:O	2.15	0.46
2:J:28:TRP:HB2	2:J:37:LEU:HD23	1.97	0.46
4:L:126:PRO:O	4:L:128:SER:N	2.48	0.46
2:B:160:THR:HG23	2:B:167:LYS:HB2	1.96	0.46
3:C:134:CYS:O	3:C:136:LEU:HD12	2.15	0.46
4:D:7:SER:HB3	4:D:21:SER:H	1.80	0.46
1:E:95:MET:CB	1:E:484:TYR:HA	2.46	0.46
1:E:215:ILE:O	1:E:215:ILE:HG13	2.15	0.46
1:E:358:THR:C	1:E:359:ILE:HD12	2.41	0.46
4:H:160:THR:O	4:H:163:VAL:HG22	2.15	0.46
1:I:354:GLY:O	1:I:357:LYS:HB2	2.16	0.46
1:I:381:GLU:HB3	1:I:420:ILE:HD13	1.96	0.46
4:L:141:LEU:HD12	4:L:179:SER:HG	1.80	0.46
4:L:169:VAL:O	4:L:176:TYR:HA	2.16	0.46
1:A:274:SER:HB3	1:A:277:PHE:CD1	2.51	0.46
1:A:390:LEU:HG	1:A:416:LEU:HD21	1.98	0.46
2:B:10:ASP:CG	2:B:11:THR:H	2.24	0.46
2:F:37:LEU:HD23	2:F:37:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:170:LEU:HD13	4:H:176:TYR:CZ	2.50	0.46
4:H:189:LEU:HB3	4:H:213:PRO:CG	2.45	0.46
1:I:94:ASN:ND2	1:I:97:LYS:CB	2.79	0.46
1:I:274:SER:HB3	1:I:277:PHE:CD1	2.51	0.46
2:J:30:ASN:O	2:J:33:GLN:N	2.48	0.46
4:L:160:THR:O	4:L:163:VAL:HG22	2.15	0.46
4:L:186:SER:C	4:L:188:SER:H	2.24	0.46
5:O:145:LYS:HB3	5:O:197:THR:OG1	2.15	0.46
1:A:358:THR:C	1:A:359:ILE:HD12	2.41	0.45
2:B:114:LEU:HD11	2:B:116:LEU:HD21	1.97	0.45
2:F:3:VAL:HG22	2:F:94:GLN:CB	2.44	0.45
4:H:126:PRO:O	4:H:128:SER:N	2.48	0.45
1:I:95:MET:CB	1:I:484:TYR:HA	2.46	0.45
1:I:390:LEU:HG	1:I:416:LEU:HD21	1.98	0.45
2:J:108:LEU:O	2:J:109:LEU:O	2.33	0.45
1:A:93:PHE:CE2	1:A:487:LYS:HG2	2.51	0.45
1:A:273:ARG:NH1	1:A:273:ARG:CG	2.78	0.45
1:E:257:THR:O	1:E:258:GLN:HB2	2.16	0.45
2:F:114:LEU:HD11	2:F:116:LEU:HD21	1.97	0.45
2:F:154:SER:OG	2:F:175:VAL:HA	2.15	0.45
3:G:134:CYS:O	3:G:136:LEU:HD12	2.15	0.45
4:H:39:GLN:NE2	4:H:44:GLY:HA2	2.23	0.45
4:H:137:ALA:HA	4:H:183:THR:HA	1.97	0.45
1:I:297:THR:C	1:I:299:ALA:H	2.24	0.45
1:I:358:THR:C	1:I:359:ILE:HD12	2.41	0.45
1:I:465:THR:O	1:I:465:THR:HG23	2.16	0.45
2:J:83:ILE:HA	2:J:92:GLU:HA	1.97	0.45
6:N:6:GLN:HB3	6:N:107:THR:CG2	2.47	0.45
6:N:38:ARG:HB3	6:N:48:ILE:HD11	1.97	0.45
1:A:368:ASP:OD2	2:B:59:ARG:NH2	2.43	0.45
2:B:110:GLN:HA	2:B:176:VAL:HG13	1.98	0.45
3:C:141:PRO:C	3:C:143:GLU:OE1	2.60	0.45
4:D:100(J):PHE:O	4:D:100(K):LEU:HD23	2.16	0.45
4:D:143:LYS:HG2	4:D:144:ASP:CG	2.41	0.45
1:E:98:ASN:HB3	1:E:101:VAL:HG23	1.99	0.45
1:E:102:GLU:OE1	1:E:476:ARG:NE	2.43	0.45
4:H:143:LYS:HG2	4:H:144:ASP:CG	2.41	0.45
1:I:104:MET:HE2	1:I:215:ILE:CD1	2.42	0.45
6:P:6:GLN:HB3	6:P:107:THR:CG2	2.47	0.45
5:Q:145:LYS:HB3	5:Q:197:THR:OG1	2.15	0.45
1:A:105:HIS:HB2	1:A:479:TRP:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:O	1:A:442:GLN:N	2.50	0.45
1:A:465:THR:O	1:A:465:THR:HG23	2.16	0.45
2:B:28:TRP:HB2	2:B:37:LEU:HD23	1.97	0.45
1:E:273:ARG:NH1	1:E:484:TYR:CD1	2.84	0.45
1:E:440:ARG:O	1:E:442:GLN:N	2.50	0.45
4:H:2:VAL:C	4:H:3:GLN:CD	2.85	0.45
2:J:110:GLN:HA	2:J:176:VAL:HG13	1.98	0.45
1:A:94:ASN:ND2	1:A:97:LYS:CB	2.79	0.45
1:A:439:ILE:HD12	1:A:439:ILE:C	2.41	0.45
2:B:30:ASN:O	2:B:33:GLN:N	2.48	0.45
3:C:73:LEU:O	3:C:73:LEU:HD13	2.17	0.45
1:E:412:ARG:HA	7:E:908:NAG:C6	2.46	0.45
1:E:460:LYS:HG3	1:E:460:LYS:O	2.16	0.45
2:F:10:ASP:CG	2:F:11:THR:H	2.24	0.45
1:I:236:THR:HG23	1:I:236:THR:O	2.16	0.45
1:I:269:GLU:CG	7:I:789:NAG:HN2	2.29	0.45
2:J:3:VAL:HG22	2:J:94:GLN:CB	2.44	0.45
2:J:54:ARG:NH1	2:J:75:LYS:HG3	2.31	0.45
2:J:94:GLN:HG3	2:J:96:LEU:HD22	1.98	0.45
3:K:25:ALA:O	3:K:26:SER:O	2.33	0.45
3:K:112:ALA:HB2	3:K:200:GLY:O	2.17	0.45
1:A:257:THR:O	1:A:258:GLN:HB2	2.17	0.45
1:A:269:GLU:CG	7:A:789:NAG:HN2	2.29	0.45
1:A:394:ASN:C	1:A:396:THR:N	2.74	0.45
1:A:460:LYS:HG3	1:A:460:LYS:O	2.16	0.45
2:B:59:ARG:H	2:B:59:ARG:HG3	1.60	0.45
4:D:186:SER:C	4:D:188:SER:H	2.24	0.45
1:E:98:ASN:ND2	1:E:486:TYR:O	2.50	0.45
1:E:274:SER:HB3	1:E:277:PHE:CD1	2.51	0.45
4:H:7:SER:HB3	4:H:21:SER:HG	1.80	0.45
1:I:448:ASN:OD1	7:I:948:NAG:H2	2.17	0.45
3:K:3:VAL:HB	3:K:26:SER:OG	2.17	0.45
3:K:133:VAL:CG2	4:L:141:LEU:HD13	2.45	0.45
1:A:95:MET:CB	1:A:484:TYR:HA	2.46	0.45
3:C:48:ILE:CD1	3:C:54:ARG:HA	2.47	0.45
1:E:439:ILE:HD12	1:E:439:ILE:C	2.41	0.45
2:F:54:ARG:NH1	2:F:75:LYS:HG3	2.32	0.45
4:H:52(A):THR:O	4:H:55:ASP:N	2.48	0.45
2:J:73:ASN:HD22	2:J:73:ASN:HA	1.65	0.45
4:L:143:LYS:HG2	4:L:144:ASP:CG	2.41	0.45
4:L:152:VAL:HG11	4:L:180:SER:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:HB3	1:A:101:VAL:HG23	1.99	0.45
3:C:79:GLN:O	3:C:82:ASP:HB2	2.17	0.45
3:C:103:ARG:HH11	3:C:103:ARG:HG3	1.82	0.45
3:C:112:ALA:HB2	3:C:200:GLY:O	2.17	0.45
4:D:52(A):THR:O	4:D:55:ASP:N	2.48	0.45
4:H:119:PRO:HB3	4:H:145:TYR:CB	2.46	0.45
1:I:95:MET:HB3	1:I:484:TYR:HA	1.99	0.45
1:I:412:ARG:HA	7:I:908:NAG:C6	2.46	0.45
1:I:439:ILE:HD12	1:I:439:ILE:C	2.41	0.45
4:L:59:TYR:CE2	4:L:68:THR:HA	2.52	0.45
1:A:354:GLY:O	1:A:357:LYS:HB2	2.16	0.45
4:D:169:VAL:O	4:D:176:TYR:HA	2.16	0.45
1:E:94:ASN:ND2	1:E:97:LYS:CB	2.79	0.45
1:E:269:GLU:CG	7:E:789:NAG:HN2	2.29	0.45
2:F:30:ASN:O	2:F:33:GLN:N	2.48	0.45
2:F:108:LEU:HD22	2:F:149:LEU:HD23	1.98	0.45
3:G:141:PRO:C	3:G:143:GLU:OE1	2.60	0.45
3:G:198:HIS:HD2	3:G:199:GLN:H	1.59	0.45
4:H:59:TYR:CE2	4:H:68:THR:HA	2.52	0.45
2:J:150:GLU:HB2	2:J:153:ASP:OD2	2.17	0.45
1:A:268:GLU:HB3	1:A:269:GLU:H	1.51	0.45
1:A:297:THR:C	1:A:299:ALA:N	2.75	0.45
3:C:94:TRP:CE3	3:C:95(A):PRO:HG3	2.49	0.45
4:H:169:VAL:O	4:H:176:TYR:HA	2.16	0.45
1:I:440:ARG:O	1:I:442:GLN:N	2.50	0.45
2:J:154:SER:OG	2:J:175:VAL:HA	2.15	0.45
1:A:279:ASN:ND2	1:A:282:LYS:HG2	2.30	0.44
3:C:3:VAL:HB	3:C:26:SER:OG	2.17	0.44
4:D:11:VAL:CG2	4:D:147:PRO:HG3	2.46	0.44
4:D:34:PHE:CG	4:D:78:VAL:HG21	2.53	0.44
1:E:279:ASN:ND2	1:E:282:LYS:HG2	2.30	0.44
3:G:3:VAL:HB	3:G:26:SER:OG	2.17	0.44
3:G:50:GLY:O	3:G:51:ALA:HB3	2.17	0.44
3:G:86:TYR:CE2	3:G:104:LEU:HD22	2.49	0.44
3:G:163:VAL:HG12	3:G:164:THR:O	2.18	0.44
4:H:152:VAL:HG11	4:H:180:SER:CB	2.47	0.44
1:I:98:ASN:ND2	1:I:486:TYR:O	2.50	0.44
3:K:120:PRO:HG3	3:K:186:TYR:CZ	2.52	0.44
4:L:28:THR:HB	4:L:31:ARG:HD2	1.99	0.44
2:B:80:ASP:HB3	2:B:82:TYR:CE1	2.52	0.44
4:D:126:PRO:HG3	4:D:138:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:ILE:HD12	2:F:70:ILE:H	1.82	0.44
2:F:80:ASP:HB3	2:F:82:TYR:CE1	2.52	0.44
3:G:6:GLN:OE1	3:G:99:GLY:HA3	2.18	0.44
4:H:66:ARG:HH22	4:H:86:ASP:CG	2.25	0.44
4:H:100(J):PHE:O	4:H:100(K):LEU:HD23	2.16	0.44
4:H:186:SER:C	4:H:188:SER:H	2.24	0.44
4:H:200:HIS:C	4:H:202:PRO:HD2	2.42	0.44
1:I:257:THR:O	1:I:258:GLN:HB2	2.17	0.44
2:J:178:ALA:C	2:J:179:PHE:HD1	2.17	0.44
3:K:50:GLY:O	3:K:51:ALA:HB3	2.17	0.44
3:K:141:PRO:C	3:K:143:GLU:OE1	2.60	0.44
1:A:297:THR:C	1:A:299:ALA:H	2.24	0.44
2:B:54:ARG:NH1	2:B:75:LYS:HG3	2.31	0.44
2:B:150:GLU:HB2	2:B:153:ASP:OD2	2.17	0.44
4:D:199:ASN:HD21	4:D:201:LYS:HG2	1.83	0.44
4:D:200:HIS:C	4:D:202:PRO:HD2	2.42	0.44
2:F:28:TRP:CE2	2:F:69:LEU:HB2	2.53	0.44
3:G:16:GLY:HA2	3:G:77:SER:OG	2.18	0.44
3:G:73:LEU:O	3:G:73:LEU:HD13	2.17	0.44
3:G:210:ASN:O	3:G:212:GLY:N	2.50	0.44
4:H:69:ILE:HG12	4:H:80:LEU:HD23	2.00	0.44
4:H:87:THR:HG23	4:H:110:THR:HA	1.99	0.44
4:H:126:PRO:HG3	4:H:138:LEU:HB3	1.98	0.44
3:K:79:GLN:O	3:K:82:ASP:HB2	2.17	0.44
3:K:163:VAL:HG12	3:K:164:THR:O	2.18	0.44
2:B:28:TRP:CE2	2:B:69:LEU:HB2	2.52	0.44
3:C:175:LEU:HD12	3:C:176:SER:N	2.29	0.44
3:C:210:ASN:O	3:C:212:GLY:N	2.51	0.44
4:D:59:TYR:CE2	4:D:68:THR:HA	2.52	0.44
4:D:152:VAL:HG11	4:D:180:SER:CB	2.47	0.44
1:E:89:VAL:HG22	1:E:90:THR:N	2.33	0.44
2:F:94:GLN:HG3	2:F:96:LEU:HD22	1.98	0.44
2:F:126:PRO:HB2	2:F:161:VAL:HG13	1.99	0.44
3:G:175:LEU:HD12	3:G:176:SER:N	2.29	0.44
1:I:460:LYS:HG3	1:I:460:LYS:O	2.16	0.44
3:K:124:GLN:O	3:K:127:SER:HB2	2.18	0.44
4:L:69:ILE:HG12	4:L:80:LEU:HD23	2.00	0.44
4:L:100(J):PHE:O	4:L:100(K):LEU:HD23	2.16	0.44
1:A:335:LYS:O	1:A:339:GLU:HB2	2.18	0.44
2:B:154:SER:HB2	2:B:176:VAL:CB	2.48	0.44
1:E:95:MET:HB3	1:E:484:TYR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:ARG:NH1	1:E:273:ARG:CG	2.78	0.44
1:I:108:ILE:HD12	1:I:253:PRO:HB2	2.00	0.44
1:I:297:THR:C	1:I:299:ALA:N	2.75	0.44
1:I:480:ARG:C	1:I:482:GLU:N	2.74	0.44
2:J:80:ASP:HB3	2:J:82:TYR:CE1	2.52	0.44
3:K:16:GLY:HA2	3:K:77:SER:OG	2.18	0.44
3:K:210:ASN:O	3:K:212:GLY:N	2.51	0.44
4:L:2:VAL:C	4:L:3:GLN:CD	2.85	0.44
1:A:205:CYS:N	1:A:206:PRO:CD	2.81	0.44
2:B:72:LYS:O	2:B:73:ASN:C	2.60	0.44
3:C:6:GLN:OE1	3:C:99:GLY:HA3	2.18	0.44
1:E:108:ILE:HD12	1:E:253:PRO:HB2	2.00	0.44
3:G:120:PRO:HG3	3:G:186:TYR:CZ	2.52	0.44
4:H:163:VAL:HG12	4:H:182:VAL:CB	2.42	0.44
4:H:199:ASN:HD21	4:H:201:LYS:HG2	1.83	0.44
1:I:98:ASN:HB3	1:I:101:VAL:HG23	1.99	0.44
1:I:335:LYS:O	1:I:339:GLU:HB2	2.18	0.44
2:J:28:TRP:CE2	2:J:69:LEU:HB2	2.52	0.44
1:A:98:ASN:ND2	1:A:486:TYR:O	2.50	0.44
1:A:359:ILE:O	1:A:395:ASP:HB2	2.18	0.44
2:B:78:ASP:O	2:B:95:LEU:HD23	2.18	0.44
3:C:86:TYR:CE2	3:C:104:LEU:HD22	2.49	0.44
4:D:28:THR:HB	4:D:31:ARG:HD2	1.99	0.44
1:E:335:LYS:O	1:E:339:GLU:HB2	2.18	0.44
1:E:480:ARG:C	1:E:482:GLU:N	2.74	0.44
2:F:150:GLU:HB2	2:F:153:ASP:OD2	2.17	0.44
3:G:79:GLN:O	3:G:82:ASP:HB2	2.17	0.44
3:G:112:ALA:HB2	3:G:200:GLY:O	2.17	0.44
4:H:34:PHE:CG	4:H:78:VAL:HG21	2.52	0.44
2:J:72:LYS:O	2:J:73:ASN:C	2.60	0.44
2:J:78:ASP:O	2:J:95:LEU:HD23	2.18	0.44
2:J:130:CYS:CA	2:J:159:CYS:HA	2.34	0.44
4:L:63:LEU:O	4:L:64:GLN:C	2.61	0.44
1:A:95:MET:HB3	1:A:484:TYR:HA	1.99	0.44
1:A:194:GLY:O	1:A:195:SER:C	2.61	0.44
1:A:448:ASN:OD1	7:A:948:NAG:H2	2.17	0.44
4:D:2:VAL:C	4:D:3:GLN:CD	2.85	0.44
4:D:54:LEU:HD12	4:D:54:LEU:HA	1.83	0.44
4:D:87:THR:HG23	4:D:110:THR:HA	1.99	0.44
1:E:105:HIS:HB2	1:E:479:TRP:HD1	1.82	0.44
1:E:108:ILE:HD12	1:E:253:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:THR:O	1:E:463:ASN:C	2.60	0.44
3:G:103:ARG:HH11	3:G:103:ARG:HG3	1.82	0.44
1:I:89:VAL:HG22	1:I:90:THR:N	2.33	0.44
1:I:108:ILE:HD12	1:I:253:PRO:HB3	1.99	0.44
3:K:48:ILE:CD1	3:K:54:ARG:HA	2.47	0.44
3:K:154:LEU:O	3:K:155:GLN:C	2.61	0.44
4:L:7:SER:CB	4:L:21:SER:H	2.31	0.44
4:L:199:ASN:HD21	4:L:201:LYS:HG2	1.83	0.44
4:L:200:HIS:C	4:L:202:PRO:HD2	2.42	0.44
1:A:105:HIS:HA	1:A:479:TRP:NE1	2.33	0.44
1:A:221:ALA:O	1:A:223:PHE:HD1	2.01	0.44
1:A:272:ILE:O	1:A:277:PHE:HZ	2.01	0.44
2:B:94:GLN:HG3	2:B:96:LEU:HD22	1.99	0.44
3:C:120:PRO:HG3	3:C:186:TYR:CZ	2.53	0.44
3:C:163:VAL:HG12	3:C:164:THR:O	2.17	0.44
4:D:39:GLN:C	4:D:88:ALA:HB1	2.43	0.44
4:D:66:ARG:HH22	4:D:86:ASP:CG	2.25	0.44
1:E:359:ILE:O	1:E:395:ASP:HB2	2.18	0.44
2:F:154:SER:HB2	2:F:176:VAL:CB	2.47	0.44
3:G:48:ILE:CD1	3:G:54:ARG:HA	2.47	0.44
1:I:340:ASN:O	1:I:343:GLU:HB2	2.18	0.44
4:D:23:LYS:NZ	4:D:75:THR:O	2.43	0.43
1:E:194:GLY:O	1:E:195:SER:C	2.61	0.43
1:E:350:LYS:HE2	1:E:359:ILE:HD13	2.00	0.43
2:F:5:LEU:HB2	2:F:168:VAL:HG13	2.00	0.43
2:F:36:ILE:HD13	2:F:49:SER:HB3	2.00	0.43
3:G:55:ALA:O	3:G:58:VAL:HG23	2.18	0.43
3:G:124:GLN:O	3:G:127:SER:HB2	2.18	0.43
1:I:105:HIS:HB2	1:I:479:TRP:HD1	1.82	0.43
1:I:359:ILE:O	1:I:395:ASP:HB2	2.18	0.43
2:J:126:PRO:HB2	2:J:161:VAL:HG13	1.99	0.43
2:J:154:SER:HB2	2:J:176:VAL:CB	2.47	0.43
3:K:6:GLN:OE1	3:K:99:GLY:HA3	2.18	0.43
3:K:161:GLU:OE2	3:K:175:LEU:HD21	2.18	0.43
5:O:22:SER:CA	5:O:72:THR:HG22	2.48	0.43
6:R:6:GLN:HB3	6:R:107:THR:CG2	2.47	0.43
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.99	0.43
1:A:221:ALA:C	1:A:223:PHE:N	2.71	0.43
1:A:280:ASN:ND2	2:B:35:LYS:HD3	2.33	0.43
2:B:178:ALA:C	2:B:179:PHE:HD1	2.17	0.43
4:D:1:GLU:O	4:D:3:GLN:NE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:CYS:HB2	1:I:434:MET:CE	2.48	0.43
1:I:221:ALA:O	1:I:223:PHE:HD1	2.01	0.43
1:I:280:ASN:ND2	2:J:35:LYS:HD3	2.33	0.43
1:I:350:LYS:HE2	1:I:359:ILE:HD13	2.00	0.43
2:J:10:ASP:CG	2:J:11:THR:N	2.77	0.43
2:J:79:SER:HA	2:J:95:LEU:O	2.18	0.43
2:J:151:LEU:HD12	2:J:176:VAL:HB	2.00	0.43
2:J:157:TRP:O	2:J:171:LYS:HA	2.18	0.43
2:J:178:ALA:HB1	2:J:180:GLN:N	2.25	0.43
3:K:73:LEU:O	3:K:73:LEU:HD13	2.17	0.43
4:L:39:GLN:C	4:L:88:ALA:HB1	2.43	0.43
1:A:89:VAL:HG22	1:A:90:THR:N	2.33	0.43
2:B:70:ILE:HD12	2:B:70:ILE:H	1.82	0.43
3:C:167:ASP:OD2	4:D:164:HIS:NE2	2.51	0.43
1:E:440:ARG:C	1:E:442:GLN:N	2.76	0.43
2:F:14:LEU:HD23	2:F:14:LEU:N	2.33	0.43
2:F:36:ILE:HA	2:F:49:SER:HB3	2.00	0.43
2:F:79:SER:HA	2:F:95:LEU:O	2.18	0.43
2:F:151:LEU:HD12	2:F:176:VAL:HB	2.00	0.43
1:I:105:HIS:HA	1:I:479:TRP:NE1	2.33	0.43
1:I:462:THR:O	1:I:463:ASN:C	2.60	0.43
1:A:108:ILE:HD12	1:A:253:PRO:HB2	2.00	0.43
2:B:151:LEU:HD12	2:B:176:VAL:HB	2.00	0.43
1:E:448:ASN:OD1	7:E:948:NAG:H2	2.17	0.43
3:G:161:GLU:OE2	3:G:175:LEU:HD21	2.18	0.43
4:H:28:THR:HB	4:H:31:ARG:HD2	1.99	0.43
4:H:39:GLN:C	4:H:88:ALA:HB1	2.43	0.43
1:I:194:GLY:O	1:I:195:SER:C	2.61	0.43
1:I:446:SER:O	7:I:948:NAG:H62	2.19	0.43
3:K:103:ARG:HH11	3:K:103:ARG:HG3	1.82	0.43
4:L:53:ILE:HG23	4:L:54:LEU:N	2.34	0.43
5:O:107:LYS:HG3	5:O:108:ARG:N	2.34	0.43
1:A:445:CYS:SG	7:A:762:NAG:O4	2.76	0.43
1:A:476:ARG:HB3	1:A:480:ARG:NH1	2.34	0.43
2:B:176:VAL:HG12	2:B:177:LEU:N	2.34	0.43
4:D:7:SER:CB	4:D:21:SER:H	2.31	0.43
1:E:297:THR:C	1:E:299:ALA:N	2.75	0.43
1:E:340:ASN:O	1:E:343:GLU:HB2	2.18	0.43
2:F:10:ASP:CG	2:F:11:THR:N	2.77	0.43
2:J:5:LEU:HB2	2:J:168:VAL:HG13	2.00	0.43
2:J:69:LEU:C	2:J:69:LEU:CD2	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HE2	1:A:235:GLY:HA3	2.00	0.43
1:E:119:CYS:HB2	1:E:434:MET:CE	2.48	0.43
1:E:258:GLN:NE2	1:E:373:THR:C	2.77	0.43
2:F:78:ASP:O	2:F:95:LEU:HD23	2.18	0.43
2:J:10:ASP:CG	2:J:11:THR:H	2.24	0.43
2:J:105:ASP:OD1	2:J:106:THR:N	2.52	0.43
3:K:142:ARG:HG3	3:K:163:VAL:HG11	2.01	0.43
1:A:480:ARG:C	1:A:482:GLU:N	2.74	0.43
2:B:69:LEU:C	2:B:69:LEU:CD2	2.92	0.43
2:B:79:SER:HA	2:B:95:LEU:O	2.18	0.43
2:B:126:PRO:HB2	2:B:161:VAL:HG13	1.99	0.43
2:B:157:TRP:O	2:B:171:LYS:HA	2.18	0.43
3:C:16:GLY:HA2	3:C:77:SER:OG	2.18	0.43
3:C:50:GLY:O	3:C:51:ALA:HB3	2.17	0.43
3:C:124:GLN:O	3:C:127:SER:HB2	2.18	0.43
4:D:119:PRO:HB3	4:D:145:TYR:CB	2.46	0.43
1:E:446:SER:O	7:E:948:NAG:H62	2.19	0.43
2:F:72:LYS:O	2:F:73:ASN:C	2.60	0.43
4:H:7:SER:CB	4:H:21:SER:H	2.31	0.43
4:H:53:ILE:HG23	4:H:54:LEU:N	2.34	0.43
1:I:272:ILE:O	1:I:277:PHE:HZ	2.01	0.43
1:I:293:VAL:O	1:I:333:LEU:HD12	2.19	0.43
2:J:79:SER:OG	2:J:96:LEU:HA	2.19	0.43
3:K:24:ARG:HH11	3:K:24:ARG:CG	2.32	0.43
4:L:34:PHE:CG	4:L:78:VAL:HG21	2.53	0.43
4:L:87:THR:HG23	4:L:110:THR:HA	2.00	0.43
4:L:123:PRO:HD3	4:L:209:LYS:HE2	2.01	0.43
1:A:252:ARG:O	1:A:254:VAL:HG23	2.19	0.43
1:A:462:THR:O	1:A:463:ASN:C	2.60	0.43
2:B:105:ASP:OD1	2:B:106:THR:N	2.52	0.43
3:C:55:ALA:O	3:C:58:VAL:HG23	2.18	0.43
3:C:135:LEU:O	3:C:136:LEU:HD12	2.19	0.43
3:C:139:PHE:N	3:C:172:THR:HB	2.34	0.43
3:C:142:ARG:HG3	3:C:163:VAL:HG11	2.00	0.43
3:C:161:GLU:OE2	3:C:175:LEU:HD21	2.18	0.43
1:E:280:ASN:ND2	2:F:35:LYS:HD3	2.33	0.43
1:E:293:VAL:O	1:E:333:LEU:HD12	2.19	0.43
2:F:27:HIS:CE1	2:F:38:GLY:HA3	2.54	0.43
3:G:95(B):ARG:HD2	4:H:61:PRO:HG3	2.01	0.43
4:H:146:PHE:H	4:H:200:HIS:HE1	1.67	0.43
1:I:252:ARG:O	1:I:254:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:135:LEU:O	3:K:136:LEU:HD12	2.19	0.43
4:L:83:ARG:HB2	4:L:85:ASP:OD1	2.19	0.43
4:D:53:ILE:HG23	4:D:54:LEU:N	2.34	0.43
4:D:67:VAL:CG2	4:D:68:THR:N	2.82	0.43
4:D:200:HIS:O	4:D:201:LYS:C	2.61	0.43
1:E:95:MET:HE2	1:E:235:GLY:HA3	2.00	0.43
3:G:135:LEU:O	3:G:136:LEU:HD12	2.19	0.43
4:H:63:LEU:O	4:H:64:GLN:C	2.61	0.43
1:I:205:CYS:N	1:I:206:PRO:CD	2.81	0.43
1:I:258:GLN:NE2	1:I:373:THR:C	2.77	0.43
2:J:27:HIS:CE1	2:J:38:GLY:HA3	2.54	0.43
2:J:36:ILE:HD13	2:J:49:SER:HB3	2.00	0.43
3:K:55:ALA:O	3:K:58:VAL:HG23	2.18	0.43
3:K:105:GLU:CD	3:K:173:TYR:HH	2.26	0.43
7:A:762:NAG:C7	7:A:762:NAG:O3	2.67	0.43
3:C:39:LYS:O	3:C:40:PRO:C	2.61	0.43
3:C:95(B):ARG:HD2	4:D:61:PRO:HG3	2.01	0.43
4:D:83:ARG:HB2	4:D:85:ASP:OD1	2.19	0.43
4:D:100:ALA:C	4:D:100(B):GLU:H	2.27	0.43
1:E:252:ARG:O	1:E:254:VAL:HG23	2.18	0.43
2:F:69:LEU:C	2:F:69:LEU:CD2	2.92	0.43
2:F:77:GLU:C	2:F:79:SER:H	2.27	0.43
4:H:200:HIS:O	4:H:201:LYS:C	2.61	0.43
4:L:66:ARG:HH22	4:L:86:ASP:CG	2.25	0.43
5:M:22:SER:CA	5:M:72:THR:HG22	2.48	0.43
5:M:107:LYS:HG3	5:M:108:ARG:N	2.34	0.43
5:Q:197:THR:HG22	5:Q:204:PRO:HB3	2.00	0.43
6:R:93:THR:HG21	6:R:100(L):PHE:CG	2.54	0.43
2:B:5:LEU:HB2	2:B:168:VAL:HG13	2.00	0.42
2:B:36:ILE:HD13	2:B:49:SER:HB3	2.01	0.42
3:C:24:ARG:HH11	3:C:24:ARG:CG	2.32	0.42
3:C:188:LYS:O	3:C:188:LYS:HG2	2.19	0.42
1:E:105:HIS:HA	1:E:479:TRP:NE1	2.33	0.42
1:E:333:LEU:HD23	1:E:390:LEU:HD21	2.01	0.42
1:E:356:ASN:HD21	7:E:856:NAG:H4	1.84	0.42
2:F:58:ARG:O	2:F:59:ARG:C	2.63	0.42
3:G:24:ARG:HH11	3:G:24:ARG:CG	2.32	0.42
1:I:356:ASN:HD21	7:I:856:NAG:H4	1.84	0.42
2:J:36:ILE:HA	2:J:49:SER:HB3	2.00	0.42
2:J:132:SER:OG	2:J:136:LYS:N	2.45	0.42
3:K:39:LYS:O	3:K:40:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:95(B):ARG:HD2	4:L:61:PRO:HG3	2.01	0.42
4:L:66:ARG:NH2	4:L:86:ASP:OD2	2.42	0.42
5:M:197:THR:HG22	5:M:204:PRO:HB3	2.00	0.42
6:P:93:THR:HG21	6:P:100(L):PHE:CG	2.54	0.42
1:A:119:CYS:HB2	1:A:434:MET:CE	2.48	0.42
1:A:258:GLN:NE2	1:A:373:THR:C	2.77	0.42
1:A:340:ASN:O	1:A:343:GLU:HB2	2.18	0.42
2:B:10:ASP:CG	2:B:11:THR:N	2.77	0.42
2:B:27:HIS:CE1	2:B:38:GLY:HA3	2.54	0.42
2:B:36:ILE:HA	2:B:49:SER:HB3	2.00	0.42
4:D:69:ILE:HG12	4:D:80:LEU:HD23	2.00	0.42
2:F:16:CYS:HB2	2:F:28:TRP:HZ2	1.84	0.42
2:F:79:SER:OG	2:F:96:LEU:HA	2.19	0.42
4:H:100:ALA:C	4:H:100(B):GLU:H	2.27	0.42
4:L:119:PRO:HB3	4:L:145:TYR:CB	2.46	0.42
4:L:200:HIS:O	4:L:201:LYS:C	2.61	0.42
1:A:350:LYS:HE2	1:A:359:ILE:HD13	2.00	0.42
1:A:446:SER:O	7:A:948:NAG:H62	2.19	0.42
1:A:489:VAL:HG22	1:A:490:LYS:N	2.35	0.42
4:D:123:PRO:HD3	4:D:209:LYS:HE2	2.01	0.42
1:E:272:ILE:O	1:E:277:PHE:HZ	2.01	0.42
2:F:157:TRP:O	2:F:171:LYS:HA	2.18	0.42
1:I:407:LEU:N	1:I:407:LEU:HD23	2.35	0.42
2:J:14:LEU:N	2:J:14:LEU:HD23	2.33	0.42
3:K:188:LYS:HG2	3:K:188:LYS:O	2.19	0.42
1:A:293:VAL:O	1:A:333:LEU:HD12	2.19	0.42
1:A:356:ASN:HD21	7:A:856:NAG:H4	1.84	0.42
2:B:58:ARG:O	2:B:59:ARG:C	2.62	0.42
1:E:222:GLY:HA2	1:E:491:ILE:HG21	2.02	0.42
7:E:762:NAG:O3	7:E:762:NAG:C7	2.67	0.42
1:I:95:MET:HE2	1:I:235:GLY:HA3	2.00	0.42
1:I:440:ARG:C	1:I:442:GLN:N	2.76	0.42
1:I:476:ARG:HB3	1:I:480:ARG:NH1	2.34	0.42
4:L:67:VAL:CG2	4:L:68:THR:N	2.82	0.42
4:L:138:LEU:HD12	4:L:211:VAL:HG12	2.01	0.42
4:L:146:PHE:H	4:L:200:HIS:HE1	1.67	0.42
5:O:197:THR:HG22	5:O:204:PRO:HB3	2.00	0.42
1:A:222:GLY:HA2	1:A:491:ILE:HG21	2.02	0.42
1:A:440:ARG:C	1:A:442:GLN:N	2.76	0.42
4:D:153:SER:HB3	4:D:157:GLY:HA2	2.01	0.42
1:E:280:ASN:HD22	1:E:458:GLY:HA3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:142:ARG:HG3	3:G:163:VAL:HG11	2.01	0.42
4:H:67:VAL:CG2	4:H:68:THR:N	2.82	0.42
4:H:82(A):ARG:O	4:H:82(B):ASN:HB2	2.20	0.42
4:H:123:PRO:HD3	4:H:209:LYS:HE2	2.01	0.42
1:I:333:LEU:HD23	1:I:390:LEU:HD21	2.01	0.42
1:I:463:ASN:O	1:I:465:THR:N	2.52	0.42
2:J:77:GLU:C	2:J:79:SER:H	2.27	0.42
3:K:175:LEU:HD12	3:K:176:SER:N	2.29	0.42
6:N:93:THR:HG21	6:N:100(L):PHE:CG	2.54	0.42
2:B:14:LEU:N	2:B:14:LEU:HD23	2.33	0.42
3:C:185:ASP:OD1	3:C:189:HIS:CD2	2.73	0.42
1:E:221:ALA:O	1:E:223:PHE:HD1	2.01	0.42
2:F:176:VAL:HG12	2:F:177:LEU:N	2.34	0.42
3:G:139:PHE:N	3:G:172:THR:HB	2.34	0.42
4:H:40:ALA:HB3	4:H:43:GLN:CG	2.49	0.42
4:H:153:SER:HB3	4:H:157:GLY:HA2	2.01	0.42
7:I:762:NAG:C7	7:I:762:NAG:O3	2.67	0.42
3:K:23:CYS:HB2	3:K:35:TRP:CH2	2.55	0.42
3:K:124:GLN:HE22	3:K:130:ALA:CA	2.32	0.42
3:K:185:ASP:OD1	3:K:189:HIS:CD2	2.73	0.42
5:Q:22:SER:CA	5:Q:72:THR:HG22	2.48	0.42
3:C:23:CYS:HB2	3:C:35:TRP:CH2	2.55	0.42
1:E:371:ILE:HD11	1:E:473:GLY:CA	2.49	0.42
3:G:33:LEU:HD13	3:G:34:ALA:N	2.35	0.42
3:G:185:ASP:OD1	3:G:189:HIS:CD2	2.73	0.42
1:I:222:GLY:HA2	1:I:491:ILE:HG21	2.02	0.42
1:I:480:ARG:O	1:I:482:GLU:N	2.53	0.42
2:J:176:VAL:HG12	2:J:177:LEU:N	2.34	0.42
4:L:14:PRO:HD3	4:L:112:SER:C	2.45	0.42
4:L:100:ALA:C	4:L:100(B):GLU:H	2.27	0.42
4:L:153:SER:HB3	4:L:157:GLY:HA2	2.01	0.42
1:A:480:ARG:O	1:A:482:GLU:N	2.53	0.42
2:B:121:PRO:O	2:B:124:SER:HB3	2.20	0.42
3:C:13:VAL:O	3:C:106:ILE:HA	2.20	0.42
4:D:154:TRP:CE2	4:D:196:CYS:HB3	2.55	0.42
2:F:105:ASP:OD1	2:F:106:THR:N	2.52	0.42
3:G:154:LEU:O	3:G:155:GLN:C	2.61	0.42
4:H:83:ARG:HB2	4:H:85:ASP:OD1	2.19	0.42
1:I:371:ILE:HD11	1:I:473:GLY:CA	2.49	0.42
1:A:292:VAL:CG1	1:A:333:LEU:HD11	2.50	0.42
1:A:357:LYS:HG3	1:A:464:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:GLN:HE22	3:C:130:ALA:CA	2.32	0.42
3:C:154:LEU:O	3:C:155:GLN:C	2.61	0.42
4:D:14:PRO:HD3	4:D:112:SER:C	2.45	0.42
4:D:40:ALA:HB3	4:D:43:GLN:CG	2.49	0.42
1:E:205:CYS:N	1:E:206:PRO:CD	2.81	0.42
2:F:10:ASP:OD1	2:F:11:THR:N	2.41	0.42
3:G:39:LYS:O	3:G:40:PRO:C	2.62	0.42
3:G:105:GLU:CD	3:G:173:TYR:HH	2.28	0.42
3:G:124:GLN:HE22	3:G:130:ALA:CA	2.32	0.42
3:G:139:PHE:HE1	3:G:174:SER:HA	1.84	0.42
1:I:268:GLU:HB3	1:I:269:GLU:H	1.51	0.42
2:J:1:LYS:HD2	2:J:1:LYS:C	2.45	0.42
2:J:77:GLU:C	2:J:79:SER:N	2.78	0.42
3:K:139:PHE:N	3:K:172:THR:HB	2.34	0.42
4:L:7:SER:OG	4:L:20:VAL:HG13	2.20	0.42
4:L:85:ASP:OD1	4:L:85:ASP:N	2.41	0.42
5:M:129:THR:HG22	5:M:130:ALA:N	2.35	0.42
1:A:333:LEU:HD23	1:A:390:LEU:HD21	2.01	0.42
1:A:407:LEU:N	1:A:407:LEU:HD23	2.35	0.42
2:B:77:GLU:C	2:B:79:SER:H	2.27	0.42
2:B:79:SER:OG	2:B:96:LEU:HA	2.19	0.42
3:C:82:ASP:O	3:C:104:LEU:HD23	2.20	0.42
4:D:63:LEU:O	4:D:64:GLN:C	2.61	0.42
4:D:66:ARG:NH2	4:D:86:ASP:OD2	2.42	0.42
2:F:104:SER:O	2:F:105:ASP:C	2.63	0.42
3:G:107:LYS:HG3	3:G:140:TYR:OH	2.20	0.42
4:H:154:TRP:CE2	4:H:196:CYS:HB3	2.55	0.42
1:I:357:LYS:HG3	1:I:464:GLY:HA3	2.02	0.42
1:I:489:VAL:HG22	1:I:490:LYS:N	2.35	0.42
2:J:70:ILE:HD12	2:J:70:ILE:H	1.82	0.42
2:J:164:ASN:C	2:J:166:LYS:N	2.77	0.42
3:K:33:LEU:HD13	3:K:34:ALA:N	2.35	0.42
2:B:36:ILE:HD13	2:B:49:SER:HB2	2.02	0.41
3:C:30:SER:OG	3:C:31:SER:N	2.52	0.41
3:C:33:LEU:HD13	3:C:34:ALA:N	2.35	0.41
4:D:125:ALA:HA	4:D:126:PRO:HD3	1.93	0.41
4:D:143:LYS:HG2	4:D:144:ASP:N	2.35	0.41
1:E:407:LEU:HD23	1:E:407:LEU:N	2.35	0.41
1:E:476:ARG:HB3	1:E:480:ARG:NH1	2.34	0.41
2:F:178:ALA:CB	2:F:180:GLN:N	2.81	0.41
3:G:13:VAL:O	3:G:106:ILE:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:125:LEU:CD1	3:G:130:ALA:HB2	2.50	0.41
3:G:153:ALA:C	3:G:155:GLN:H	2.29	0.41
4:H:143:LYS:HG2	4:H:144:ASP:N	2.35	0.41
3:K:82:ASP:O	3:K:104:LEU:HD23	2.20	0.41
4:L:154:TRP:CE2	4:L:196:CYS:HB3	2.55	0.41
5:Q:107:LYS:HG3	5:Q:108:ARG:N	2.34	0.41
1:A:463:ASN:O	1:A:465:THR:N	2.52	0.41
2:B:104:SER:O	2:B:105:ASP:C	2.63	0.41
4:D:82(A):ARG:O	4:D:82(B):ASN:HB2	2.20	0.41
1:E:252:ARG:HA	1:E:253:PRO:HD2	1.91	0.41
1:E:333:LEU:HB3	1:E:414:ILE:HB	2.02	0.41
1:E:477:ASP:O	1:E:480:ARG:HB2	2.20	0.41
2:F:51:LEU:O	2:F:55:ALA:N	2.53	0.41
3:G:23:CYS:HB2	3:G:35:TRP:CH2	2.55	0.41
1:I:95:MET:CE	1:I:273:ARG:HG2	2.49	0.41
1:I:477:ASP:O	1:I:480:ARG:HB2	2.20	0.41
2:J:36:ILE:HD13	2:J:49:SER:HB2	2.02	0.41
3:K:153:ALA:C	3:K:155:GLN:H	2.29	0.41
4:L:27:ASP:CG	4:L:28:THR:N	2.79	0.41
4:L:88:ALA:O	4:L:108:LEU:HD12	2.21	0.41
6:N:81:GLU:OE2	6:N:82(A):LYS:CE	2.66	0.41
5:Q:121:SER:O	5:Q:125:LEU:HG	2.21	0.41
1:A:274:SER:HB3	1:A:277:PHE:CE1	2.55	0.41
1:A:333:LEU:HB3	1:A:414:ILE:HB	2.02	0.41
7:A:963:NAG:H3	7:A:963:NAG:C8	2.37	0.41
3:C:125:LEU:CD1	3:C:130:ALA:HB2	2.50	0.41
1:E:350:LYS:HE2	1:E:357:LYS:O	2.20	0.41
2:F:1:LYS:HD2	2:F:1:LYS:C	2.45	0.41
2:F:121:PRO:O	2:F:124:SER:HB3	2.20	0.41
3:G:188:LYS:O	3:G:188:LYS:HG2	2.19	0.41
4:H:14:PRO:HD3	4:H:112:SER:C	2.45	0.41
1:I:280:ASN:O	2:J:35:LYS:CD	2.60	0.41
2:J:58:ARG:O	2:J:59:ARG:C	2.63	0.41
3:K:2:ILE:HG12	3:K:27:GLU:CD	2.45	0.41
3:K:14:SER:OG	3:K:15:PRO:HD2	2.19	0.41
3:K:125:LEU:CD1	3:K:130:ALA:HB2	2.50	0.41
4:L:5:VAL:HB	4:L:23:LYS:HB3	2.02	0.41
4:L:52(A):THR:O	4:L:55:ASP:N	2.48	0.41
6:P:81:GLU:OE2	6:P:82(A):LYS:CE	2.66	0.41
1:A:350:LYS:HE2	1:A:357:LYS:O	2.20	0.41
1:A:478:ASN:HD22	1:A:478:ASN:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:LYS:HD2	2:B:1:LYS:C	2.45	0.41
2:B:178:ALA:CB	2:B:180:GLN:N	2.81	0.41
3:C:107:LYS:HG3	3:C:140:TYR:OH	2.20	0.41
3:C:150:VAL:HG11	3:C:189:HIS:CD2	2.56	0.41
4:D:146:PHE:H	4:D:200:HIS:HE1	1.67	0.41
1:E:463:ASN:O	1:E:465:THR:N	2.52	0.41
1:E:480:ARG:O	1:E:482:GLU:N	2.53	0.41
3:K:13:VAL:O	3:K:106:ILE:HA	2.19	0.41
3:K:30:SER:OG	3:K:31:SER:N	2.52	0.41
1:A:248:THR:HG22	1:A:486:TYR:CD2	2.56	0.41
1:A:341:THR:HG22	1:A:345:ILE:HD12	2.03	0.41
2:B:51:LEU:O	2:B:55:ALA:N	2.53	0.41
3:C:105:GLU:OE2	3:C:173:TYR:HE2	2.03	0.41
3:C:105:GLU:OE2	3:C:173:TYR:CE2	2.73	0.41
4:D:40:ALA:HB1	4:D:41:PRO:HD2	2.02	0.41
4:D:138:LEU:HD23	4:D:138:LEU:H	1.85	0.41
1:E:489:VAL:HG22	1:E:490:LYS:N	2.35	0.41
2:F:128:VAL:HG23	2:F:141:GLY:O	2.21	0.41
3:G:105:GLU:OE2	3:G:173:TYR:CE2	2.73	0.41
1:I:333:LEU:HB3	1:I:414:ILE:HB	2.02	0.41
3:K:107:LYS:HG3	3:K:140:TYR:OH	2.20	0.41
3:K:139:PHE:HE1	3:K:174:SER:HA	1.84	0.41
2:B:116:LEU:O	2:B:143:THR:HG23	2.21	0.41
3:C:14:SER:OG	3:C:15:PRO:HD2	2.20	0.41
2:F:116:LEU:O	2:F:143:THR:HG23	2.21	0.41
3:G:105:GLU:OE2	3:G:173:TYR:HE2	2.03	0.41
2:J:121:PRO:O	2:J:124:SER:HB3	2.20	0.41
4:L:40:ALA:HB1	4:L:41:PRO:HD2	2.02	0.41
4:L:138:LEU:HD23	4:L:138:LEU:H	1.85	0.41
5:O:129:THR:HG22	5:O:130:ALA:N	2.35	0.41
5:Q:124:GLN:HG2	5:Q:129:THR:O	2.21	0.41
1:A:371:ILE:HD11	1:A:473:GLY:CA	2.49	0.41
1:A:457:ASP:CG	1:A:469:ARG:HE	2.29	0.41
4:D:88:ALA:O	4:D:108:LEU:HD12	2.21	0.41
1:E:248:THR:HG22	1:E:486:TYR:CD2	2.56	0.41
3:G:2:ILE:HG12	3:G:27:GLU:CD	2.45	0.41
3:G:82:ASP:O	3:G:104:LEU:HD23	2.20	0.41
3:G:187:GLU:O	3:G:211:ARG:CZ	2.69	0.41
4:H:138:LEU:H	4:H:138:LEU:HD23	1.85	0.41
4:H:138:LEU:HD23	4:H:138:LEU:N	2.36	0.41
4:H:195:ILE:CG1	4:H:210:LYS:HA	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:ILE:HG12	1:I:288:LEU:HA	2.03	0.41
1:I:478:ASN:HD22	1:I:478:ASN:N	2.19	0.41
2:J:30:ASN:O	2:J:31:SER:C	2.64	0.41
2:J:128:VAL:HG23	2:J:141:GLY:O	2.21	0.41
4:L:54:LEU:HD12	4:L:54:LEU:HA	1.82	0.41
4:L:82(A):ARG:O	4:L:82(B):ASN:HB2	2.20	0.41
6:N:189:LEU:HD23	6:N:189:LEU:HA	1.88	0.41
5:Q:129:THR:HG22	5:Q:130:ALA:N	2.35	0.41
1:A:371:ILE:HG21	2:B:45:THR:HG22	2.03	0.41
1:A:477:ASP:O	1:A:480:ARG:HB2	2.20	0.41
4:D:138:LEU:HD23	4:D:138:LEU:N	2.36	0.41
1:E:270:ILE:HG12	1:E:288:LEU:HA	2.03	0.41
2:F:2:LYS:HB3	2:F:93:VAL:HG23	2.03	0.41
2:F:100:LEU:HD12	2:F:170:PHE:CG	2.55	0.41
3:G:45:ARG:NH1	3:G:47:LEU:HD23	2.36	0.41
4:H:54:LEU:HD12	4:H:54:LEU:HA	1.83	0.41
1:I:89:VAL:HG22	1:I:90:THR:H	1.86	0.41
1:I:274:SER:HB3	1:I:277:PHE:CE1	2.55	0.41
1:I:478:ASN:O	1:I:479:TRP:C	2.63	0.41
2:J:87:GLU:O	2:J:88:ASP:HB2	2.21	0.41
1:A:387:SER:O	1:A:391:PHE:HD1	2.04	0.41
2:B:152:GLN:CD	2:B:152:GLN:H	2.29	0.41
3:C:139:PHE:HE1	3:C:174:SER:HA	1.84	0.41
3:C:153:ALA:C	3:C:155:GLN:H	2.29	0.41
3:C:170:ASP:O	3:C:171:SER:HB2	2.21	0.41
1:E:95:MET:CE	1:E:273:ARG:HG2	2.48	0.41
1:E:341:THR:HG22	1:E:345:ILE:HD12	2.03	0.41
2:F:27:HIS:ND1	2:F:38:GLY:HA3	2.36	0.41
3:G:94:TRP:CE3	3:G:95(A):PRO:HG3	2.49	0.41
3:G:134:CYS:HB2	3:G:148:TRP:CH2	2.56	0.41
4:H:5:VAL:HB	4:H:23:LYS:HB3	2.02	0.41
4:H:186:SER:HA	4:H:189:LEU:HG	2.03	0.41
1:I:292:VAL:CG1	1:I:333:LEU:HD11	2.50	0.41
1:I:350:LYS:HE2	1:I:357:LYS:O	2.20	0.41
1:I:358:THR:O	1:I:359:ILE:HD12	2.21	0.41
2:J:51:LEU:O	2:J:55:ALA:N	2.53	0.41
2:J:152:GLN:CD	2:J:152:GLN:H	2.29	0.41
3:K:105:GLU:OE2	3:K:173:TYR:CE2	2.73	0.41
3:K:105:GLU:OE2	3:K:173:TYR:HE2	2.03	0.41
3:K:187:GLU:O	3:K:211:ARG:CZ	2.69	0.41
5:O:121:SER:O	5:O:125:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:124:GLN:HG2	5:O:129:THR:O	2.21	0.41
1:A:202:THR:CG2	3:C:95:PRO:HG3	2.48	0.41
1:A:270:ILE:HG12	1:A:288:LEU:HA	2.03	0.41
2:B:100:LEU:HD12	2:B:170:PHE:CG	2.56	0.41
1:E:274:SER:HB3	1:E:277:PHE:CE1	2.55	0.41
1:E:351:GLU:HG2	1:E:351:GLU:O	2.21	0.41
1:E:358:THR:O	1:E:359:ILE:HD12	2.21	0.41
1:E:371:ILE:HG21	2:F:45:THR:HG22	2.03	0.41
1:E:478:ASN:O	1:E:479:TRP:C	2.64	0.41
2:F:73:ASN:HD22	2:F:73:ASN:HA	1.65	0.41
3:G:170:ASP:O	3:G:171:SER:HB2	2.21	0.41
4:H:88:ALA:O	4:H:108:LEU:HD12	2.21	0.41
1:I:202:THR:CG2	3:K:95:PRO:HG3	2.48	0.41
2:J:100:LEU:HD12	2:J:170:PHE:CG	2.56	0.41
3:K:141:PRO:O	3:K:143:GLU:N	2.54	0.41
3:K:150:VAL:HG11	3:K:189:HIS:CD2	2.56	0.41
1:A:478:ASN:O	1:A:479:TRP:C	2.63	0.40
2:B:30:ASN:O	2:B:31:SER:C	2.64	0.40
2:B:80:ASP:CG	2:B:81:THR:H	2.29	0.40
2:B:128:VAL:HG23	2:B:141:GLY:O	2.21	0.40
3:C:141:PRO:O	3:C:143:GLU:N	2.54	0.40
4:D:7:SER:OG	4:D:20:VAL:HG13	2.20	0.40
4:D:186:SER:HA	4:D:189:LEU:HG	2.03	0.40
1:E:89:VAL:HG22	1:E:90:THR:H	1.86	0.40
2:F:30:ASN:O	2:F:31:SER:C	2.64	0.40
3:G:94:TRP:CA	3:G:95:PRO:O	2.69	0.40
1:I:341:THR:HG22	1:I:345:ILE:CD1	2.51	0.40
2:J:74:LEU:HD12	2:J:74:LEU:HA	1.90	0.40
3:K:170:ASP:O	3:K:171:SER:HB2	2.21	0.40
4:L:138:LEU:HD23	4:L:138:LEU:N	2.36	0.40
6:R:189:LEU:HD23	6:R:189:LEU:HA	1.88	0.40
2:B:136:LYS:HB3	2:B:138:ILE:HG23	2.02	0.40
1:E:202:THR:CG2	3:G:95:PRO:HG3	2.48	0.40
1:E:478:ASN:HD22	1:E:478:ASN:N	2.19	0.40
2:F:152:GLN:CD	2:F:152:GLN:H	2.29	0.40
3:G:14:SER:OG	3:G:15:PRO:HD2	2.20	0.40
4:H:100:ALA:C	4:H:100(B):GLU:N	2.80	0.40
1:I:100:MET:HE1	1:I:487:LYS:N	2.36	0.40
1:I:248:THR:HG22	1:I:486:TYR:CD2	2.56	0.40
2:J:104:SER:O	2:J:105:ASP:C	2.63	0.40
3:K:45:ARG:NH1	3:K:47:LEU:HD23	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:212:GLU:C	4:L:214:LYS:N	2.73	0.40
6:R:123:PRO:HD3	6:R:209:LYS:HD3	2.03	0.40
1:A:277:PHE:HB3	1:A:353:PHE:CZ	2.56	0.40
2:B:16:CYS:HB2	2:B:28:TRP:HZ2	1.84	0.40
2:B:83:ILE:H	2:B:83:ILE:HG13	1.73	0.40
2:B:87:GLU:O	2:B:88:ASP:HB2	2.21	0.40
2:B:136:LYS:HZ3	2:B:146:VAL:HG13	1.87	0.40
3:C:158:ASN:O	3:C:179:LEU:HD12	2.22	0.40
4:D:163:VAL:HG12	4:D:182:VAL:CB	2.42	0.40
2:F:36:ILE:HD13	2:F:49:SER:HB2	2.02	0.40
3:G:141:PRO:O	3:G:143:GLU:N	2.54	0.40
4:H:40:ALA:HB1	4:H:41:PRO:HD2	2.02	0.40
2:J:54:ARG:HH12	2:J:75:LYS:HG3	1.86	0.40
2:J:140:GLY:O	2:J:144:LEU:HD11	2.21	0.40
4:L:143:LYS:HG2	4:L:144:ASP:N	2.35	0.40
6:R:146:PHE:HA	6:R:147:PRO:HA	1.88	0.40
1:A:122:LEU:HB3	1:A:198:THR:CG2	2.52	0.40
1:A:335:LYS:CD	1:A:408:ASN:HA	2.52	0.40
2:B:2:LYS:HB3	2:B:93:VAL:HG23	2.03	0.40
2:B:75:LYS:N	2:B:78:ASP:OD2	2.41	0.40
3:C:2:ILE:HG12	3:C:27:GLU:CD	2.45	0.40
3:C:12:SER:HB3	3:C:105:GLU:OE1	2.22	0.40
1:E:292:VAL:CG1	1:E:333:LEU:HD11	2.50	0.40
1:E:387:SER:O	1:E:391:PHE:HD1	2.04	0.40
2:F:136:LYS:HB3	2:F:138:ILE:HG23	2.02	0.40
2:F:164:ASN:C	2:F:166:LYS:N	2.78	0.40
3:G:108:ARG:NE	3:G:170:ASP:O	2.54	0.40
3:G:174:SER:HG	4:H:164:HIS:CE1	2.38	0.40
4:H:186:SER:C	4:H:188:SER:N	2.80	0.40
1:I:117:LYS:HA	1:I:118:PRO:HD3	1.85	0.40
1:I:377:ASN:HD21	1:I:380:GLY:C	2.30	0.40
2:J:116:LEU:O	2:J:143:THR:HG23	2.21	0.40
3:K:108:ARG:NE	3:K:170:ASP:O	2.54	0.40
3:K:135:LEU:CD2	3:K:137:ASN:N	2.85	0.40
3:C:108:ARG:NE	3:C:170:ASP:O	2.54	0.40
3:C:187:GLU:O	3:C:211:ARG:CZ	2.69	0.40
4:D:139:GLY:HA2	4:D:154:TRP:CZ2	2.57	0.40
1:E:100:MET:HE1	1:E:487:LYS:N	2.36	0.40
1:E:122:LEU:HB3	1:E:198:THR:CG2	2.52	0.40
2:F:54:ARG:HH12	2:F:75:LYS:HG3	1.86	0.40
3:G:150:VAL:HG11	3:G:189:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:139:GLY:HA2	4:H:154:TRP:CZ2	2.57	0.40
2:J:10:ASP:OD1	2:J:11:THR:N	2.41	0.40
2:J:27:HIS:ND1	2:J:38:GLY:HA3	2.36	0.40
3:K:150:VAL:O	3:K:153:ALA:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	17
1	E	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	17
1	I	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	17
2	B	179/181 (99%)	127 (71%)	38 (21%)	14 (8%)	1	10
2	F	179/181 (99%)	127 (71%)	38 (21%)	14 (8%)	1	10
2	J	179/181 (99%)	128 (72%)	37 (21%)	14 (8%)	1	10
3	C	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	1	13
3	G	212/214 (99%)	171 (81%)	29 (14%)	12 (6%)	1	14
3	K	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	1	13
4	D	227/229 (99%)	185 (82%)	35 (15%)	7 (3%)	3	22
4	H	227/229 (99%)	185 (82%)	35 (15%)	7 (3%)	3	22
4	L	227/229 (99%)	184 (81%)	36 (16%)	7 (3%)	3	22
5	M	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
5	O	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
5	Q	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
6	N	220/244 (90%)	219 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	P	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
6	R	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
All	All	4062/4188 (97%)	3465 (85%)	454 (11%)	143 (4%)	4	20

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	A	409	ASN
1	A	475	MET
2	B	109	LEU
2	B	165	GLN
2	B	179	PHE
3	C	26	SER
3	C	76	SER
3	C	138	ASN
4	D	127	SER
1	E	268	GLU
1	E	409	ASN
1	E	475	MET
2	F	109	LEU
2	F	165	GLN
2	F	179	PHE
3	G	26	SER
3	G	76	SER
3	G	138	ASN
4	H	127	SER
1	I	268	GLU
1	I	409	ASN
1	I	475	MET
2	J	109	LEU
2	J	165	GLN
2	J	179	PHE
3	K	26	SER
3	K	76	SER
3	K	138	ASN
4	L	127	SER
1	A	194	GLY
1	A	220	PRO
1	A	253	PRO
1	A	395	ASP

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Mol	Chain	Res	Type
1	A	463	ASN
1	A	464	GLY
2	B	68	PRO
2	B	105	ASP
2	B	178	ALA
2	B	180	GLN
3	C	158	ASN
3	C	211	ARG
4	D	52(A)	THR
4	D	99	GLU
4	D	148	GLU
1	E	194	GLY
1	E	220	PRO
1	E	253	PRO
1	E	395	ASP
1	E	463	ASN
1	E	464	GLY
2	F	68	PRO
2	F	105	ASP
2	F	178	ALA
2	F	180	GLN
3	G	158	ASN
3	G	211	ARG
4	H	52(A)	THR
4	H	99	GLU
4	H	148	GLU
1	I	194	GLY
1	I	220	PRO
1	I	253	PRO
1	I	395	ASP
1	I	463	ASN
1	I	464	GLY
2	J	68	PRO
2	J	105	ASP
2	J	178	ALA
2	J	180	GLN
3	K	158	ASN
3	K	211	ARG
4	L	52(A)	THR
4	L	99	GLU
4	L	148	GLU
1	A	210	PHE

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Mol	Chain	Res	Type
1	A	276	ASN
2	B	154	SER
3	C	78	LEU
1	E	210	PHE
1	E	276	ASN
2	F	154	SER
3	G	78	LEU
1	I	210	PHE
1	I	276	ASN
2	J	154	SER
3	K	78	LEU
4	L	213	PRO
1	A	481	SER
2	B	16	CYS
2	B	164	ASN
3	C	110	VAL
3	C	142	ARG
4	D	193	THR
4	D	213	PRO
1	E	481	SER
2	F	16	CYS
2	F	164	ASN
3	G	110	VAL
3	G	142	ARG
4	H	193	THR
4	H	213	PRO
1	I	481	SER
2	J	16	CYS
2	J	164	ASN
3	K	110	VAL
3	K	142	ARG
4	L	193	THR
1	A	407	LEU
2	B	2	LYS
2	B	56	ASP
2	B	147	SER
3	C	182	SER
1	E	407	LEU
2	F	56	ASP
2	F	147	SER
3	G	182	SER
1	I	407	LEU

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Mol	Chain	Res	Type
2	J	56	ASP
2	J	147	SER
3	K	182	SER
2	B	135	GLY
2	F	2	LYS
2	F	135	GLY
2	J	2	LYS
2	J	135	GLY
1	A	441	GLY
1	E	441	GLY
1	I	441	GLY
3	C	44	PRO
3	G	44	PRO
3	K	44	PRO
3	C	128	GLY
3	G	128	GLY
3	K	128	GLY
3	C	157	GLY
3	G	157	GLY
3	K	157	GLY
4	D	147	PRO
4	H	147	PRO
4	L	147	PRO
3	C	95	PRO
3	K	95	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/276 (98%)	257 (95%)	14 (5%)	21	42
1	E	271/276 (98%)	257 (95%)	14 (5%)	21	42
1	I	271/276 (98%)	257 (95%)	14 (5%)	21	42
2	B	164/164 (100%)	147 (90%)	17 (10%)	7	22
2	F	164/164 (100%)	147 (90%)	17 (10%)	7	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	164/164 (100%)	147 (90%)	17 (10%)	7	22
3	C	184/184 (100%)	170 (92%)	14 (8%)	12	33
3	G	184/184 (100%)	171 (93%)	13 (7%)	13	35
3	K	184/184 (100%)	167 (91%)	17 (9%)	8	27
4	D	193/193 (100%)	181 (94%)	12 (6%)	16	38
4	H	193/193 (100%)	181 (94%)	12 (6%)	16	38
4	L	193/193 (100%)	181 (94%)	12 (6%)	16	38
5	M	174/182 (96%)	162 (93%)	12 (7%)	14	36
5	O	174/182 (96%)	162 (93%)	12 (7%)	14	36
5	Q	174/182 (96%)	162 (93%)	12 (7%)	14	36
6	N	183/210 (87%)	173 (94%)	10 (6%)	19	41
6	P	183/210 (87%)	173 (94%)	10 (6%)	19	41
6	R	183/210 (87%)	173 (94%)	10 (6%)	19	41
All	All	3507/3627 (97%)	3268 (93%)	239 (7%)	16	36

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	120	VAL
1	A	123	THR
1	A	126	CYS
1	A	205	CYS
1	A	211	GLU
1	A	226	LEU
1	A	242	VAL
1	A	268	GLU
1	A	339	GLU
1	A	416	LEU
1	A	432	LYS
1	A	447	SER
1	A	488	VAL
2	B	1	LYS
2	B	2	LYS
2	B	14	LEU
2	B	40	GLN
2	B	64	GLN

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Mol	Chain	Res	Type
2	B	69	LEU
2	B	73	ASN
2	B	76	ILE
2	B	77	GLU
2	B	89	GLN
2	B	103	ASN
2	B	128	VAL
2	B	137	ASN
2	B	148	GLN
2	B	152	GLN
2	B	167	LYS
2	B	177	LEU
3	C	3	VAL
3	C	17	GLU
3	C	46	LEU
3	C	53	THR
3	C	73	LEU
3	C	74	THR
3	C	92	ASN
3	C	103	ARG
3	C	105	GLU
3	C	106	ILE
3	C	137	ASN
3	C	138	ASN
3	C	141	PRO
3	C	169	LYS
4	D	37	VAL
4	D	38	ARG
4	D	46	GLU
4	D	54	LEU
4	D	66	ARG
4	D	74	SER
4	D	105	GLN
4	D	110	THR
4	D	148	GLU
4	D	149	PRO
4	D	178	LEU
4	D	206	LYS
1	E	103	GLN
1	E	120	VAL
1	E	123	THR
1	E	126	CYS

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Mol	Chain	Res	Type
1	E	205	CYS
1	E	211	GLU
1	E	226	LEU
1	E	242	VAL
1	E	268	GLU
1	E	339	GLU
1	E	416	LEU
1	E	432	LYS
1	E	447	SER
1	E	488	VAL
2	F	1	LYS
2	F	2	LYS
2	F	14	LEU
2	F	40	GLN
2	F	64	GLN
2	F	69	LEU
2	F	73	ASN
2	F	76	ILE
2	F	77	GLU
2	F	89	GLN
2	F	103	ASN
2	F	128	VAL
2	F	137	ASN
2	F	148	GLN
2	F	152	GLN
2	F	167	LYS
2	F	177	LEU
3	G	3	VAL
3	G	17	GLU
3	G	46	LEU
3	G	53	THR
3	G	73	LEU
3	G	74	THR
3	G	92	ASN
3	G	103	ARG
3	G	106	ILE
3	G	137	ASN
3	G	138	ASN
3	G	141	PRO
3	G	169	LYS
4	H	37	VAL
4	H	38	ARG

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Mol	Chain	Res	Type
4	H	46	GLU
4	H	54	LEU
4	H	66	ARG
4	H	74	SER
4	H	105	GLN
4	H	110	THR
4	H	148	GLU
4	H	149	PRO
4	H	178	LEU
4	H	206	LYS
1	I	103	GLN
1	I	120	VAL
1	I	123	THR
1	I	126	CYS
1	I	205	CYS
1	I	211	GLU
1	I	226	LEU
1	I	242	VAL
1	I	268	GLU
1	I	339	GLU
1	I	416	LEU
1	I	432	LYS
1	I	447	SER
1	I	488	VAL
2	J	1	LYS
2	J	2	LYS
2	J	14	LEU
2	J	40	GLN
2	J	64	GLN
2	J	69	LEU
2	J	73	ASN
2	J	76	ILE
2	J	77	GLU
2	J	89	GLN
2	J	103	ASN
2	J	128	VAL
2	J	137	ASN
2	J	148	GLN
2	J	152	GLN
2	J	167	LYS
2	J	177	LEU
3	K	3	VAL

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Mol	Chain	Res	Type
3	K	17	GLU
3	K	46	LEU
3	K	53	THR
3	K	73	LEU
3	K	74	THR
3	K	92	ASN
3	K	95	PRO
3	K	95(A)	PRO
3	K	95(B)	ARG
3	K	103	ARG
3	K	105	GLU
3	K	106	ILE
3	K	137	ASN
3	K	138	ASN
3	K	141	PRO
3	K	169	LYS
4	L	37	VAL
4	L	38	ARG
4	L	46	GLU
4	L	54	LEU
4	L	66	ARG
4	L	74	SER
4	L	105	GLN
4	L	110	THR
4	L	148	GLU
4	L	149	PRO
4	L	178	LEU
4	L	206	LYS
5	M	1	ASP
5	M	7	SER
5	M	12	SER
5	M	19	VAL
5	M	50	ARG
5	M	78	LEU
5	M	79	GLN
5	M	93	THR
5	M	108	ARG
5	M	123	GLU
5	M	146	VAL
5	M	181	LEU
6	N	66	ARG
6	N	67	VAL

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Mol	Chain	Res	Type
6	N	94	THR
6	N	107	THR
6	N	116	THR
6	N	161	SER
6	N	178	LEU
6	N	182	VAL
6	N	207	VAL
6	N	209	LYS
5	O	1	ASP
5	O	7	SER
5	O	12	SER
5	O	19	VAL
5	O	50	ARG
5	O	78	LEU
5	O	79	GLN
5	O	93	THR
5	O	108	ARG
5	O	123	GLU
5	O	146	VAL
5	O	181	LEU
6	P	66	ARG
6	P	67	VAL
6	P	94	THR
6	P	107	THR
6	P	116	THR
6	P	161	SER
6	P	178	LEU
6	P	182	VAL
6	P	207	VAL
6	P	209	LYS
5	Q	1	ASP
5	Q	7	SER
5	Q	12	SER
5	Q	19	VAL
5	Q	50	ARG
5	Q	78	LEU
5	Q	79	GLN
5	Q	93	THR
5	Q	108	ARG
5	Q	123	GLU
5	Q	146	VAL
5	Q	181	LEU

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Mol	Chain	Res	Type
6	R	66	ARG
6	R	67	VAL
6	R	94	THR
6	R	107	THR
6	R	116	THR
6	R	161	SER
6	R	178	LEU
6	R	182	VAL
6	R	207	VAL
6	R	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	94	ASN
1	A	114	GLN
1	A	246	GLN
1	A	279	ASN
1	A	340	ASN
1	A	344	GLN
1	A	355	ASN
1	A	362	ASN
1	A	425	ASN
1	A	478	ASN
2	B	20	GLN
2	B	33	GLN
2	B	73	ASN
2	B	103	ASN
2	B	137	ASN
2	B	165	GLN
3	C	79	GLN
3	C	100	GLN
3	C	198	HIS
3	C	199	GLN
3	C	210	ASN
4	D	82(B)	ASN
4	D	199	ASN
4	D	200	HIS
1	E	92	ASN
1	E	94	ASN
1	E	114	GLN

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Mol	Chain	Res	Type
1	E	246	GLN
1	E	279	ASN
1	E	340	ASN
1	E	344	GLN
1	E	355	ASN
1	E	362	ASN
1	E	478	ASN
2	F	20	GLN
2	F	33	GLN
2	F	73	ASN
2	F	103	ASN
2	F	165	GLN
3	G	100	GLN
3	G	198	HIS
3	G	199	GLN
4	H	82(B)	ASN
4	H	199	ASN
4	H	200	HIS
1	I	92	ASN
1	I	94	ASN
1	I	114	GLN
1	I	246	GLN
1	I	279	ASN
1	I	330	HIS
1	I	332	ASN
1	I	340	ASN
1	I	344	GLN
1	I	355	ASN
1	I	362	ASN
1	I	478	ASN
2	J	20	GLN
2	J	33	GLN
2	J	73	ASN
2	J	103	ASN
2	J	165	GLN
3	K	100	GLN
3	K	198	HIS
3	K	199	GLN
4	L	82(B)	ASN
4	L	199	ASN
4	L	200	HIS
5	M	38	GLN

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Mol	Chain	Res	Type
5	M	155	GLN
5	M	160	GLN
6	N	39	GLN
6	N	62	HIS
6	N	100(F)	HIS
6	N	199	ASN
5	O	38	GLN
5	O	155	GLN
5	O	160	GLN
6	P	39	GLN
6	P	62	HIS
6	P	100(F)	HIS
6	P	199	ASN
5	Q	38	GLN
5	Q	155	GLN
5	Q	160	GLN
6	R	39	GLN
6	R	62	HIS
6	R	100(F)	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

45 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	856	1	14,14,15	0.80	0	17,19,21	0.73	0
7	NAG	I	734	1	14,14,15	0.64	0	17,19,21	0.54	0
7	NAG	I	776	1	14,14,15	0.60	0	17,19,21	0.81	1 (5%)
7	NAG	I	908	1	14,14,15	0.63	0	17,19,21	0.64	0
7	NAG	R	1000	6	14,14,15	1.60	1 (7%)	17,19,21	1.38	1 (5%)
7	NAG	N	1000	6	14,14,15	1.60	1 (7%)	17,19,21	1.39	1 (5%)
7	NAG	I	886	1	14,14,15	0.69	0	17,19,21	1.07	2 (11%)
7	NAG	I	894	1	14,14,15	0.68	0	17,19,21	0.77	1 (5%)
7	NAG	A	697	1	14,14,15	0.68	0	17,19,21	0.67	0
7	NAG	E	795	1	14,14,15	0.52	0	17,19,21	0.76	0
7	NAG	E	741	1	14,14,15	0.58	0	17,19,21	0.64	0
7	NAG	A	776	1	14,14,15	0.61	0	17,19,21	0.80	1 (5%)
7	NAG	A	894	1	14,14,15	0.68	0	17,19,21	0.77	1 (5%)
7	NAG	A	908	1	14,14,15	0.66	0	17,19,21	0.64	0
7	NAG	I	948	1	14,14,15	0.93	1 (7%)	17,19,21	0.98	1 (5%)
7	NAG	E	963	1	14,14,15	0.78	0	17,19,21	0.68	0
7	NAG	A	762	1	14,14,15	0.64	0	17,19,21	0.76	1 (5%)
7	NAG	I	789	1	14,14,15	0.67	0	17,19,21	0.92	1 (5%)
7	NAG	I	856	1	14,14,15	0.80	0	17,19,21	0.74	0
7	NAG	E	908	1	14,14,15	0.65	0	17,19,21	0.64	0
7	NAG	E	886	1	14,14,15	0.69	0	17,19,21	1.06	2 (11%)
7	NAG	I	588	1	14,14,15	0.64	0	17,19,21	0.82	0
7	NAG	I	795	1	14,14,15	0.51	0	17,19,21	0.77	0
7	NAG	I	963	1	14,14,15	0.78	0	17,19,21	0.68	0
7	NAG	A	795	1	14,14,15	0.52	0	17,19,21	0.76	0
7	NAG	E	762	1	14,14,15	0.64	0	17,19,21	0.76	1 (5%)
7	NAG	A	789	1	14,14,15	0.67	0	17,19,21	0.90	0
7	NAG	A	886	1	14,14,15	0.69	0	17,19,21	1.07	2 (11%)
7	NAG	E	697	1	14,14,15	0.68	0	17,19,21	0.68	0
7	NAG	E	776	1	14,14,15	0.60	0	17,19,21	0.80	1 (5%)
7	NAG	A	588	1	14,14,15	0.66	0	17,19,21	0.83	1 (5%)
7	NAG	I	762	1	14,14,15	0.63	0	17,19,21	0.75	1 (5%)
7	NAG	A	734	1	14,14,15	0.64	0	17,19,21	0.53	0
7	NAG	I	741	1	14,14,15	0.59	0	17,19,21	0.63	0
7	NAG	A	963	1	14,14,15	0.79	0	17,19,21	0.68	0
7	NAG	E	789	1	14,14,15	0.67	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	E	948	1	14,14,15	0.94	1 (7%)	17,19,21	0.98	1 (5%)
7	NAG	I	697	1	14,14,15	0.67	0	17,19,21	0.67	0
7	NAG	E	588	1	14,14,15	0.65	0	17,19,21	0.81	0
7	NAG	E	856	1	14,14,15	0.79	0	17,19,21	0.74	0
7	NAG	E	734	1	14,14,15	0.65	0	17,19,21	0.53	0
7	NAG	A	948	1	14,14,15	0.92	1 (7%)	17,19,21	0.98	1 (5%)
7	NAG	P	1000	6	14,14,15	1.61	1 (7%)	17,19,21	1.39	1 (5%)
7	NAG	E	894	1	14,14,15	0.70	0	17,19,21	0.76	1 (5%)
7	NAG	A	741	1	14,14,15	0.59	0	17,19,21	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	856	1	-	5/6/23/26	0/1/1/1
7	NAG	I	734	1	-	5/6/23/26	0/1/1/1
7	NAG	I	776	1	-	2/6/23/26	0/1/1/1
7	NAG	I	908	1	-	2/6/23/26	0/1/1/1
7	NAG	R	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	N	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	I	886	1	-	4/6/23/26	0/1/1/1
7	NAG	I	894	1	-	4/6/23/26	0/1/1/1
7	NAG	A	697	1	-	5/6/23/26	0/1/1/1
7	NAG	E	795	1	-	2/6/23/26	0/1/1/1
7	NAG	E	741	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	776	1	-	2/6/23/26	0/1/1/1
7	NAG	A	894	1	-	4/6/23/26	0/1/1/1
7	NAG	A	908	1	-	2/6/23/26	0/1/1/1
7	NAG	I	948	1	-	4/6/23/26	0/1/1/1
7	NAG	E	963	1	-	5/6/23/26	0/1/1/1
7	NAG	A	762	1	-	5/6/23/26	0/1/1/1
7	NAG	I	789	1	-	4/6/23/26	0/1/1/1
7	NAG	I	856	1	-	5/6/23/26	0/1/1/1
7	NAG	E	908	1	-	2/6/23/26	0/1/1/1
7	NAG	E	886	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	588	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	I	795	1	-	2/6/23/26	0/1/1/1
7	NAG	I	963	1	-	5/6/23/26	0/1/1/1
7	NAG	A	795	1	-	2/6/23/26	0/1/1/1
7	NAG	E	762	1	-	5/6/23/26	0/1/1/1
7	NAG	A	789	1	-	4/6/23/26	0/1/1/1
7	NAG	A	886	1	-	4/6/23/26	0/1/1/1
7	NAG	E	697	1	-	5/6/23/26	0/1/1/1
7	NAG	E	776	1	-	2/6/23/26	0/1/1/1
7	NAG	A	588	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	I	762	1	-	5/6/23/26	0/1/1/1
7	NAG	A	734	1	-	5/6/23/26	0/1/1/1
7	NAG	I	741	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	963	1	-	5/6/23/26	0/1/1/1
7	NAG	E	789	1	-	4/6/23/26	0/1/1/1
7	NAG	E	948	1	-	4/6/23/26	0/1/1/1
7	NAG	I	697	1	-	5/6/23/26	0/1/1/1
7	NAG	E	588	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	E	856	1	-	5/6/23/26	0/1/1/1
7	NAG	E	734	1	-	5/6/23/26	0/1/1/1
7	NAG	A	948	1	-	4/6/23/26	0/1/1/1
7	NAG	P	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	E	894	1	-	4/6/23/26	0/1/1/1
7	NAG	A	741	1	1/1/5/7	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	1000	NAG	O5-C1	-5.60	1.34	1.43
7	N	1000	NAG	O5-C1	-5.59	1.34	1.43
7	R	1000	NAG	O5-C1	-5.57	1.34	1.43
7	I	948	NAG	C1-C2	2.79	1.56	1.52
7	E	948	NAG	C1-C2	2.76	1.56	1.52
7	A	948	NAG	C1-C2	2.74	1.56	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	1000	NAG	C1-O5-C5	-4.78	105.78	112.19
7	N	1000	NAG	C1-O5-C5	-4.76	105.81	112.19
7	R	1000	NAG	C1-O5-C5	-4.75	105.82	112.19
7	I	886	NAG	C2-N2-C7	-2.85	119.08	122.90
7	A	886	NAG	C2-N2-C7	-2.82	119.12	122.90
7	E	886	NAG	C2-N2-C7	-2.81	119.13	122.90
7	A	762	NAG	C2-N2-C7	-2.38	119.71	122.90
7	E	762	NAG	C2-N2-C7	-2.33	119.78	122.90
7	I	762	NAG	C2-N2-C7	-2.31	119.80	122.90
7	A	894	NAG	C2-N2-C7	-2.27	119.85	122.90
7	I	894	NAG	C2-N2-C7	-2.26	119.87	122.90
7	E	894	NAG	C2-N2-C7	-2.22	119.93	122.90
7	I	948	NAG	C2-N2-C7	-2.19	119.97	122.90
7	E	948	NAG	C2-N2-C7	-2.15	120.02	122.90
7	A	948	NAG	C2-N2-C7	-2.14	120.04	122.90
7	I	776	NAG	C2-N2-C7	-2.13	120.05	122.90
7	A	776	NAG	C2-N2-C7	-2.12	120.06	122.90
7	E	776	NAG	C2-N2-C7	-2.11	120.08	122.90
7	A	886	NAG	C4-C3-C2	-2.09	107.95	111.02
7	I	886	NAG	C4-C3-C2	-2.08	107.97	111.02
7	A	588	NAG	C2-N2-C7	-2.07	120.12	122.90
7	I	789	NAG	C2-N2-C7	-2.06	120.14	122.90
7	E	886	NAG	C4-C3-C2	-2.04	108.02	111.02
7	E	789	NAG	C2-N2-C7	-2.02	120.19	122.90

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	588	NAG	C1
7	A	741	NAG	C1
7	E	588	NAG	C1
7	E	741	NAG	C1
7	I	588	NAG	C1
7	I	741	NAG	C1

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	588	NAG	C8-C7-N2-C2
7	A	588	NAG	O7-C7-N2-C2
7	A	697	NAG	C1-C2-N2-C7
7	A	697	NAG	C8-C7-N2-C2
7	A	697	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	734	NAG	C8-C7-N2-C2
7	A	734	NAG	O7-C7-N2-C2
7	A	741	NAG	C8-C7-N2-C2
7	A	741	NAG	O7-C7-N2-C2
7	A	762	NAG	C8-C7-N2-C2
7	A	762	NAG	O7-C7-N2-C2
7	A	776	NAG	C8-C7-N2-C2
7	A	776	NAG	O7-C7-N2-C2
7	A	789	NAG	C8-C7-N2-C2
7	A	789	NAG	O7-C7-N2-C2
7	A	795	NAG	C8-C7-N2-C2
7	A	795	NAG	O7-C7-N2-C2
7	A	856	NAG	C8-C7-N2-C2
7	A	856	NAG	O7-C7-N2-C2
7	A	886	NAG	C8-C7-N2-C2
7	A	886	NAG	O7-C7-N2-C2
7	A	894	NAG	C8-C7-N2-C2
7	A	894	NAG	O7-C7-N2-C2
7	A	908	NAG	C8-C7-N2-C2
7	A	908	NAG	O7-C7-N2-C2
7	A	948	NAG	C8-C7-N2-C2
7	A	948	NAG	O7-C7-N2-C2
7	A	963	NAG	C8-C7-N2-C2
7	A	963	NAG	O7-C7-N2-C2
7	E	588	NAG	C8-C7-N2-C2
7	E	588	NAG	O7-C7-N2-C2
7	E	697	NAG	C1-C2-N2-C7
7	E	697	NAG	C8-C7-N2-C2
7	E	697	NAG	O7-C7-N2-C2
7	E	734	NAG	C8-C7-N2-C2
7	E	734	NAG	O7-C7-N2-C2
7	E	741	NAG	C8-C7-N2-C2
7	E	741	NAG	O7-C7-N2-C2
7	E	762	NAG	C8-C7-N2-C2
7	E	762	NAG	O7-C7-N2-C2
7	E	776	NAG	C8-C7-N2-C2
7	E	776	NAG	O7-C7-N2-C2
7	E	789	NAG	C8-C7-N2-C2
7	E	789	NAG	O7-C7-N2-C2
7	E	795	NAG	C8-C7-N2-C2
7	E	795	NAG	O7-C7-N2-C2
7	E	856	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	E	856	NAG	O7-C7-N2-C2
7	E	886	NAG	C8-C7-N2-C2
7	E	886	NAG	O7-C7-N2-C2
7	E	894	NAG	C8-C7-N2-C2
7	E	894	NAG	O7-C7-N2-C2
7	E	908	NAG	C8-C7-N2-C2
7	E	908	NAG	O7-C7-N2-C2
7	E	948	NAG	C8-C7-N2-C2
7	E	948	NAG	O7-C7-N2-C2
7	E	963	NAG	C8-C7-N2-C2
7	E	963	NAG	O7-C7-N2-C2
7	I	588	NAG	C8-C7-N2-C2
7	I	588	NAG	O7-C7-N2-C2
7	I	697	NAG	C1-C2-N2-C7
7	I	697	NAG	C8-C7-N2-C2
7	I	697	NAG	O7-C7-N2-C2
7	I	734	NAG	C8-C7-N2-C2
7	I	734	NAG	O7-C7-N2-C2
7	I	741	NAG	C8-C7-N2-C2
7	I	741	NAG	O7-C7-N2-C2
7	I	762	NAG	C8-C7-N2-C2
7	I	762	NAG	O7-C7-N2-C2
7	I	776	NAG	C8-C7-N2-C2
7	I	776	NAG	O7-C7-N2-C2
7	I	789	NAG	C8-C7-N2-C2
7	I	789	NAG	O7-C7-N2-C2
7	I	795	NAG	C8-C7-N2-C2
7	I	795	NAG	O7-C7-N2-C2
7	I	856	NAG	C8-C7-N2-C2
7	I	856	NAG	O7-C7-N2-C2
7	I	886	NAG	C8-C7-N2-C2
7	I	886	NAG	O7-C7-N2-C2
7	I	894	NAG	C8-C7-N2-C2
7	I	894	NAG	O7-C7-N2-C2
7	I	908	NAG	C8-C7-N2-C2
7	I	908	NAG	O7-C7-N2-C2
7	I	948	NAG	C8-C7-N2-C2
7	I	948	NAG	O7-C7-N2-C2
7	I	963	NAG	C8-C7-N2-C2
7	I	963	NAG	O7-C7-N2-C2
7	A	734	NAG	C4-C5-C6-O6
7	E	734	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	I	734	NAG	C4-C5-C6-O6
7	A	948	NAG	C4-C5-C6-O6
7	E	948	NAG	C4-C5-C6-O6
7	I	948	NAG	C4-C5-C6-O6
7	A	894	NAG	O5-C5-C6-O6
7	E	894	NAG	O5-C5-C6-O6
7	I	894	NAG	O5-C5-C6-O6
7	A	697	NAG	C4-C5-C6-O6
7	E	697	NAG	C4-C5-C6-O6
7	I	697	NAG	C4-C5-C6-O6
7	A	697	NAG	O5-C5-C6-O6
7	E	697	NAG	O5-C5-C6-O6
7	I	697	NAG	O5-C5-C6-O6
7	A	963	NAG	O5-C5-C6-O6
7	E	963	NAG	O5-C5-C6-O6
7	I	963	NAG	O5-C5-C6-O6
7	E	734	NAG	O5-C5-C6-O6
7	A	734	NAG	O5-C5-C6-O6
7	I	734	NAG	O5-C5-C6-O6
7	A	762	NAG	O5-C5-C6-O6
7	E	762	NAG	O5-C5-C6-O6
7	I	762	NAG	O5-C5-C6-O6
7	A	762	NAG	C4-C5-C6-O6
7	E	762	NAG	C4-C5-C6-O6
7	I	762	NAG	C4-C5-C6-O6
7	A	894	NAG	C4-C5-C6-O6
7	E	894	NAG	C4-C5-C6-O6
7	I	894	NAG	C4-C5-C6-O6
7	A	948	NAG	O5-C5-C6-O6
7	E	948	NAG	O5-C5-C6-O6
7	I	948	NAG	O5-C5-C6-O6
7	A	963	NAG	C4-C5-C6-O6
7	E	963	NAG	C4-C5-C6-O6
7	I	963	NAG	C4-C5-C6-O6
7	A	588	NAG	O5-C5-C6-O6
7	E	588	NAG	O5-C5-C6-O6
7	I	588	NAG	O5-C5-C6-O6
7	A	886	NAG	O5-C5-C6-O6
7	E	886	NAG	O5-C5-C6-O6
7	I	886	NAG	O5-C5-C6-O6
7	E	789	NAG	O5-C5-C6-O6
7	A	789	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	I	789	NAG	O5-C5-C6-O6
7	A	886	NAG	C4-C5-C6-O6
7	E	886	NAG	C4-C5-C6-O6
7	I	886	NAG	C4-C5-C6-O6
7	A	734	NAG	C3-C2-N2-C7
7	A	762	NAG	C3-C2-N2-C7
7	A	963	NAG	C3-C2-N2-C7
7	E	734	NAG	C3-C2-N2-C7
7	E	762	NAG	C3-C2-N2-C7
7	E	963	NAG	C3-C2-N2-C7
7	I	734	NAG	C3-C2-N2-C7
7	I	762	NAG	C3-C2-N2-C7
7	I	963	NAG	C3-C2-N2-C7
7	I	741	NAG	C4-C5-C6-O6
7	A	741	NAG	C4-C5-C6-O6
7	E	741	NAG	C4-C5-C6-O6
7	A	856	NAG	C4-C5-C6-O6
7	E	856	NAG	C4-C5-C6-O6
7	I	856	NAG	C4-C5-C6-O6
7	A	856	NAG	C1-C2-N2-C7
7	E	856	NAG	C1-C2-N2-C7
7	I	856	NAG	C1-C2-N2-C7
7	A	856	NAG	C3-C2-N2-C7
7	E	856	NAG	C3-C2-N2-C7
7	I	856	NAG	C3-C2-N2-C7
7	E	588	NAG	C4-C5-C6-O6
7	A	588	NAG	C4-C5-C6-O6
7	I	789	NAG	C4-C5-C6-O6
7	A	741	NAG	O5-C5-C6-O6
7	I	741	NAG	O5-C5-C6-O6
7	I	588	NAG	C4-C5-C6-O6
7	E	741	NAG	O5-C5-C6-O6
7	E	789	NAG	C4-C5-C6-O6
7	A	789	NAG	C4-C5-C6-O6

There are no ring outliers.

27 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	856	NAG	1	0
7	I	776	NAG	1	0
7	I	908	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	894	NAG	3	0
7	E	741	NAG	1	0
7	A	776	NAG	1	0
7	A	894	NAG	3	0
7	A	908	NAG	3	0
7	I	948	NAG	3	0
7	E	963	NAG	1	0
7	A	762	NAG	2	0
7	I	789	NAG	5	0
7	I	856	NAG	1	0
7	E	908	NAG	3	0
7	I	963	NAG	1	0
7	E	762	NAG	1	0
7	A	789	NAG	5	0
7	E	776	NAG	1	0
7	I	762	NAG	1	0
7	I	741	NAG	1	0
7	A	963	NAG	2	0
7	E	789	NAG	5	0
7	E	948	NAG	3	0
7	E	856	NAG	1	0
7	A	948	NAG	3	0
7	E	894	NAG	3	0
7	A	741	NAG	1	0

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-3086. These allow visual inspection of the internal detail of the map and identification of artifacts.

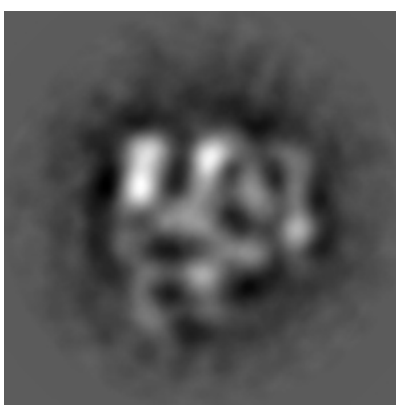
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

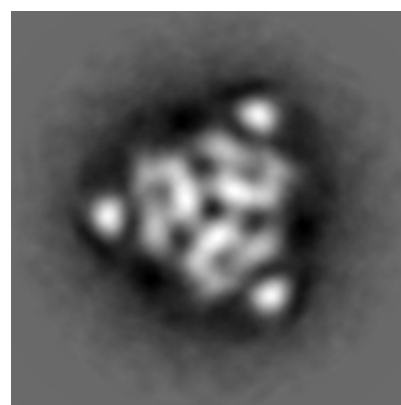
6.1.1 Primary map



X



Y

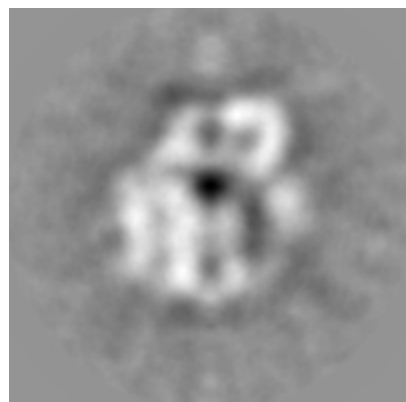


Z

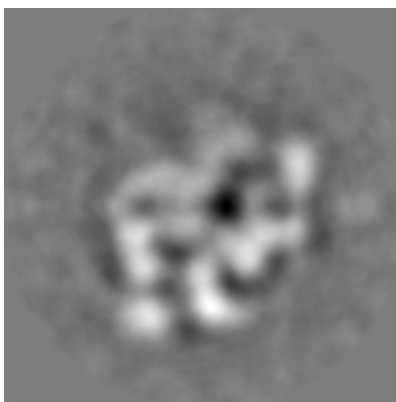
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

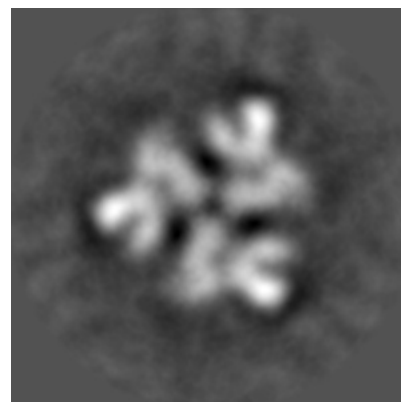
6.2.1 Primary map



X Index: 64



Y Index: 64

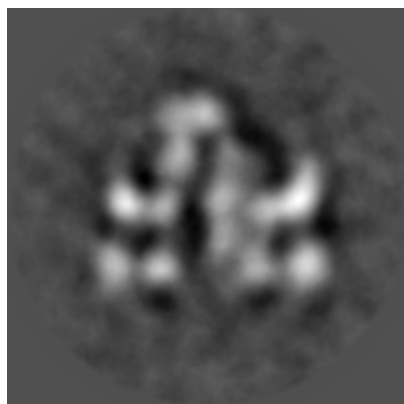


Z Index: 64

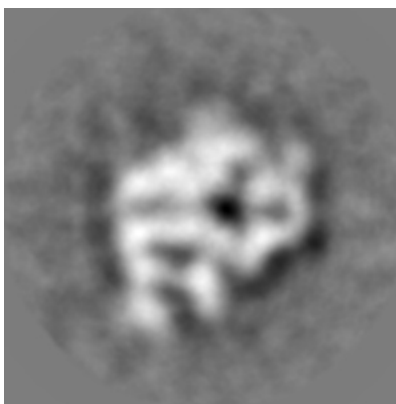
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

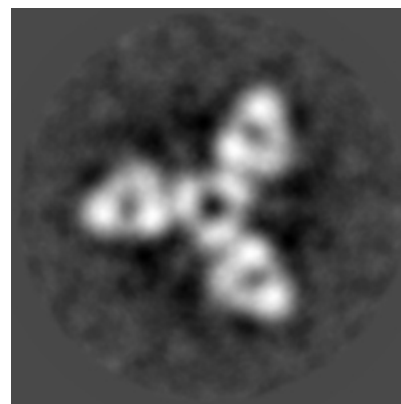
6.3.1 Primary map



X Index: 79



Y Index: 68

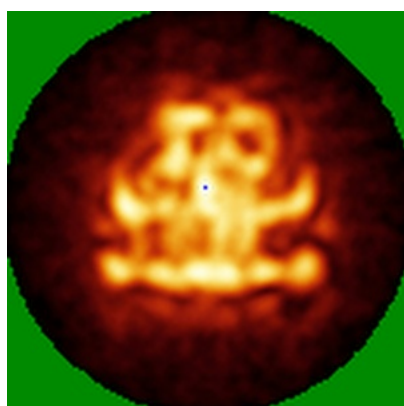


Z Index: 44

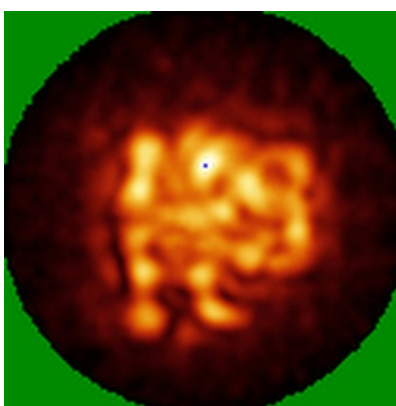
The images above show the largest variance slices of the map in three orthogonal directions.

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

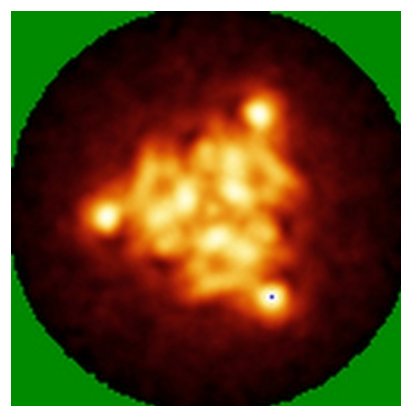
6.4.1 Primary map



X



Y

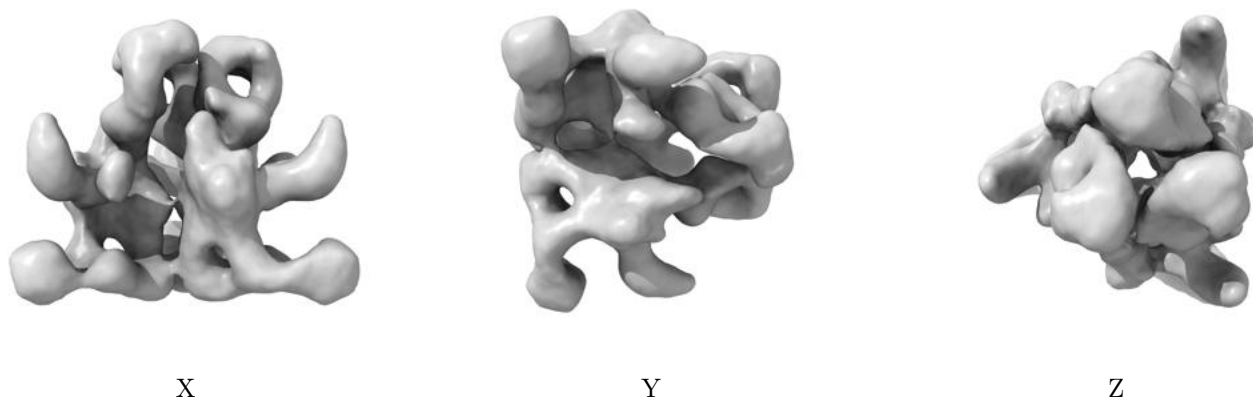


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0269. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

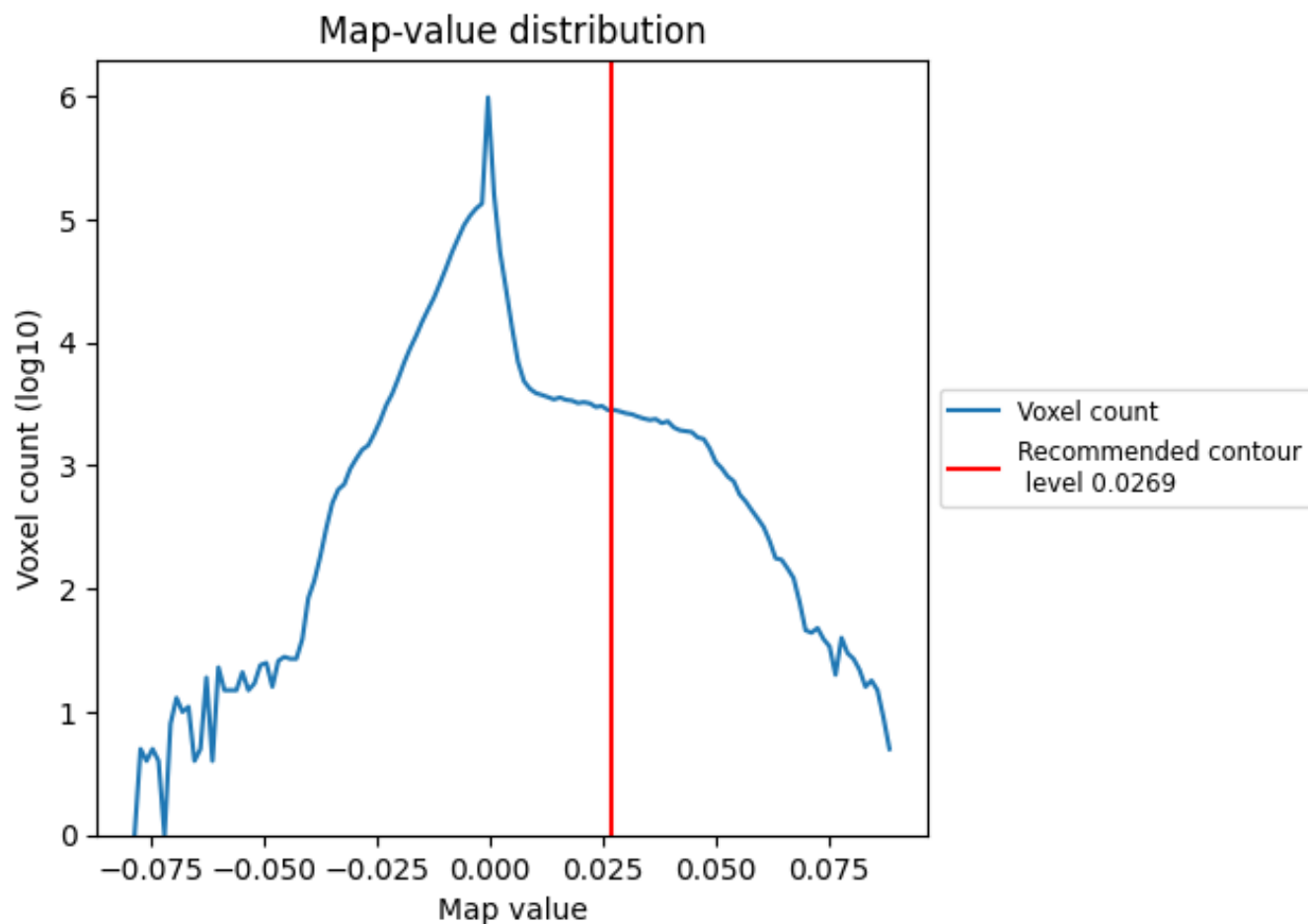
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

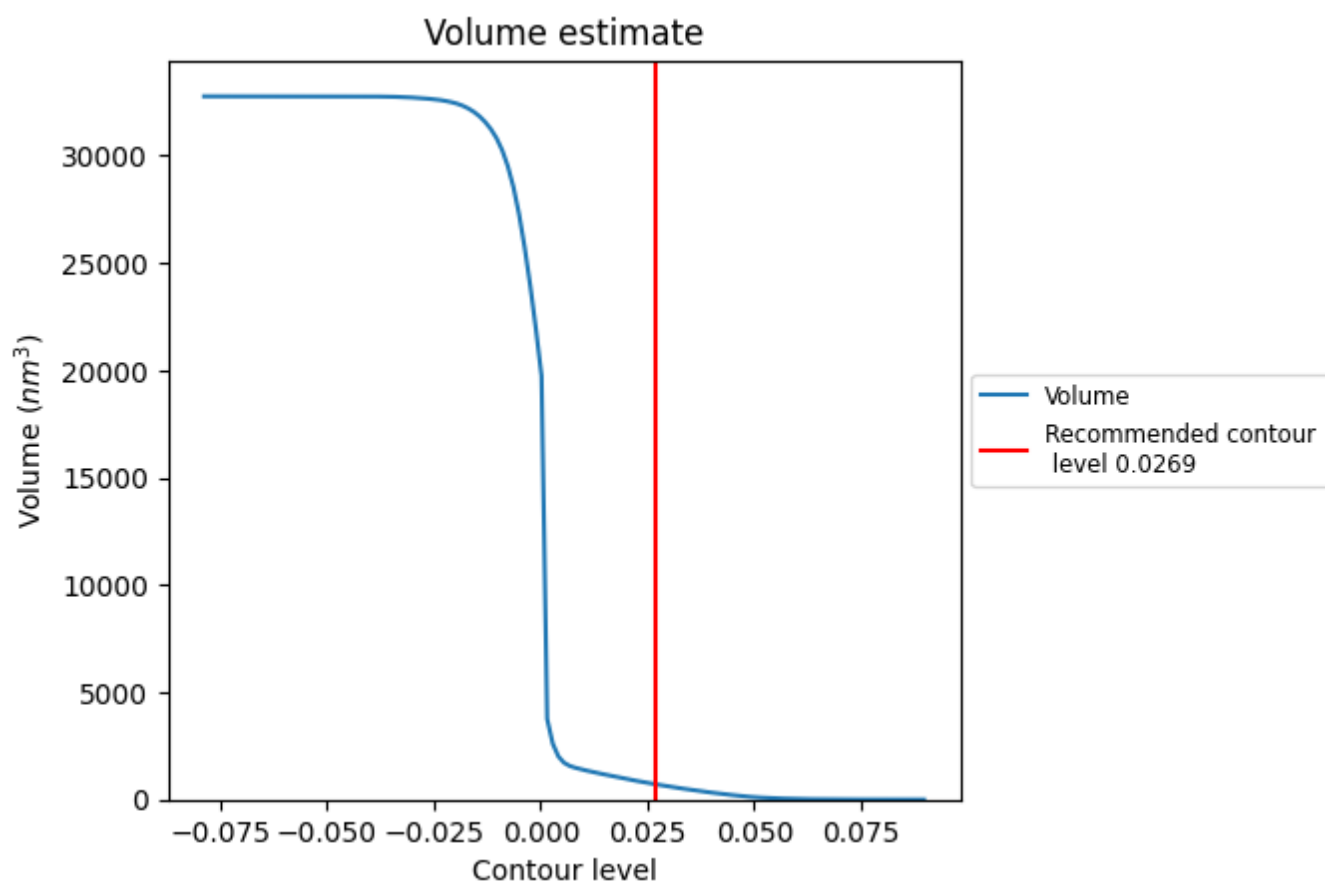
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

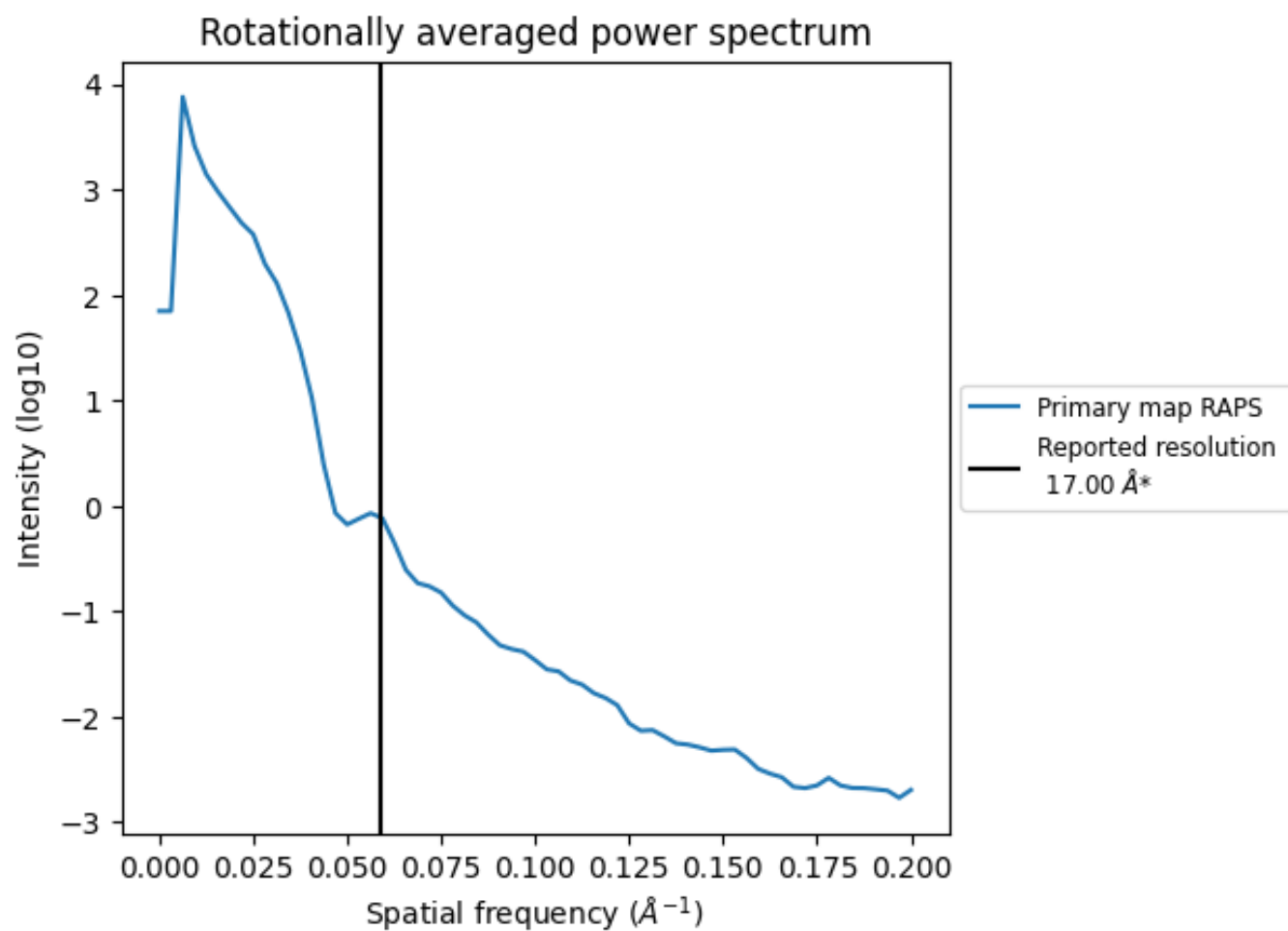
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 714 nm³; this corresponds to an approximate mass of 645 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 ⓘ

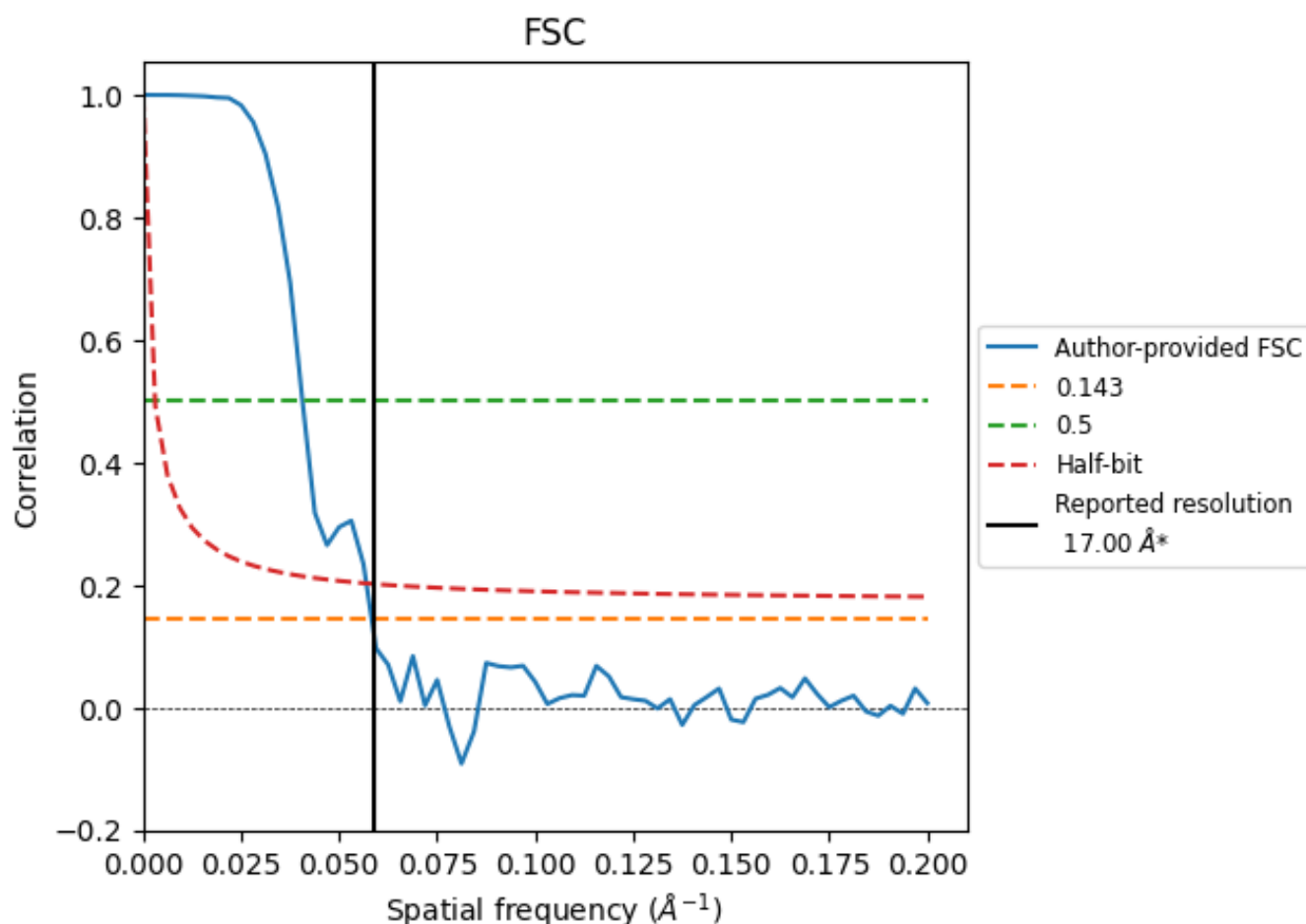


*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

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 0.059 Å⁻¹

8.2 Resolution estimates [i](#)

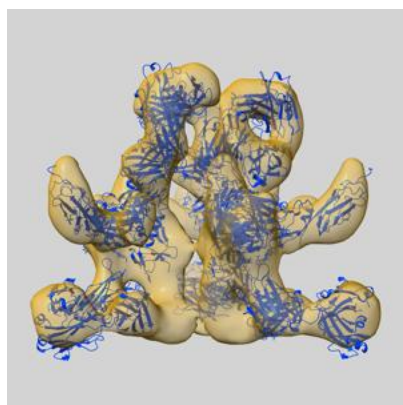
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	17.15	24.57	17.54
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

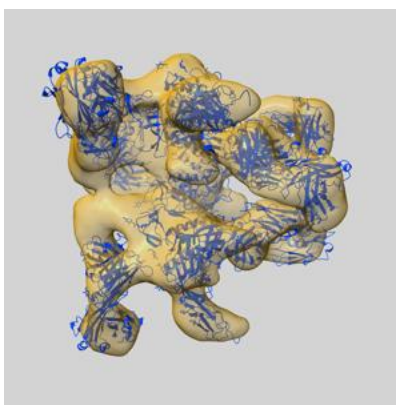
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3086 and PDB model 5A7X. Per-residue inclusion information can be found in section [3](#) on page [9](#).

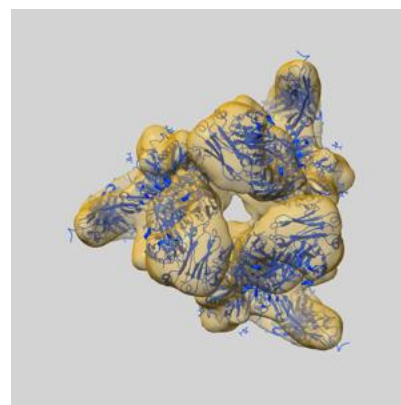
9.1 Map-model overlay [i](#)



X



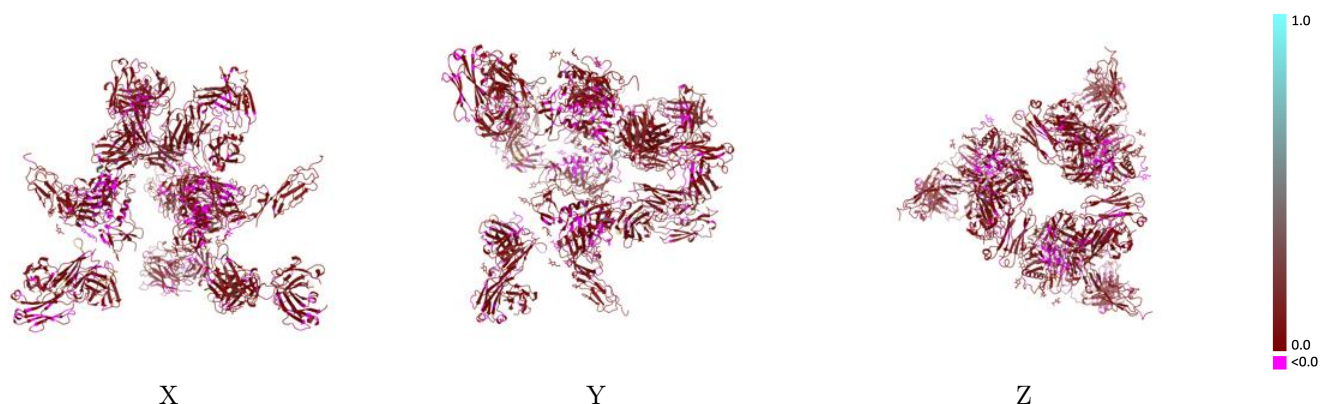
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0269 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

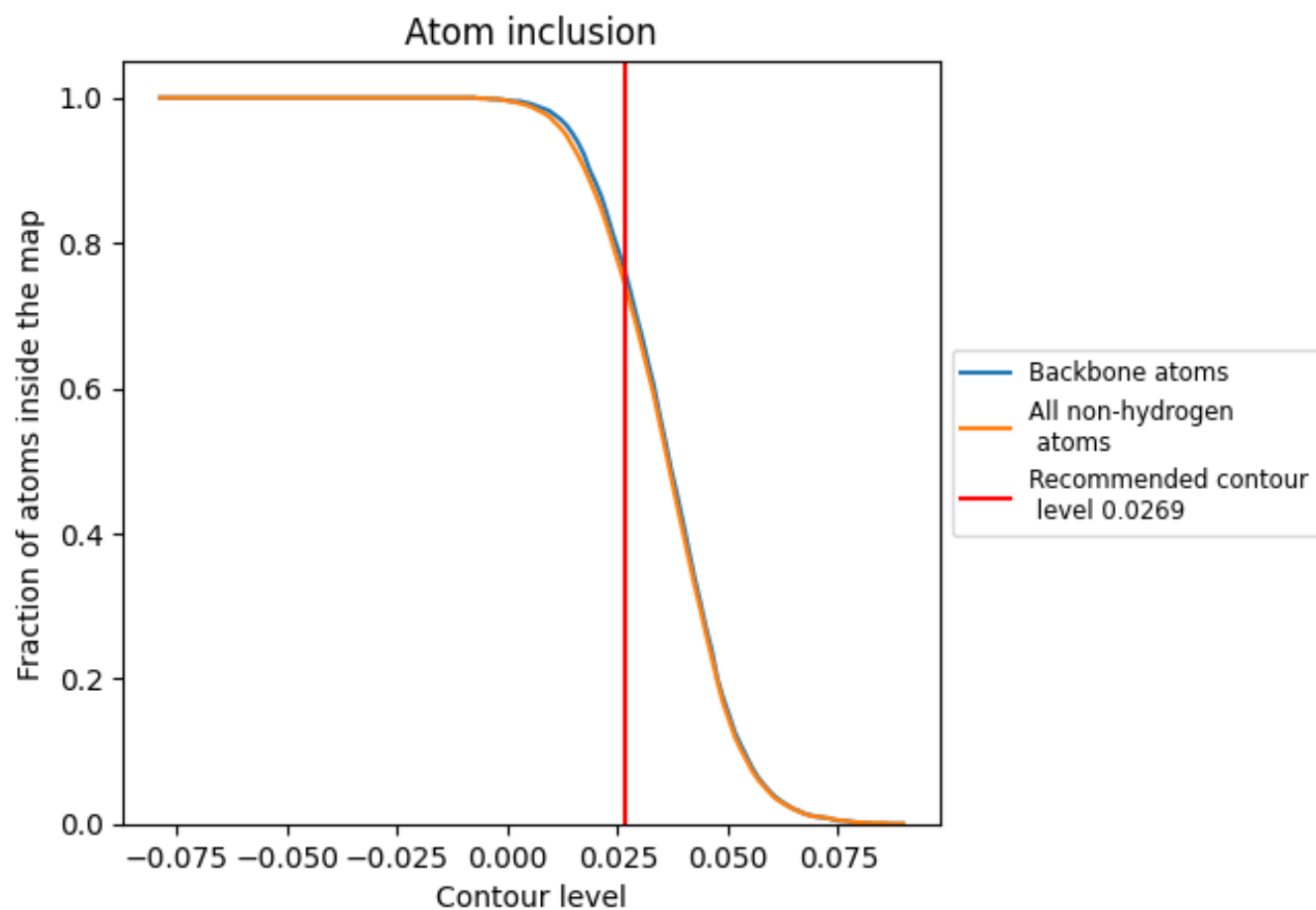


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.0269) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7380	 0.0650
A	 0.7520	 0.0580
B	 0.7560	 0.0730
C	 0.7900	 0.0780
D	 0.7410	 0.0650
E	 0.7530	 0.0550
F	 0.7530	 0.0730
G	 0.7890	 0.0760
H	 0.7420	 0.0680
I	 0.7520	 0.0570
J	 0.7550	 0.0760
K	 0.7890	 0.0760
L	 0.7420	 0.0650
M	 0.6610	 0.0530
N	 0.7160	 0.0680
O	 0.6590	 0.0520
P	 0.7210	 0.0710
Q	 0.6680	 0.0540
R	 0.7180	 0.0690

