



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 08:44 PM UTC

PDB ID : 3J0J / pdb_00003j0j
EMDB ID : EMD-5335
Title : Fitted atomic models of Thermus thermophilus V-ATPase subunits into cryo-EM map
Authors : Lau, W.C.Y.; Rubinstein, J.L.
Deposited on : 2011-08-24
Resolution : 9.70 Å (reported)
Based on initial models : 3K5B, 3A5C, 1R5Z

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:

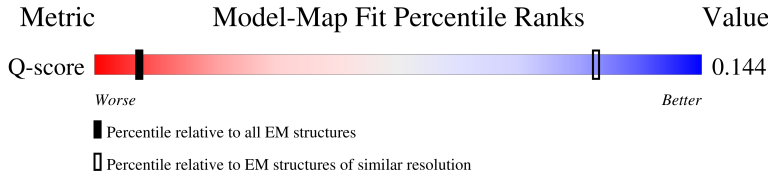
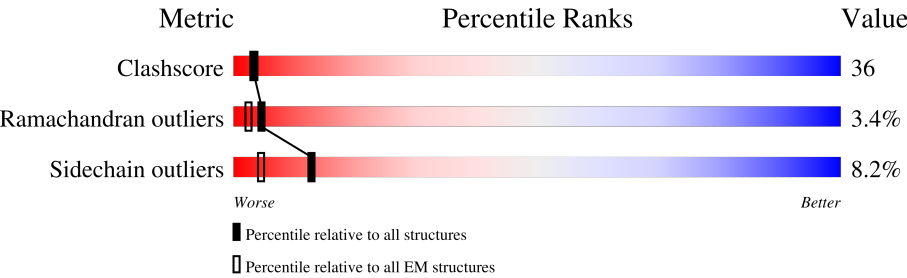
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 9.70 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	165 (9.20 - 10.20)

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	578	 79% 15% ...
1	B	578	 10% 82% 12% ...
1	C	578	 6% 81% 13% ...
2	D	478	 6% 81% 11% • 6%

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Mol	Chain	Length	Quality of chain
2	E	478	
2	F	478	
3	G	223	
4	H	104	
5	I	104	
5	K	104	
6	J	188	
6	L	188	
7	M	323	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22726 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	561	Total	C	N	O	0	0
			2752	1630	561	561		
1	B	561	Total	C	N	O	0	0
			2752	1630	561	561		
1	C	561	Total	C	N	O	0	0
			2752	1630	561	561		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	450	Total	C	N	O	0	0
			2212	1312	450	450		
2	E	450	Total	C	N	O	0	0
			2212	1312	450	450		
2	F	450	Total	C	N	O	0	0
			2212	1312	450	450		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	129	Total	C	N	O	0	0
			639	381	129	129		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	104	Total	C	N	O	0	0
			509	301	104	104		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	100	Total	C	N	O	S	0	0
			747	460	136	150	1		
5	K	100	Total	C	N	O	S	0	0
			747	460	136	150	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	17	GLY	-	expression tag	UNP Q5SIT5
K	17	GLY	-	expression tag	UNP Q5SIT5

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	184	Total	C	N	O	S	0	0
			1312	815	242	252	3		
6	L	184	Total	C	N	O	S	0	0
			1312	815	242	252	3		

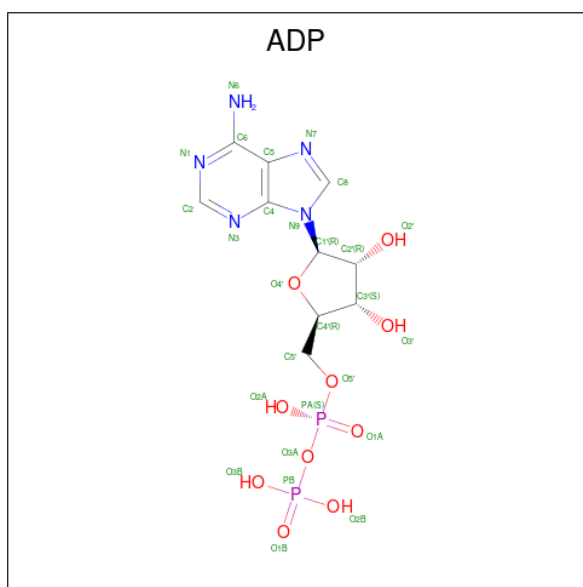
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

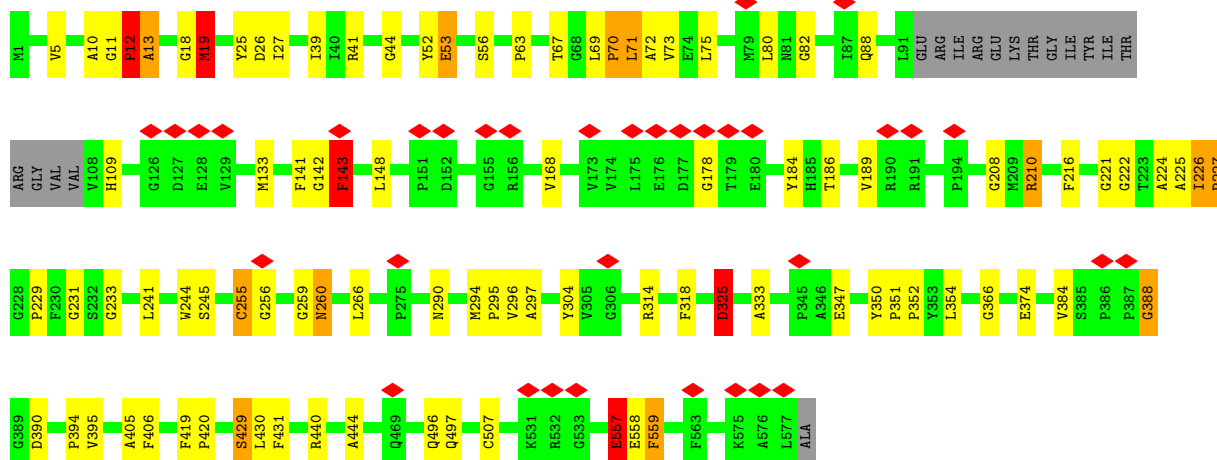
Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	320	Total	C	N	O	S	0	0
			2514	1599	460	451	4		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



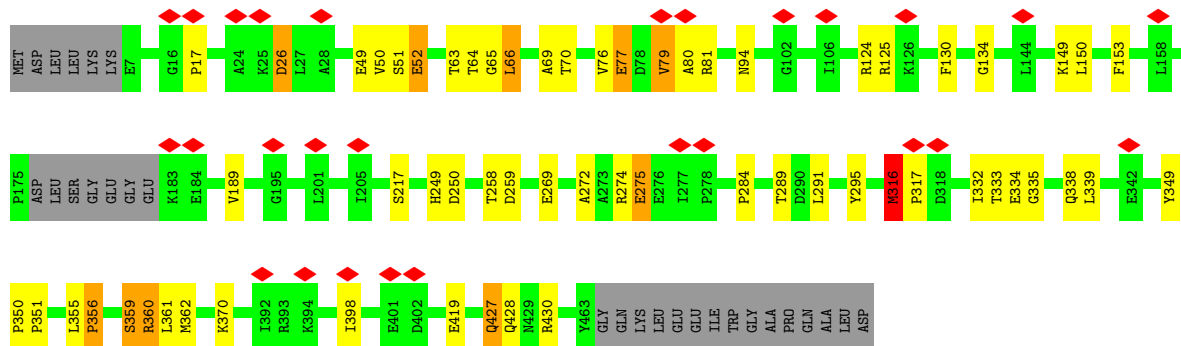
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0
8	C	1	Total 27	C 10	N 5	O 10	P 2	0

Chain C: 



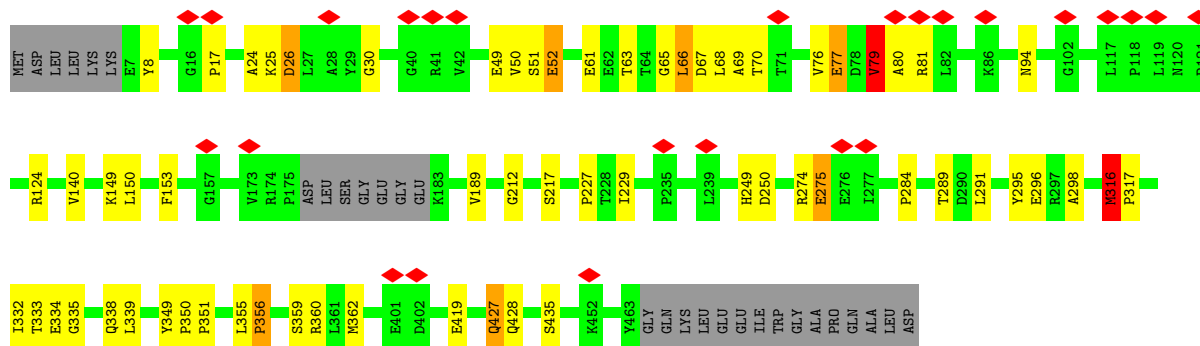
• Molecule 2: V-type ATP synthase beta chain

Chain D: 



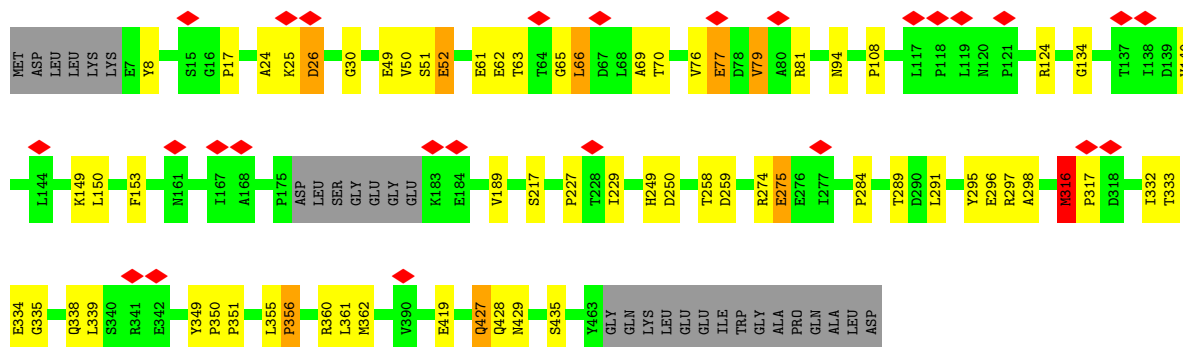
• Molecule 2: V-type ATP synthase beta chain

Chain E: 

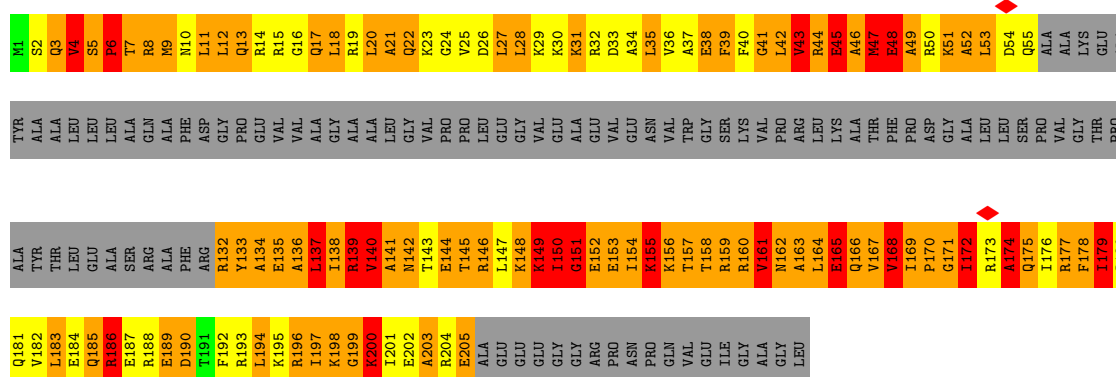


• Molecule 2: V-type ATP synthase beta chain

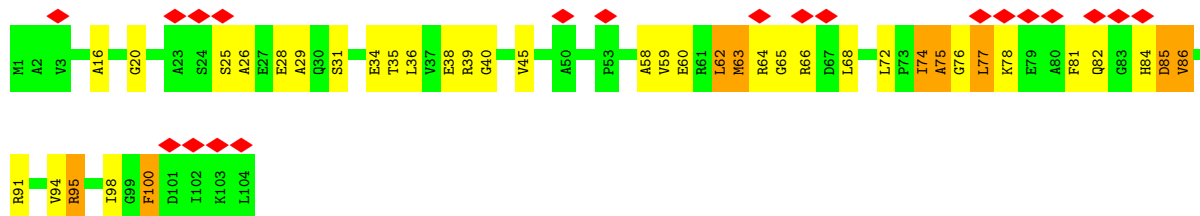
Chain F: 



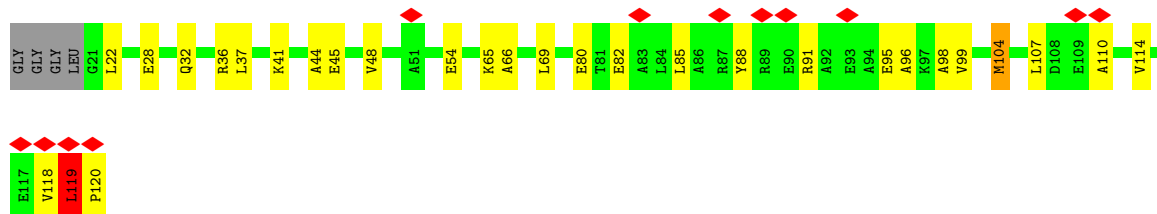
• Molecule 3: V-type ATP synthase subunit D



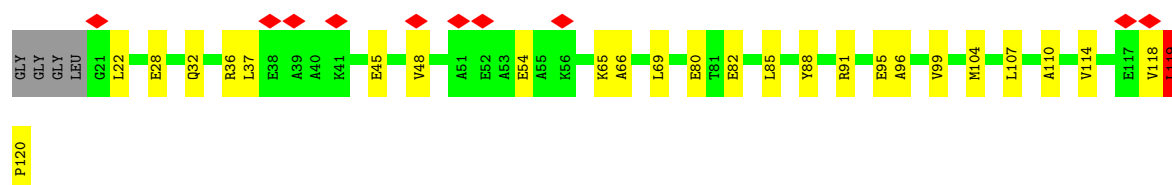
• Molecule 4: V-type ATP synthase subunit F



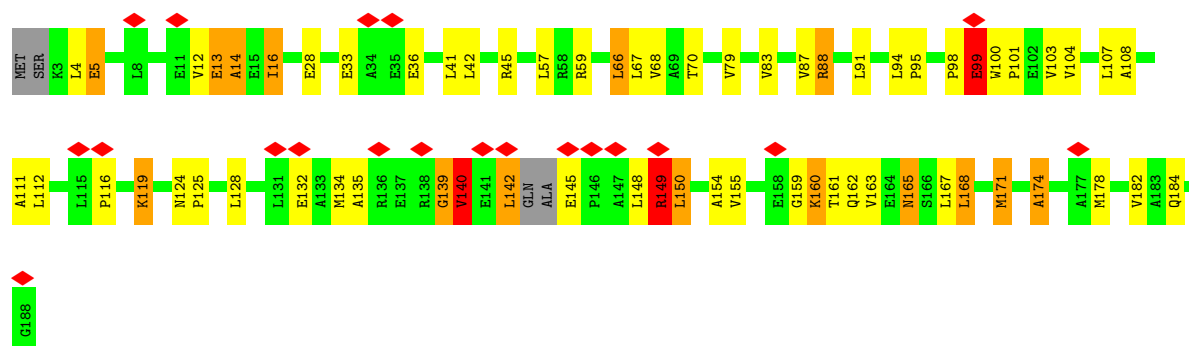
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



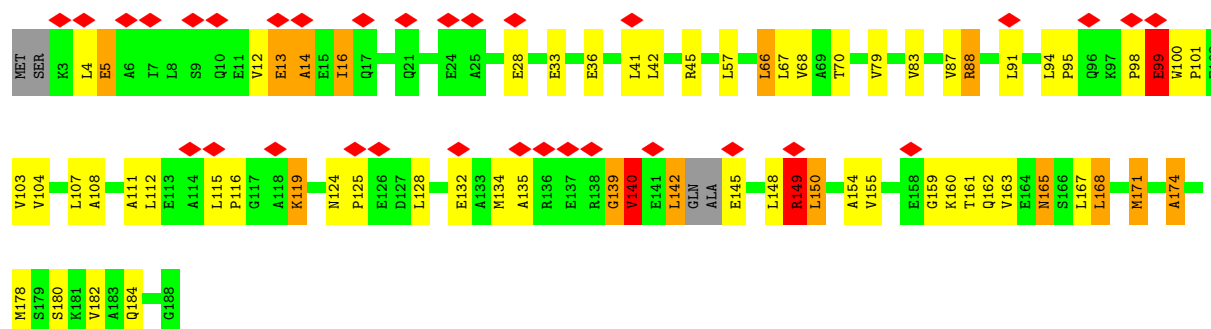
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



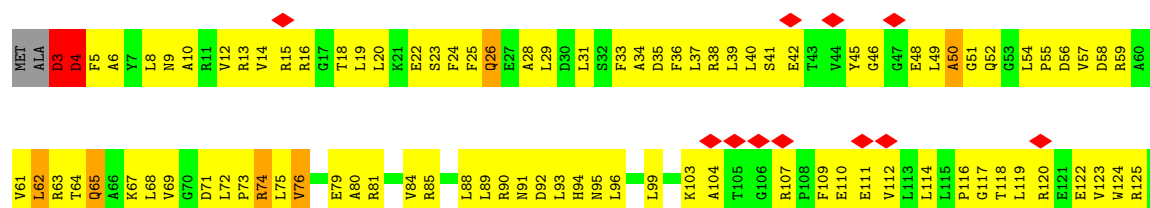
• Molecule 6: V-type ATP synthase subunit E

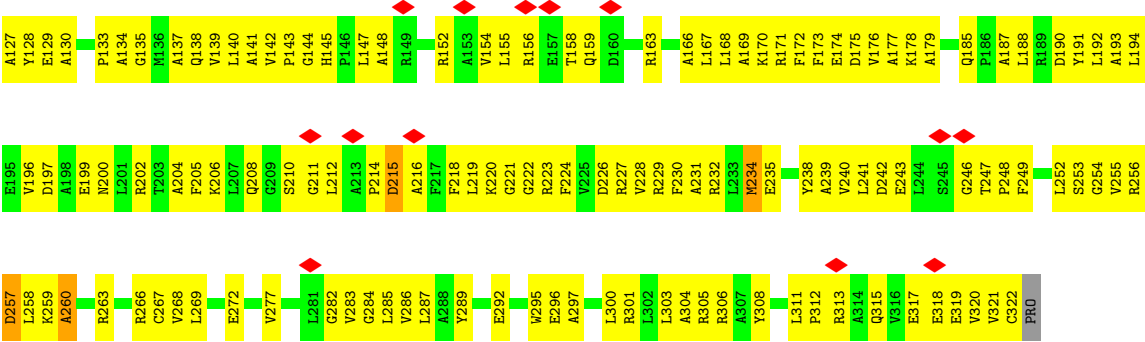


• Molecule 6: V-type ATP synthase subunit E



• Molecule 7: V-type ATP synthase subunit C





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46105	Depositor
Resolution determination method	Not provided	
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.18	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	50000	Depositor
Image detector	GENERIC FILM	Depositor
Maximum map value	1.571	Depositor
Minimum map value	-0.417	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.548	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.94	4/2750 (0.1%)	2.01	36/3815 (0.9%)
1	B	0.94	4/2750 (0.1%)	1.77	31/3815 (0.8%)
1	C	0.95	5/2750 (0.2%)	1.97	34/3815 (0.9%)
2	D	1.15	12/2210 (0.5%)	1.59	17/3068 (0.6%)
2	E	1.16	13/2210 (0.6%)	1.56	15/3068 (0.5%)
2	F	1.13	10/2210 (0.5%)	1.54	13/3068 (0.4%)
3	G	6.38	247/637 (38.8%)	4.09	159/885 (18.0%)
4	H	2.73	21/508 (4.1%)	3.50	28/703 (4.0%)
5	I	0.59	2/749 (0.3%)	0.73	0/1004
5	K	0.59	2/749 (0.3%)	0.73	0/1004
6	J	0.64	6/1325 (0.5%)	0.80	0/1798
6	L	0.64	6/1325 (0.5%)	0.80	0/1798
7	M	1.45	8/2553 (0.3%)	1.21	2/3447 (0.1%)
All	All	1.52	340/22726 (1.5%)	1.76	335/31288 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
2	D	0	4
2	E	0	3
2	F	0	3
4	H	0	2
7	M	0	1
All	All	0	31

All (340) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	47	MET	CA-CB	-32.25	0.98	1.53
3	G	196	ARG	CA-C	23.85	1.84	1.52
3	G	167	VAL	CA-C	23.24	1.81	1.52
4	H	75	ALA	CA-C	21.74	1.81	1.52
3	G	138	ILE	CA-CB	-21.60	1.27	1.54
4	H	75	ALA	N-CA	21.54	1.73	1.45
3	G	7	THR	CA-CB	20.39	1.86	1.53
3	G	4	VAL	CA-C	20.20	1.78	1.52
3	G	27	LEU	CA-CB	19.80	1.87	1.53
3	G	31	LYS	N-CA	19.30	1.71	1.46
3	G	194	LEU	CA-C	17.15	1.75	1.52
4	H	34	GLU	C-O	16.83	1.43	1.24
3	G	168	VAL	CA-CB	-16.76	1.31	1.54
3	G	163	ALA	CA-C	16.28	1.74	1.52
4	H	76	GLY	CA-C	16.01	1.71	1.51
3	G	19	ARG	N-CA	15.17	1.65	1.46
3	G	20	LEU	CA-C	14.85	1.71	1.52
3	G	184	GLU	N-CA	14.85	1.64	1.46
3	G	16	GLY	CA-C	14.53	1.69	1.51
3	G	52	ALA	CA-CB	14.47	1.75	1.53
3	G	38	GLU	N-CA	14.28	1.63	1.46
3	G	32	ARG	C-O	14.13	1.40	1.24
3	G	142	ASN	CA-CB	14.09	1.75	1.53
3	G	189	GLU	CA-CB	14.03	1.76	1.53
3	G	32	ARG	CA-C	13.86	1.70	1.52
3	G	156	LYS	CA-C	13.86	1.70	1.52
3	G	164	LEU	C-O	13.22	1.40	1.24
3	G	167	VAL	CA-CB	13.13	1.69	1.54
3	G	184	GLU	CA-CB	13.10	1.73	1.53
3	G	189	GLU	CA-C	13.02	1.69	1.52
3	G	163	ALA	C-O	12.91	1.40	1.24
3	G	6	PRO	C-O	12.78	1.40	1.24
3	G	182	VAL	N-CA	12.64	1.62	1.46
3	G	155	LYS	N-CA	12.63	1.62	1.46
3	G	195	LYS	N-CA	12.61	1.62	1.46
3	G	205	GLU	CA-CB	12.60	1.78	1.53
3	G	50	ARG	C-O	12.52	1.41	1.24
3	G	170	PRO	CA-C	12.42	1.68	1.52
3	G	183	LEU	C-O	12.42	1.39	1.24
3	G	169	ILE	C-O	12.40	1.40	1.24
3	G	33	ASP	N-CA	12.25	1.61	1.46
3	G	9	MET	CA-C	-12.24	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	171	GLY	CA-C	12.03	1.68	1.51
3	G	28	LEU	CA-C	11.93	1.69	1.52
3	G	192	PHE	CA-C	11.90	1.69	1.52
3	G	52	ALA	N-CA	11.75	1.60	1.46
3	G	169	ILE	CA-C	11.75	1.65	1.52
3	G	4	VAL	CA-CB	11.71	1.70	1.54
3	G	134	ALA	N-CA	11.56	1.61	1.46
3	G	188	ARG	N-CA	11.54	1.60	1.46
3	G	16	GLY	C-O	11.53	1.40	1.23
3	G	32	ARG	C-N	11.49	1.49	1.33
3	G	187	GLU	CA-C	11.49	1.67	1.52
3	G	172	ILE	N-CA	11.46	1.60	1.46
3	G	7	THR	CA-C	11.44	1.68	1.52
3	G	193	ARG	N-CA	11.42	1.60	1.46
3	G	185	GLN	C-O	11.38	1.38	1.24
3	G	53	LEU	N-CA	11.32	1.60	1.46
4	H	76	GLY	N-CA	11.14	1.60	1.44
3	G	198	LYS	C-O	11.12	1.38	1.24
4	H	40	GLY	C-O	10.94	1.36	1.24
3	G	36	VAL	CA-C	10.91	1.67	1.52
3	G	46	ALA	C-O	10.84	1.37	1.24
3	G	51	LYS	C-O	10.78	1.37	1.24
3	G	27	LEU	N-CA	10.73	1.60	1.46
3	G	49	ALA	CA-C	-10.67	1.39	1.52
3	G	192	PHE	C-O	10.60	1.37	1.24
3	G	169	ILE	N-CA	10.59	1.59	1.46
3	G	34	ALA	CA-CB	-10.56	1.35	1.53
3	G	24	GLY	CA-C	10.47	1.64	1.51
3	G	22	GLN	C-O	10.42	1.37	1.24
3	G	201	ILE	CA-CB	-10.40	1.41	1.54
3	G	14	ARG	N-CA	10.38	1.58	1.46
3	G	179	ILE	C-O	10.33	1.36	1.24
3	G	138	ILE	CA-C	-10.30	1.39	1.52
3	G	4	VAL	C-O	10.29	1.36	1.24
3	G	204	ARG	N-CA	10.26	1.59	1.46
3	G	154	ILE	C-O	10.26	1.36	1.24
2	D	289	THR	C-N	10.10	1.46	1.33
3	G	200	LYS	CA-C	10.01	1.66	1.52
7	M	234	MET	SD-CE	-9.95	1.54	1.79
3	G	6	PRO	CA-CB	9.87	1.67	1.53
2	E	66	LEU	CA-CB	-9.83	1.42	1.54
2	F	289	THR	C-N	9.83	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	66	LEU	CA-CB	-9.82	1.42	1.54
2	E	289	THR	C-N	9.81	1.46	1.33
3	G	146	ARG	CA-CB	9.78	1.70	1.53
3	G	205	GLU	CA-C	9.73	1.73	1.52
3	G	14	ARG	C-O	9.70	1.35	1.24
3	G	11	LEU	CA-CB	9.69	1.69	1.53
3	G	164	LEU	N-CA	9.65	1.58	1.46
2	D	66	LEU	CA-CB	-9.65	1.42	1.54
3	G	184	GLU	CA-C	9.58	1.65	1.52
3	G	35	LEU	CA-C	9.46	1.65	1.52
3	G	203	ALA	N-CA	-9.40	1.34	1.46
3	G	163	ALA	C-N	9.36	1.46	1.34
3	G	50	ARG	CA-C	9.31	1.65	1.52
4	H	75	ALA	C-N	9.30	1.45	1.33
3	G	49	ALA	N-CA	9.18	1.57	1.46
3	G	5	SER	CA-C	-9.13	1.41	1.52
3	G	17	GLN	CA-CB	-9.12	1.39	1.53
3	G	31	LYS	C-O	9.08	1.35	1.24
3	G	194	LEU	C-O	9.03	1.34	1.24
3	G	196	ARG	CA-CB	9.01	1.68	1.53
3	G	22	GLN	CA-C	8.92	1.64	1.52
3	G	23	LYS	N-CA	8.92	1.57	1.46
3	G	51	LYS	CA-C	8.90	1.64	1.52
3	G	18	LEU	CA-C	8.81	1.64	1.52
2	E	81	ARG	CA-C	8.80	1.63	1.52
3	G	175	GLN	CA-CB	-8.80	1.39	1.53
3	G	52	ALA	C-O	8.73	1.34	1.24
3	G	45	GLU	C-O	8.72	1.34	1.24
3	G	158	THR	CA-CB	-8.65	1.39	1.53
3	G	14	ARG	CA-CB	8.60	1.66	1.53
3	G	166	GLN	CA-C	8.60	1.64	1.52
3	G	36	VAL	CA-CB	8.57	1.65	1.54
3	G	134	ALA	CA-CB	8.55	1.68	1.53
3	G	193	ARG	CA-C	-8.54	1.41	1.52
3	G	12	LEU	CA-C	-8.50	1.42	1.52
3	G	148	LYS	CA-CB	8.47	1.68	1.53
3	G	22	GLN	C-N	8.46	1.45	1.34
3	G	164	LEU	CA-C	8.43	1.64	1.52
3	G	183	LEU	C-N	8.41	1.44	1.33
3	G	198	LYS	CA-C	8.39	1.64	1.52
3	G	148	LYS	N-CA	8.36	1.57	1.46
3	G	143	THR	N-CA	8.33	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	24	GLY	C-O	8.31	1.33	1.23
3	G	25	VAL	N-CA	8.30	1.57	1.46
3	G	48	GLU	CA-C	8.29	1.63	1.52
3	G	7	THR	N-CA	8.21	1.56	1.46
3	G	170	PRO	N-CA	8.21	1.56	1.47
1	B	13	ALA	CA-CB	-8.15	1.39	1.53
3	G	21	ALA	C-O	8.15	1.34	1.24
1	C	13	ALA	CA-CB	-8.11	1.39	1.53
3	G	175	GLN	N-CA	-8.08	1.36	1.46
7	M	34	ALA	CA-CB	8.06	1.65	1.53
3	G	15	ARG	CA-CB	8.04	1.66	1.53
3	G	142	ASN	CA-C	8.03	1.63	1.52
1	A	13	ALA	CA-CB	-8.02	1.40	1.53
3	G	149	LYS	CA-C	8.01	1.63	1.52
3	G	153	GLU	N-CA	7.96	1.56	1.46
3	G	165	GLU	N-CA	7.95	1.56	1.46
2	E	81	ARG	N-CA	7.91	1.55	1.46
3	G	47	MET	C-O	7.88	1.33	1.24
3	G	166	GLN	CA-CB	-7.88	1.41	1.53
3	G	136	ALA	N-CA	7.88	1.56	1.46
3	G	49	ALA	CA-CB	-7.87	1.41	1.53
3	G	168	VAL	N-CA	7.86	1.56	1.46
3	G	15	ARG	C-O	7.80	1.33	1.24
3	G	195	LYS	CA-C	-7.80	1.42	1.52
2	F	77	GLU	CA-CB	-7.80	1.43	1.54
1	A	352	PRO	CA-CB	-7.79	1.43	1.53
3	G	160	ARG	CA-C	7.74	1.63	1.52
3	G	187	GLU	C-N	7.73	1.44	1.33
2	E	77	GLU	CA-CB	-7.71	1.43	1.54
3	G	183	LEU	CA-C	7.64	1.63	1.52
1	C	325	ASP	C-N	-7.64	1.23	1.33
4	H	29	ALA	CA-CB	-7.62	1.41	1.53
3	G	194	LEU	C-N	7.61	1.44	1.34
1	A	325	ASP	C-N	-7.59	1.23	1.33
3	G	196	ARG	C-O	7.58	1.33	1.24
3	G	12	LEU	N-CA	7.58	1.55	1.46
3	G	17	GLN	N-CA	7.54	1.55	1.46
3	G	19	ARG	CA-C	7.52	1.62	1.52
3	G	201	ILE	C-O	7.50	1.33	1.24
1	B	325	ASP	C-N	-7.49	1.24	1.33
2	D	77	GLU	CA-CB	-7.47	1.44	1.54
3	G	199	GLY	N-CA	7.45	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	26	ASP	C-O	7.43	1.32	1.24
3	G	16	GLY	C-N	7.41	1.43	1.33
2	E	80	ALA	CA-C	7.39	1.63	1.53
3	G	36	VAL	C-O	7.39	1.32	1.24
3	G	7	THR	C-O	7.38	1.33	1.24
4	H	29	ALA	N-CA	-7.37	1.37	1.46
3	G	52	ALA	CA-C	7.33	1.62	1.52
3	G	28	LEU	C-O	7.33	1.33	1.24
3	G	29	LYS	CA-C	7.32	1.61	1.52
1	B	352	PRO	CA-CB	-7.30	1.43	1.53
3	G	22	GLN	N-CA	7.29	1.55	1.46
3	G	133	TYR	CA-C	7.29	1.62	1.52
3	G	162	ASN	CA-CB	-7.28	1.41	1.53
3	G	38	GLU	C-O	7.27	1.32	1.24
1	C	352	PRO	CA-CB	-7.26	1.43	1.53
3	G	170	PRO	C-O	7.26	1.32	1.24
3	G	49	ALA	C-O	7.24	1.32	1.24
3	G	167	VAL	C-O	7.23	1.32	1.24
3	G	165	GLU	C-O	7.21	1.33	1.24
3	G	162	ASN	C-O	7.20	1.33	1.24
3	G	30	LYS	C-N	7.15	1.43	1.33
3	G	37	ALA	CA-CB	-7.15	1.40	1.53
3	G	189	GLU	C-O	7.13	1.32	1.24
3	G	192	PHE	C-N	7.11	1.43	1.34
4	H	36	LEU	C-N	7.10	1.42	1.33
2	D	275	GLU	CA-CB	-7.09	1.41	1.53
7	M	297	ALA	CA-CB	7.09	1.64	1.53
2	F	275	GLU	CA-CB	-7.08	1.41	1.53
3	G	48	GLU	C-N	7.07	1.43	1.33
3	G	144	GLU	N-CA	-7.02	1.37	1.46
2	E	275	GLU	CA-CB	-6.98	1.41	1.53
3	G	20	LEU	C-O	6.98	1.32	1.24
3	G	172	ILE	CA-C	-6.96	1.44	1.52
3	G	160	ARG	C-O	6.91	1.32	1.24
3	G	37	ALA	C-O	6.89	1.32	1.24
3	G	184	GLU	C-O	6.87	1.31	1.24
3	G	203	ALA	CA-CB	-6.83	1.42	1.53
2	D	81	ARG	N-CA	6.81	1.53	1.46
3	G	25	VAL	CA-CB	6.80	1.63	1.54
3	G	154	ILE	C-N	6.79	1.43	1.33
3	G	139	ARG	CA-CB	6.77	1.65	1.53
3	G	188	ARG	C-O	6.72	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	MET	CA-CB	-6.72	1.42	1.53
1	A	19	MET	CA-CB	-6.71	1.42	1.53
1	C	19	MET	CA-CB	-6.66	1.42	1.53
3	G	181	GLN	C-O	6.59	1.32	1.24
3	G	155	LYS	CA-CB	6.59	1.64	1.53
3	G	133	TYR	C-N	6.55	1.42	1.33
3	G	35	LEU	C-O	6.53	1.32	1.24
2	D	80	ALA	CA-C	6.50	1.61	1.53
4	H	58	ALA	CA-CB	-6.50	1.43	1.53
3	G	150	ILE	N-CA	6.49	1.54	1.46
6	L	178	MET	SD-CE	6.46	1.95	1.79
6	J	134	MET	SD-CE	6.43	1.95	1.79
3	G	141	ALA	N-CA	6.42	1.54	1.46
6	J	178	MET	SD-CE	6.42	1.95	1.79
5	I	104	MET	SD-CE	6.42	1.95	1.79
3	G	161	VAL	C-O	6.40	1.31	1.24
5	K	104	MET	SD-CE	6.40	1.95	1.79
3	G	178	PHE	C-O	6.40	1.31	1.24
6	L	134	MET	SD-CE	6.38	1.95	1.79
3	G	202	GLU	N-CA	6.36	1.53	1.46
3	G	181	GLN	CA-C	6.33	1.61	1.52
3	G	190	ASP	C-O	6.33	1.31	1.24
5	I	104	MET	CG-SD	6.31	1.96	1.80
3	G	171	GLY	C-O	6.29	1.32	1.23
5	K	104	MET	CG-SD	6.29	1.96	1.80
2	E	80	ALA	N-CA	6.27	1.53	1.45
3	G	183	LEU	N-CA	6.27	1.54	1.46
3	G	141	ALA	CA-CB	6.26	1.64	1.53
3	G	13	GLN	C-N	6.21	1.41	1.33
3	G	149	LYS	N-CA	-6.20	1.38	1.46
4	H	28	GLU	CA-C	6.16	1.60	1.52
3	G	133	TYR	C-O	6.14	1.31	1.24
3	G	38	GLU	CA-C	6.13	1.60	1.52
3	G	190	ASP	CA-C	6.09	1.60	1.52
3	G	188	ARG	C-N	6.09	1.42	1.33
3	G	31	LYS	CA-CB	6.07	1.63	1.53
3	G	142	ASN	C-O	6.06	1.31	1.24
3	G	159	ARG	C-O	6.04	1.31	1.24
2	D	81	ARG	CA-C	6.04	1.59	1.52
4	H	40	GLY	C-N	6.04	1.44	1.33
2	F	250	ASP	C-O	-6.02	1.15	1.23
6	J	134	MET	CG-SD	5.98	1.95	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	134	MET	CG-SD	5.97	1.95	1.80
2	D	250	ASP	C-O	-5.97	1.15	1.23
6	J	171	MET	SD-CE	5.96	1.94	1.79
6	L	171	MET	SD-CE	5.96	1.94	1.79
3	G	42	LEU	C-O	5.95	1.31	1.24
4	H	45	VAL	CA-C	-5.95	1.45	1.52
4	H	31	SER	N-CA	-5.94	1.39	1.46
3	G	139	ARG	CA-C	5.92	1.60	1.52
2	E	250	ASP	C-O	-5.90	1.15	1.23
3	G	200	LYS	CA-CB	5.86	1.63	1.53
3	G	29	LYS	C-O	5.86	1.30	1.24
3	G	135	GLU	CA-CB	5.85	1.62	1.53
3	G	142	ASN	C-N	5.80	1.41	1.33
6	L	178	MET	CG-SD	5.80	1.95	1.80
4	H	35	THR	CA-C	5.78	1.60	1.52
6	J	178	MET	CG-SD	5.78	1.95	1.80
3	G	186	ARG	C-O	5.75	1.31	1.24
2	F	26	ASP	CA-CB	-5.75	1.43	1.53
3	G	5	SER	CA-CB	5.74	1.62	1.53
2	D	26	ASP	CA-CB	-5.73	1.43	1.53
3	G	41	GLY	C-O	5.71	1.31	1.23
3	G	177	ARG	N-CA	5.69	1.53	1.46
3	G	166	GLN	C-O	5.67	1.30	1.24
2	E	26	ASP	CA-CB	-5.67	1.43	1.53
7	M	260	ALA	CA-CB	-5.66	1.44	1.53
3	G	43	VAL	N-CA	5.63	1.53	1.46
3	G	30	LYS	N-CA	5.63	1.53	1.46
3	G	182	VAL	C-O	5.63	1.30	1.24
3	G	159	ARG	N-CA	5.61	1.53	1.46
3	G	11	LEU	C-N	5.61	1.40	1.33
3	G	43	VAL	C-O	5.59	1.30	1.24
2	F	249	HIS	C-O	-5.59	1.16	1.24
3	G	205	GLU	C-O	5.58	1.34	1.23
2	D	249	HIS	C-O	-5.57	1.16	1.24
3	G	190	ASP	CA-CB	-5.55	1.44	1.53
2	E	249	HIS	C-O	-5.52	1.16	1.24
3	G	158	THR	N-CA	5.52	1.53	1.46
3	G	181	GLN	C-N	5.51	1.40	1.33
3	G	15	ARG	N-CA	5.50	1.52	1.46
4	H	76	GLY	C-O	-5.50	1.19	1.24
3	G	43	VAL	CA-CB	5.49	1.61	1.54
3	G	37	ALA	C-N	5.49	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	81	ARG	CA-C	5.48	1.59	1.52
3	G	156	LYS	CA-CB	5.48	1.62	1.54
1	C	70	PRO	C-N	5.47	1.41	1.33
4	H	91	ARG	C-O	5.45	1.30	1.24
3	G	166	GLN	N-CA	-5.43	1.39	1.46
7	M	28	ALA	CA-CB	5.43	1.61	1.53
3	G	198	LYS	C-N	5.40	1.41	1.33
7	M	6	ALA	CA-CB	5.40	1.62	1.53
3	G	8	ARG	CA-C	5.39	1.60	1.52
3	G	133	TYR	N-CA	-5.38	1.39	1.46
3	G	24	GLY	N-CA	5.37	1.52	1.45
3	G	135	GLU	CA-C	5.37	1.59	1.52
3	G	204	ARG	C-O	5.37	1.30	1.24
3	G	186	ARG	CA-CB	5.37	1.62	1.53
2	F	63	THR	CA-CB	-5.36	1.44	1.53
2	E	63	THR	CA-CB	-5.35	1.44	1.53
3	G	177	ARG	C-O	5.35	1.30	1.24
2	D	63	THR	CA-CB	-5.33	1.44	1.53
3	G	135	GLU	N-CA	5.30	1.52	1.46
3	G	21	ALA	C-N	5.28	1.41	1.33
4	H	76	GLY	C-N	5.28	1.40	1.33
3	G	44	ARG	CA-CB	-5.27	1.43	1.53
2	E	291	LEU	C-O	-5.26	1.17	1.24
3	G	149	LYS	CA-CB	-5.25	1.44	1.53
3	G	179	ILE	CA-C	5.24	1.59	1.52
3	G	145	THR	C-O	5.23	1.30	1.24
3	G	38	GLU	CA-CB	5.23	1.61	1.53
7	M	112	VAL	CA-C	5.23	1.58	1.52
3	G	182	VAL	C-N	5.23	1.41	1.33
3	G	194	LEU	N-CA	5.22	1.52	1.46
4	H	20	GLY	C-O	-5.21	1.16	1.23
3	G	42	LEU	CA-C	5.19	1.59	1.52
3	G	11	LEU	CA-C	5.19	1.59	1.52
3	G	134	ALA	CA-C	5.17	1.59	1.52
3	G	199	GLY	CA-C	-5.17	1.44	1.51
3	G	22	GLN	CA-CB	5.15	1.62	1.53
2	F	291	LEU	C-O	-5.14	1.17	1.24
6	J	171	MET	CG-SD	5.13	1.93	1.80
6	L	171	MET	CG-SD	5.12	1.93	1.80
3	G	21	ALA	N-CA	5.11	1.52	1.46
2	D	291	LEU	C-O	-5.10	1.17	1.24
7	M	50	ALA	C-O	-5.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	47	MET	CA-C	5.06	1.59	1.52
4	H	72	LEU	N-CA	-5.05	1.41	1.46
3	G	139	ARG	C-O	5.05	1.30	1.24
3	G	157	THR	CA-CB	-5.03	1.44	1.53

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASP	O-C-N	-47.93	58.85	122.59
1	B	325	ASP	O-C-N	-47.92	58.85	122.59
1	C	325	ASP	O-C-N	-47.85	58.95	122.59
4	H	76	GLY	N-CA-C	47.09	179.94	112.60
1	C	70	PRO	CA-C-N	-35.85	53.06	121.54
1	C	70	PRO	C-N-CA	-35.85	53.06	121.54
1	A	429	SER	CA-C-N	-33.69	68.49	122.73
1	A	429	SER	C-N-CA	-33.69	68.49	122.73
1	A	429	SER	O-C-N	33.50	163.87	123.33
4	H	74	ILE	O-C-N	-28.60	92.50	123.10
1	C	325	ASP	CA-C-N	-27.91	76.09	121.87
1	C	325	ASP	C-N-CA	-27.91	76.09	121.87
1	B	325	ASP	CA-C-N	-27.89	76.13	121.87
1	B	325	ASP	C-N-CA	-27.89	76.13	121.87
1	A	325	ASP	CA-C-N	-27.80	76.28	121.87
1	A	325	ASP	C-N-CA	-27.80	76.28	121.87
2	D	316	MET	O-C-N	-26.03	91.39	121.32
2	E	316	MET	O-C-N	-25.93	91.50	121.32
2	F	316	MET	O-C-N	-25.87	91.57	121.32
4	H	75	ALA	N-CA-C	23.74	143.97	110.50
4	H	76	GLY	CA-C-O	-21.50	99.97	121.90
3	G	133	TYR	N-CA-C	-16.85	91.82	112.38
4	H	77	LEU	CA-C-N	-16.84	92.05	120.68
4	H	77	LEU	C-N-CA	-16.84	92.05	120.68
3	G	157	THR	N-CA-C	-16.81	92.03	112.54
3	G	12	LEU	N-CA-C	-16.46	93.03	110.97
1	C	70	PRO	O-C-N	15.94	144.16	122.64
3	G	203	ALA	N-CA-C	-15.38	89.89	112.04
4	H	75	ALA	CA-C-N	15.38	141.44	122.83
4	H	75	ALA	C-N-CA	15.38	141.44	122.83
4	H	63	MET	N-CA-C	15.26	130.88	108.60
2	D	360	ARG	N-CA-C	-14.77	94.36	112.38
3	G	142	ASN	N-CA-C	-14.15	95.94	111.36
4	H	76	GLY	CA-C-N	14.05	146.99	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	76	GLY	C-N-CA	14.05	146.99	121.70
3	G	6	PRO	CA-C-N	-13.86	97.13	120.68
3	G	6	PRO	C-N-CA	-13.86	97.13	120.68
3	G	187	GLU	N-CA-C	13.81	133.59	113.02
3	G	153	GLU	N-CA-C	13.70	129.88	112.89
3	G	47	MET	N-CA-C	13.60	139.76	110.80
1	C	430	LEU	N-CA-C	-13.38	97.01	113.20
3	G	139	ARG	N-CA-C	-13.18	82.73	110.80
3	G	194	LEU	N-CA-C	12.81	127.03	111.40
3	G	186	ARG	CA-C-N	-12.59	102.06	122.08
3	G	186	ARG	C-N-CA	-12.59	102.06	122.08
4	H	76	GLY	O-C-N	-12.26	109.82	122.82
1	B	429	SER	O-C-N	-12.00	107.77	123.14
3	G	9	MET	CA-C-N	-11.83	98.27	121.94
3	G	9	MET	C-N-CA	-11.83	98.27	121.94
3	G	188	ARG	N-CA-C	-11.79	98.42	111.28
3	G	49	ALA	CA-C-N	-11.55	98.84	121.94
3	G	49	ALA	C-N-CA	-11.55	98.84	121.94
3	G	7	THR	CA-C-N	-11.35	103.82	120.38
3	G	7	THR	C-N-CA	-11.35	103.82	120.38
3	G	167	VAL	O-C-N	-11.34	110.80	121.91
2	F	351	PRO	N-CA-CB	11.29	110.37	102.81
2	E	351	PRO	N-CA-CB	11.26	110.36	102.81
3	G	47	MET	CA-C-N	-11.16	100.23	121.54
3	G	47	MET	C-N-CA	-11.16	100.23	121.54
1	A	63	PRO	N-CA-CB	11.15	113.78	103.19
2	D	351	PRO	N-CA-CB	11.11	110.25	102.81
2	E	81	ARG	N-CA-C	11.01	124.67	108.60
1	C	63	PRO	N-CA-CB	10.99	113.63	103.19
1	B	63	PRO	N-CA-CB	10.90	113.55	103.19
1	A	70	PRO	N-CA-C	-10.89	98.39	113.53
3	G	6	PRO	N-CA-CB	10.88	114.67	103.25
3	G	38	GLU	N-CA-C	10.49	122.40	110.97
3	G	167	VAL	CA-C-N	-10.27	103.48	121.97
3	G	167	VAL	C-N-CA	-10.27	103.48	121.97
3	G	163	ALA	N-CA-C	10.27	123.73	111.82
3	G	183	LEU	CA-C-N	10.07	134.13	120.54
3	G	183	LEU	C-N-CA	10.07	134.13	120.54
3	G	156	LYS	N-CA-C	9.96	129.63	113.89
3	G	19	ARG	N-CA-C	9.87	123.06	111.71
4	H	68	LEU	CA-C-N	9.63	130.24	119.93
4	H	68	LEU	C-N-CA	9.63	130.24	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LEU	CA-C-N	9.48	129.57	119.05
1	A	69	LEU	C-N-CA	9.48	129.57	119.05
4	H	86	VAL	N-CA-C	9.41	120.21	110.62
3	G	30	LYS	CA-C-N	9.37	139.44	121.54
3	G	30	LYS	C-N-CA	9.37	139.44	121.54
3	G	178	PHE	N-CA-C	-9.23	100.16	111.33
3	G	204	ARG	N-CA-C	9.21	122.50	111.82
3	G	14	ARG	N-CA-C	9.14	120.85	111.07
3	G	11	LEU	N-CA-C	-9.09	101.62	112.89
3	G	156	LYS	CA-C-N	-9.05	105.60	120.72
3	G	156	LYS	C-N-CA	-9.05	105.60	120.72
3	G	49	ALA	CA-C-O	9.03	130.00	120.70
3	G	181	GLN	N-CA-C	9.03	123.84	113.01
3	G	174	ALA	CA-C-N	-8.86	108.24	120.38
3	G	174	ALA	C-N-CA	-8.86	108.24	120.38
3	G	31	LYS	O-C-N	8.85	134.37	122.59
3	G	192	PHE	N-CA-C	8.82	123.34	112.23
2	D	359	SER	N-CA-C	-8.80	96.41	109.62
3	G	155	LYS	CA-C-N	-8.80	108.25	121.99
3	G	155	LYS	C-N-CA	-8.80	108.25	121.99
3	G	37	ALA	CA-C-N	8.75	132.20	120.65
3	G	37	ALA	C-N-CA	8.75	132.20	120.65
4	H	35	THR	CB-CA-C	-8.62	97.01	110.81
2	F	81	ARG	N-CA-C	8.52	121.66	108.96
2	D	289	THR	O-C-N	-8.42	111.05	122.33
1	A	244	TRP	N-CA-C	8.39	126.19	113.61
1	C	244	TRP	N-CA-C	8.38	126.18	113.61
1	B	244	TRP	N-CA-C	8.37	126.17	113.61
2	F	289	THR	O-C-N	-8.27	111.25	122.33
2	E	289	THR	O-C-N	-8.24	111.29	122.33
3	G	170	PRO	N-CA-CB	8.16	111.78	102.88
2	D	284	PRO	N-CA-CB	8.11	110.39	103.25
2	F	284	PRO	N-CA-CB	8.11	110.39	103.25
2	E	284	PRO	N-CA-CB	8.01	110.30	103.25
3	G	13	GLN	CA-C-N	7.97	130.81	120.44
3	G	13	GLN	C-N-CA	7.97	130.81	120.44
3	G	182	VAL	O-C-N	7.91	133.90	122.04
3	G	12	LEU	O-C-N	7.90	130.25	122.03
3	G	158	THR	N-CA-C	7.87	122.65	112.89
1	C	351	PRO	N-CA-CB	7.84	107.58	103.19
1	A	351	PRO	N-CA-CB	7.82	107.57	103.19
3	G	140	VAL	N-CA-C	7.77	125.50	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	160	ARG	N-CA-C	-7.74	102.93	112.38
3	G	163	ALA	CA-C-N	7.71	131.39	120.28
3	G	163	ALA	C-N-CA	7.71	131.39	120.28
2	E	80	ALA	N-CA-C	7.71	120.48	110.53
1	C	12	PRO	N-CA-CB	7.66	111.29	103.25
3	G	165	GLU	CA-C-N	-7.61	109.95	120.38
3	G	165	GLU	C-N-CA	-7.61	109.95	120.38
3	G	47	MET	CA-C-O	7.60	131.38	120.51
1	B	12	PRO	N-CA-CB	7.60	111.23	103.25
1	B	351	PRO	N-CA-CB	7.57	107.43	103.19
2	D	17	PRO	N-CA-CB	7.57	110.39	103.20
1	A	12	PRO	N-CA-CB	7.56	111.19	103.25
3	G	154	ILE	N-CA-C	-7.56	93.61	109.34
2	F	17	PRO	N-CA-CB	7.53	110.35	103.20
2	E	17	PRO	N-CA-CB	7.50	110.33	103.20
3	G	196	ARG	N-CA-CB	-7.47	99.06	110.20
3	G	21	ALA	O-C-N	7.47	132.52	122.59
3	G	149	LYS	N-CA-C	-7.42	95.00	110.80
4	H	62	LEU	CA-C-N	-7.41	109.12	121.80
4	H	62	LEU	C-N-CA	-7.41	109.12	121.80
3	G	166	GLN	CA-C-N	-7.37	111.27	120.56
3	G	166	GLN	C-N-CA	-7.37	111.27	120.56
3	G	188	ARG	N-CA-CB	7.36	120.94	110.12
3	G	32	ARG	CA-C-O	-7.35	112.76	120.55
3	G	151	GLY	N-CA-C	-7.24	96.02	113.18
3	G	136	ALA	N-CA-C	-7.21	95.45	110.80
3	G	202	GLU	CA-C-O	7.20	128.14	119.78
3	G	51	LYS	CA-C-N	7.19	130.25	120.54
3	G	51	LYS	C-N-CA	7.19	130.25	120.54
2	D	81	ARG	CA-C-N	-7.14	112.87	122.72
2	D	81	ARG	C-N-CA	-7.14	112.87	122.72
3	G	5	SER	O-C-N	7.13	129.52	121.32
4	H	77	LEU	O-C-N	-7.13	111.59	123.00
3	G	51	LYS	N-CA-C	-7.12	103.52	111.71
3	G	193	ARG	N-CA-C	-7.01	103.65	111.71
3	G	137	LEU	CA-C-N	-7.00	110.05	121.19
3	G	137	LEU	C-N-CA	-7.00	110.05	121.19
3	G	195	LYS	CA-C-O	7.00	128.01	120.10
7	M	277	VAL	CB-CA-C	-6.97	102.73	112.14
3	G	31	LYS	CA-C-N	6.92	129.55	120.28
3	G	31	LYS	C-N-CA	6.92	129.55	120.28
1	B	557	GLU	O-C-N	-6.87	113.46	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	15	ARG	N-CA-C	-6.84	103.44	111.03
3	G	196	ARG	CB-CA-C	6.81	123.16	110.70
4	H	40	GLY	N-CA-C	6.81	120.86	113.58
1	C	557	GLU	O-C-N	-6.79	113.57	122.39
1	A	557	GLU	O-C-N	-6.77	113.59	122.39
3	G	187	GLU	CA-C-O	-6.73	112.00	119.34
4	H	81	PHE	N-CA-C	-6.71	104.73	113.12
4	H	40	GLY	O-C-N	6.66	128.04	122.71
3	G	179	ILE	CA-C-N	-6.66	111.26	120.38
3	G	179	ILE	C-N-CA	-6.66	111.26	120.38
3	G	199	GLY	N-CA-C	-6.62	97.49	113.18
2	E	66	LEU	N-CA-CB	-6.59	107.51	114.10
3	G	32	ARG	CA-C-N	6.54	129.33	120.44
3	G	32	ARG	C-N-CA	6.54	129.33	120.44
2	F	66	LEU	N-CA-CB	-6.53	107.57	114.10
2	D	66	LEU	N-CA-CB	-6.48	107.62	114.10
4	H	62	LEU	O-C-N	-6.46	115.38	122.09
7	M	4	ASP	CB-CA-C	6.41	122.62	110.56
3	G	161	VAL	O-C-N	6.41	130.58	122.57
4	H	95	ARG	N-CA-C	-6.40	104.22	111.07
4	H	34	GLU	CA-C-O	-6.36	114.14	120.82
1	B	226	ILE	N-CA-CB	6.31	119.80	111.40
1	A	142	GLY	CA-C-N	6.31	133.05	121.70
1	A	142	GLY	C-N-CA	6.31	133.05	121.70
1	C	39	ILE	CB-CA-C	-6.30	104.48	111.35
1	C	142	GLY	CA-C-N	6.29	133.03	121.70
1	C	142	GLY	C-N-CA	6.29	133.03	121.70
3	G	10	ASN	CA-C-N	-6.29	110.14	121.14
3	G	10	ASN	C-N-CA	-6.29	110.14	121.14
1	A	39	ILE	CB-CA-C	-6.27	104.51	111.35
3	G	167	VAL	CB-CA-C	6.26	119.98	111.97
1	B	142	GLY	CA-C-N	6.26	132.97	121.70
1	B	142	GLY	C-N-CA	6.26	132.97	121.70
1	B	39	ILE	CB-CA-C	-6.25	104.54	111.35
4	H	64	ARG	N-CA-C	-6.25	105.24	112.92
3	G	182	VAL	CB-CA-C	-6.24	102.86	111.65
1	A	226	ILE	N-CA-CB	6.22	119.68	111.40
3	G	145	THR	N-CA-C	6.22	118.06	111.28
1	C	226	ILE	N-CA-CB	6.21	119.67	111.40
1	A	143	PHE	N-CA-C	6.20	128.37	111.00
1	C	143	PHE	N-CA-C	6.17	128.27	111.00
3	G	169	ILE	N-CA-C	6.17	122.20	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	PRO	N-CA-CB	6.16	110.90	103.45
3	G	138	ILE	N-CA-C	6.15	121.00	113.00
1	B	143	PHE	N-CA-C	6.14	128.20	111.00
3	G	203	ALA	CA-C-N	6.12	129.62	120.31
3	G	203	ALA	C-N-CA	6.12	129.62	120.31
3	G	137	LEU	O-C-N	-6.11	114.47	122.59
3	G	172	ILE	O-C-N	6.10	130.19	122.57
1	C	354	LEU	N-CA-C	6.09	117.92	111.28
1	A	354	LEU	N-CA-C	6.09	117.92	111.28
1	B	229	PRO	N-CA-CB	6.08	110.81	103.45
1	B	354	LEU	N-CA-C	6.07	117.90	111.28
3	G	29	LYS	N-CA-C	-6.07	104.35	110.97
2	D	81	ARG	N-CA-C	6.07	117.45	108.60
1	A	350	TYR	CA-C-N	6.05	124.07	119.66
1	A	350	TYR	C-N-CA	6.05	124.07	119.66
3	G	164	LEU	CA-C-O	6.04	126.93	120.10
1	A	559	PHE	CA-C-N	6.04	125.72	119.56
1	A	559	PHE	C-N-CA	6.04	125.72	119.56
1	C	229	PRO	N-CA-CB	6.01	110.72	103.45
1	C	559	PHE	CA-C-N	6.00	125.68	119.56
1	C	559	PHE	C-N-CA	6.00	125.68	119.56
1	C	210	ARG	CA-C-O	-5.97	114.55	120.82
3	G	47	MET	N-CA-CB	-5.97	100.41	110.49
1	B	559	PHE	CA-C-N	5.95	125.62	119.56
1	B	559	PHE	C-N-CA	5.95	125.62	119.56
1	B	199	LEU	N-CA-C	5.94	118.20	110.53
3	G	193	ARG	O-C-N	5.93	129.16	122.22
3	G	201	ILE	CA-C-O	5.90	127.11	120.85
2	F	94	ASN	CA-C-N	5.90	127.56	120.13
2	F	94	ASN	C-N-CA	5.90	127.56	120.13
3	G	47	MET	O-C-N	-5.89	114.75	122.59
1	A	210	ARG	CA-C-O	-5.86	114.66	120.82
3	G	27	LEU	N-CA-C	5.86	119.69	112.54
2	D	94	ASN	CA-C-N	5.86	127.51	120.13
2	D	94	ASN	C-N-CA	5.86	127.51	120.13
1	B	210	ARG	CA-C-O	-5.85	114.67	120.82
2	E	94	ASN	CA-C-N	5.82	127.46	120.13
2	E	94	ASN	C-N-CA	5.82	127.46	120.13
3	G	143	THR	CA-C-O	5.79	127.56	120.56
1	C	168	VAL	N-CA-CB	-5.77	104.10	110.51
1	A	168	VAL	N-CA-CB	-5.76	104.11	110.51
3	G	196	ARG	N-CA-C	5.75	118.77	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	7	THR	N-CA-C	5.75	119.47	112.23
1	A	41	ARG	CA-C-O	-5.73	114.23	120.36
2	D	289	THR	CA-C-N	5.73	127.89	120.44
2	D	289	THR	C-N-CA	5.73	127.89	120.44
3	G	201	ILE	N-CA-C	5.71	116.48	110.72
1	C	143	PHE	CA-C-O	5.67	130.45	120.80
2	F	289	THR	CA-C-N	5.67	127.82	120.44
2	F	289	THR	C-N-CA	5.67	127.82	120.44
1	B	143	PHE	CA-C-O	5.67	130.43	120.80
3	G	165	GLU	N-CA-C	5.66	122.85	110.80
1	C	350	TYR	CA-C-N	5.65	123.78	119.66
1	C	350	TYR	C-N-CA	5.65	123.78	119.66
3	G	7	THR	O-C-N	-5.65	114.76	122.33
1	A	143	PHE	CA-C-O	5.64	130.39	120.80
1	C	41	ARG	CA-C-O	-5.64	114.33	120.36
1	B	350	TYR	CA-C-N	5.63	123.77	119.66
1	B	350	TYR	C-N-CA	5.63	123.77	119.66
3	G	163	ALA	CA-C-O	-5.62	113.50	119.97
1	B	168	VAL	N-CA-CB	-5.61	104.28	110.51
3	G	140	VAL	CA-C-N	5.59	131.76	122.54
3	G	140	VAL	C-N-CA	5.59	131.76	122.54
2	E	289	THR	CA-C-N	5.58	127.69	120.44
2	E	289	THR	C-N-CA	5.58	127.69	120.44
4	H	38	GLU	N-CA-C	-5.57	105.36	111.82
1	B	41	ARG	CA-C-O	-5.56	114.41	120.36
3	G	39	PHE	N-CA-C	5.55	117.41	111.36
3	G	159	ARG	O-C-N	5.55	128.55	122.11
3	G	171	GLY	N-CA-C	-5.54	100.05	113.18
1	A	222	GLY	CA-C-N	-5.54	115.30	123.05
1	A	222	GLY	C-N-CA	-5.54	115.30	123.05
3	G	31	LYS	N-CA-C	5.54	122.59	110.80
3	G	182	VAL	CA-C-N	5.52	132.08	121.54
3	G	182	VAL	C-N-CA	5.52	132.08	121.54
3	G	202	GLU	O-C-N	5.50	129.80	122.26
3	G	46	ALA	N-CA-C	-5.50	99.08	110.80
3	G	157	THR	N-CA-CB	5.48	119.49	110.39
3	G	23	LYS	N-CA-C	-5.46	105.49	111.82
3	G	15	ARG	CA-C-O	-5.43	115.30	120.90
1	C	222	GLY	CA-C-N	-5.42	115.46	123.05
1	C	222	GLY	C-N-CA	-5.42	115.46	123.05
1	B	222	GLY	CA-C-N	-5.40	115.49	123.05
1	B	222	GLY	C-N-CA	-5.40	115.49	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	30	LYS	O-C-N	5.36	127.80	122.12
3	G	132	ARG	CA-C-N	-5.35	112.03	120.60
3	G	132	ARG	C-N-CA	-5.35	112.03	120.60
1	C	294	MET	CA-C-N	5.35	125.29	119.78
1	C	294	MET	C-N-CA	5.35	125.29	119.78
3	G	178	PHE	O-C-N	5.33	127.77	122.12
1	B	294	MET	CA-C-N	5.32	125.26	119.78
1	B	294	MET	C-N-CA	5.32	125.26	119.78
3	G	172	ILE	CB-CA-C	-5.31	102.58	111.29
3	G	165	GLU	CA-C-O	5.28	128.06	120.51
2	E	419	GLU	CA-C-O	5.27	126.01	120.42
2	D	356	PRO	N-CA-CB	5.27	108.78	103.25
2	D	419	GLU	CA-C-O	5.26	125.99	120.42
1	C	67	THR	N-CA-CB	5.25	117.97	110.67
2	E	356	PRO	N-CA-CB	5.25	108.76	103.25
4	H	77	LEU	CA-C-O	-5.24	111.90	120.80
1	A	67	THR	N-CA-CB	5.23	117.94	110.67
1	C	347	GLU	CA-C-O	-5.21	115.28	120.96
2	F	356	PRO	N-CA-CB	5.21	108.72	103.25
3	G	31	LYS	CB-CA-C	-5.20	100.06	110.42
3	G	203	ALA	CA-C-O	-5.20	113.81	120.31
3	G	136	ALA	O-C-N	5.20	129.51	122.59
3	G	156	LYS	O-C-N	-5.20	116.57	122.23
2	E	79	VAL	O-C-N	-5.19	116.08	122.57
3	G	194	LEU	CA-C-O	-5.19	115.00	120.55
1	B	67	THR	N-CA-CB	5.18	117.86	110.67
1	A	294	MET	CA-C-N	5.17	125.11	119.78
1	A	294	MET	C-N-CA	5.17	125.11	119.78
3	G	189	GLU	CB-CA-C	5.17	119.48	110.79
3	G	25	VAL	CA-C-O	5.15	125.82	120.25
3	G	54	ASP	CA-C-N	-5.13	112.46	121.70
3	G	54	ASP	C-N-CA	-5.13	112.46	121.70
1	B	347	GLU	CA-C-O	-5.13	115.37	120.96
3	G	174	ALA	N-CA-C	5.12	121.70	110.80
3	G	170	PRO	CA-C-O	5.11	125.22	118.98
3	G	23	LYS	CA-C-N	5.10	125.75	119.99
3	G	23	LYS	C-N-CA	5.10	125.75	119.99
3	G	43	VAL	CA-C-N	-5.09	112.43	120.63
3	G	43	VAL	C-N-CA	-5.09	112.43	120.63
3	G	49	ALA	CB-CA-C	-5.09	102.85	110.90
3	G	144	GLU	CA-C-N	5.09	127.10	120.28
3	G	144	GLU	C-N-CA	5.09	127.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	429	SER	N-CA-C	-5.06	100.04	108.34
2	F	419	GLU	CA-C-O	5.06	125.78	120.42
3	G	47	MET	CB-CA-C	-5.05	100.38	110.42
1	A	13	ALA	CA-C-N	-5.04	116.58	122.93
1	A	13	ALA	C-N-CA	-5.04	116.58	122.93
3	G	4	VAL	N-CA-C	5.04	119.82	109.34
3	G	185	GLN	N-CA-C	-5.03	100.08	110.80

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	557	GLU	Mainchain
1	A	69	LEU	Peptide
1	B	178	GLY	Peptide
1	B	210	ARG	Mainchain
1	B	297	ALA	Mainchain
1	B	325	ASP	Mainchain
1	B	429	SER	Mainchain
1	B	557	GLU	Mainchain
1	C	178	GLY	Peptide
1	C	210	ARG	Mainchain
1	C	297	ALA	Mainchain
1	C	325	ASP	Mainchain
1	C	557	GLU	Mainchain
1	C	70	PRO	Mainchain
2	D	316	MET	Mainchain
2	D	427	GLN	Peptide
2	D	79	VAL	Mainchain,Peptide
2	E	316	MET	Mainchain
2	E	427	GLN	Peptide
2	E	79	VAL	Mainchain
2	F	316	MET	Mainchain
2	F	427	GLN	Peptide
2	F	79	VAL	Mainchain
4	H	39	ARG	Peptide
4	H	82	GLN	Peptide
7	M	3	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	1300	127	0
1	B	2752	0	1303	61	0
1	C	2752	0	1302	89	0
2	D	2212	0	1009	85	0
2	E	2212	0	1009	84	0
2	F	2212	0	1009	84	0
3	G	639	0	299	145	0
4	H	509	0	255	27	0
5	I	747	0	726	22	0
5	K	747	0	726	19	0
6	J	1312	0	1240	77	0
6	L	1312	0	1240	59	0
7	M	2514	0	2583	639	0
8	A	27	0	12	0	0
8	C	27	0	12	4	0
All	All	22726	0	14025	1336	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 36.

All (1336) 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)
7:M:33:PHE:CG	7:M:308:TYR:HD1	1.08	1.66
7:M:33:PHE:CD2	7:M:308:TYR:CD1	1.83	1.64
7:M:20:LEU:HD23	7:M:24:PHE:CD1	1.11	1.61
2:E:25:LYS:CA	6:J:161:THR:HG23	1.14	1.61
3:G:189:GLU:CA	3:G:189:GLU:CB	1.76	1.61
3:G:194:LEU:C	3:G:194:LEU:CA	1.75	1.60
3:G:142:ASN:CB	3:G:142:ASN:CA	1.75	1.60
3:G:205:GLU:CB	3:G:205:GLU:CA	1.78	1.60
7:M:229:ARG:CZ	7:M:243:GLU:HB3	1.26	1.59
7:M:20:LEU:CD2	7:M:24:PHE:CD1	1.83	1.59
3:G:52:ALA:CB	3:G:52:ALA:CA	1.76	1.58
7:M:266:ARG:NE	7:M:295:TRP:CH2	1.70	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:266:ARG:CD	7:M:295:TRP:CZ2	1.87	1.57
1:B:475:ALA:HB1	4:H:100:PHE:CB	1.33	1.57
3:G:4:VAL:C	3:G:4:VAL:CA	1.78	1.57
3:G:163:ALA:C	3:G:163:ALA:CA	1.74	1.57
7:M:15:ARG:HH11	7:M:68:LEU:CD2	1.14	1.56
1:C:52:TYR:HA	1:C:295:PRO:CB	1.08	1.55
7:M:178:LYS:CE	7:M:221:GLY:CA	1.84	1.55
7:M:214:PRO:HG2	7:M:231:ALA:CB	1.17	1.55
1:C:52:TYR:CA	1:C:295:PRO:CB	1.85	1.54
4:H:75:ALA:C	4:H:75:ALA:CA	1.81	1.52
7:M:266:ARG:CZ	7:M:295:TRP:CZ3	1.90	1.52
1:A:71:LEU:CB	1:A:188:PRO:HA	1.09	1.52
2:F:140:VAL:CB	2:F:435:SER:CB	1.84	1.52
1:A:267:VAL:N	2:F:124:ARG:CB	1.70	1.51
3:G:196:ARG:C	3:G:196:ARG:CA	1.84	1.51
3:G:31:LYS:N	3:G:31:LYS:CA	1.71	1.50
3:G:7:THR:CB	3:G:7:THR:CA	1.86	1.50
3:G:27:LEU:CA	3:G:27:LEU:CB	1.87	1.49
1:A:24:MET:HA	2:D:66:LEU:CA	1.38	1.49
3:G:167:VAL:C	3:G:167:VAL:CA	1.81	1.49
7:M:57:VAL:HG12	7:M:301:ARG:NH1	1.28	1.49
7:M:229:ARG:CZ	7:M:243:GLU:CB	1.91	1.49
7:M:33:PHE:CD2	7:M:308:TYR:HD1	1.15	1.48
7:M:137:ALA:CB	7:M:152:ARG:HD2	1.42	1.47
4:H:75:ALA:CA	4:H:75:ALA:N	1.73	1.47
7:M:178:LYS:HE3	7:M:221:GLY:CA	1.05	1.46
7:M:229:ARG:NH2	7:M:243:GLU:HB3	1.18	1.46
2:E:25:LYS:N	6:J:161:THR:HA	1.14	1.46
7:M:266:ARG:HD3	7:M:295:TRP:CE2	1.50	1.45
1:A:25:TYR:N	2:D:66:LEU:H	0.97	1.44
7:M:229:ARG:NH1	7:M:243:GLU:CB	1.76	1.44
7:M:15:ARG:NH1	7:M:68:LEU:CD2	1.81	1.44
2:E:25:LYS:CB	6:J:161:THR:CB	1.93	1.43
1:A:266:LEU:C	2:F:124:ARG:CB	1.93	1.42
7:M:33:PHE:CD1	7:M:308:TYR:HB2	1.52	1.42
1:A:24:MET:CA	2:D:66:LEU:HA	1.48	1.41
7:M:33:PHE:CG	7:M:308:TYR:CD1	1.95	1.41
1:A:25:TYR:H	2:D:66:LEU:N	1.16	1.40
7:M:266:ARG:HD3	7:M:295:TRP:CZ2	1.52	1.38
1:B:475:ALA:CB	4:H:100:PHE:CB	1.99	1.37
1:B:419:PHE:O	1:B:496:GLN:HA	1.25	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:ARG:O	3:G:47:MET:CB	1.72	1.36
7:M:266:ARG:CZ	7:M:295:TRP:CH2	2.03	1.36
4:H:75:ALA:HB3	4:H:85:ASP:CB	1.53	1.36
1:C:259:GLY:N	2:E:296:GLU:CA	1.83	1.35
1:A:11:GLY:CA	2:F:50:VAL:H	1.36	1.35
7:M:88:LEU:HB3	7:M:117:GLY:C	1.48	1.35
1:A:71:LEU:CB	1:A:188:PRO:CA	2.05	1.34
7:M:312:PRO:CG	7:M:315:GLN:OE1	1.74	1.34
7:M:266:ARG:NH1	7:M:295:TRP:CZ3	1.95	1.33
1:B:9:ILE:CB	2:D:50:VAL:O	1.75	1.33
7:M:33:PHE:CE2	7:M:308:TYR:CD1	2.17	1.33
7:M:5:PHE:CD2	7:M:286:VAL:HG11	1.64	1.32
1:A:259:GLY:O	2:F:296:GLU:C	1.73	1.31
2:E:24:ALA:C	6:J:161:THR:HA	1.49	1.31
7:M:33:PHE:CD1	7:M:308:TYR:CB	2.11	1.31
7:M:226:ASP:OD1	7:M:229:ARG:HD2	1.30	1.31
1:C:69:LEU:CB	1:C:72:ALA:HB3	1.61	1.30
7:M:147:LEU:CD1	7:M:172:PHE:HE1	1.44	1.29
7:M:20:LEU:HD23	7:M:24:PHE:CG	1.67	1.29
1:A:11:GLY:HA3	2:F:50:VAL:CA	1.63	1.28
1:A:11:GLY:HA3	2:F:50:VAL:C	1.58	1.28
7:M:20:LEU:CD2	7:M:24:PHE:CE1	2.16	1.28
7:M:214:PRO:CG	7:M:231:ALA:CB	2.12	1.28
7:M:214:PRO:CG	7:M:231:ALA:HA	1.62	1.28
1:C:224:ALA:CB	1:C:405:ALA:HB3	1.66	1.26
7:M:147:LEU:HD13	7:M:172:PHE:CE1	1.71	1.26
7:M:5:PHE:CG	7:M:286:VAL:HG11	1.71	1.26
7:M:170:LYS:HG3	7:M:174:GLU:OE2	1.33	1.26
1:C:44:GLY:HA2	2:F:69:ALA:CB	1.64	1.25
1:B:224:ALA:CB	1:B:405:ALA:HB3	1.65	1.25
7:M:33:PHE:CD2	7:M:308:TYR:CE1	2.24	1.25
7:M:137:ALA:HB3	7:M:152:ARG:CD	1.67	1.25
4:H:74:ILE:O	4:H:75:ALA:HA	1.35	1.24
1:A:224:ALA:CB	1:A:405:ALA:HB3	1.65	1.24
7:M:20:LEU:HD23	7:M:24:PHE:CE1	1.71	1.24
2:F:360:ARG:O	2:F:362:MET:N	1.70	1.23
1:A:25:TYR:N	2:D:66:LEU:N	1.76	1.23
7:M:214:PRO:CG	7:M:231:ALA:CA	2.17	1.23
7:M:15:ARG:NH1	7:M:68:LEU:HD21	1.39	1.22
7:M:220:LYS:HD3	7:M:227:ARG:NH2	1.52	1.22
1:A:11:GLY:CA	2:F:50:VAL:N	2.00	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:89:LEU:HD21	7:M:145:HIS:CD2	1.74	1.21
7:M:123:VAL:CG1	7:M:139:VAL:HG13	1.70	1.21
7:M:147:LEU:CD1	7:M:172:PHE:CE1	2.23	1.21
1:B:263:THR:CB	2:D:125:ARG:C	2.15	1.20
2:E:25:LYS:N	6:J:161:THR:CA	2.05	1.20
7:M:33:PHE:CE1	7:M:308:TYR:HB2	1.75	1.20
7:M:123:VAL:CG1	7:M:139:VAL:CG1	2.18	1.19
4:H:75:ALA:CB	4:H:85:ASP:CB	2.18	1.19
2:E:24:ALA:CB	6:J:159:GLY:O	1.88	1.19
2:F:61:GLU:O	2:F:227:PRO:CB	1.90	1.18
2:E:24:ALA:HB1	6:J:159:GLY:C	1.69	1.18
1:A:259:GLY:C	2:F:296:GLU:C	2.06	1.17
7:M:51:GLY:HA3	7:M:56:ASP:HB3	1.26	1.17
6:L:87:VAL:HG12	6:L:171:MET:HE2	1.20	1.17
7:M:123:VAL:HG13	7:M:139:VAL:CG1	1.72	1.17
7:M:33:PHE:CE2	7:M:308:TYR:CE1	2.33	1.16
1:A:24:MET:C	2:D:66:LEU:H	1.53	1.16
7:M:170:LYS:CG	7:M:174:GLU:OE2	1.92	1.15
7:M:92:ASP:HA	7:M:124:TRP:CZ2	1.80	1.15
7:M:33:PHE:CD1	7:M:308:TYR:CD1	2.34	1.15
2:E:25:LYS:CA	6:J:161:THR:CG2	1.88	1.15
1:A:11:GLY:HA3	2:F:50:VAL:O	1.47	1.14
7:M:267:CYS:N	7:M:322:CYS:SG	2.21	1.14
1:C:266:LEU:CB	2:E:124:ARG:CB	2.26	1.14
7:M:259:LYS:NZ	7:M:318:GLU:HB3	1.63	1.14
7:M:223:ARG:HG2	7:M:224:PHE:CE2	1.81	1.13
1:C:44:GLY:HA2	2:F:69:ALA:HB3	1.15	1.13
1:C:259:GLY:N	2:E:296:GLU:HA	1.36	1.13
7:M:119:LEU:HD11	7:M:140:LEU:HD23	1.31	1.13
7:M:57:VAL:HG21	7:M:305:ARG:HH12	1.08	1.13
7:M:214:PRO:HG2	7:M:231:ALA:CA	1.77	1.13
1:A:11:GLY:HA3	2:F:50:VAL:N	1.59	1.12
7:M:88:LEU:HB3	7:M:118:THR:N	1.62	1.13
4:H:84:HIS:O	4:H:86:VAL:N	1.81	1.12
7:M:137:ALA:CB	7:M:152:ARG:CD	2.27	1.12
7:M:223:ARG:HG2	7:M:224:PHE:CD2	1.85	1.12
1:B:419:PHE:O	1:B:496:GLN:CA	1.99	1.11
1:C:69:LEU:CB	1:C:72:ALA:CB	2.27	1.11
7:M:194:LEU:HD11	7:M:268:VAL:HG11	1.33	1.11
2:E:25:LYS:CB	6:J:161:THR:HG21	1.69	1.10
6:J:87:VAL:HG12	6:J:171:MET:HE2	1.20	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:214:PRO:HG3	7:M:231:ALA:CA	1.79	1.09
2:E:24:ALA:HB1	6:J:159:GLY:O	0.92	1.09
7:M:99:LEU:HD22	7:M:128:TYR:CD1	1.87	1.09
1:A:266:LEU:CB	2:F:124:ARG:CB	2.30	1.09
1:B:24:MET:HA	2:E:67:ASP:O	1.52	1.09
7:M:99:LEU:HD22	7:M:128:TYR:HD1	1.13	1.09
7:M:214:PRO:HG2	7:M:231:ALA:HB2	1.27	1.09
2:D:334:GLU:O	2:D:361:LEU:N	1.86	1.09
7:M:232:ARG:HH12	7:M:243:GLU:CD	1.60	1.08
1:C:259:GLY:O	2:E:296:GLU:C	1.97	1.08
2:E:149:LYS:O	2:E:334:GLU:N	1.87	1.08
7:M:51:GLY:CA	7:M:56:ASP:HB3	1.83	1.08
7:M:214:PRO:HG2	7:M:231:ALA:HB1	1.12	1.08
7:M:57:VAL:CG1	7:M:301:ARG:NH1	2.16	1.07
1:C:10:ALA:O	2:E:50:VAL:CB	2.03	1.07
2:D:149:LYS:O	2:D:334:GLU:N	1.87	1.07
7:M:178:LYS:HE3	7:M:221:GLY:HA3	1.15	1.06
7:M:163:ARG:HB3	7:M:167:LEU:CD1	1.85	1.06
7:M:229:ARG:NH1	7:M:243:GLU:HB2	1.45	1.06
2:F:149:LYS:O	2:F:334:GLU:N	1.87	1.06
7:M:266:ARG:CD	7:M:295:TRP:CH2	2.23	1.06
3:G:176:ILE:O	3:G:179:ILE:CB	2.03	1.06
2:F:108:PRO:O	6:L:180:SER:HB3	1.56	1.05
7:M:266:ARG:HD2	7:M:295:TRP:CZ2	1.82	1.05
1:C:259:GLY:O	2:E:296:GLU:O	1.74	1.05
3:G:7:THR:O	3:G:8:ARG:C	1.98	1.05
7:M:147:LEU:HD13	7:M:172:PHE:CD1	1.91	1.05
7:M:204:ALA:HA	7:M:234:MET:CE	1.87	1.04
7:M:3:ASP:HB3	7:M:79:GLU:HB3	1.35	1.04
1:C:52:TYR:CB	1:C:295:PRO:CB	2.34	1.04
7:M:89:LEU:N	7:M:118:THR:HG23	1.72	1.04
7:M:89:LEU:CG	7:M:118:THR:HG21	1.88	1.04
7:M:172:PHE:O	7:M:176:VAL:HG23	1.58	1.04
7:M:263:ARG:HG3	7:M:321:VAL:O	1.56	1.04
7:M:204:ALA:CA	7:M:234:MET:HE2	1.86	1.04
7:M:15:ARG:HH11	7:M:68:LEU:HD22	1.17	1.03
7:M:33:PHE:CD1	7:M:308:TYR:HD1	1.74	1.03
7:M:89:LEU:HG	7:M:118:THR:CG2	1.88	1.03
2:F:360:ARG:C	2:F:362:MET:H	1.67	1.03
7:M:5:PHE:CD2	7:M:286:VAL:CG1	2.42	1.03
7:M:220:LYS:HD3	7:M:227:ARG:HH22	0.91	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:266:ARG:NH1	7:M:295:TRP:CE3	2.26	1.02
1:A:11:GLY:CA	2:F:50:VAL:O	2.07	1.02
7:M:168:LEU:O	7:M:172:PHE:HB3	1.60	1.02
7:M:5:PHE:CG	7:M:286:VAL:CG1	2.43	1.01
7:M:312:PRO:HG3	7:M:315:GLN:OE1	0.84	1.01
1:C:224:ALA:HB1	1:C:405:ALA:HB3	1.41	1.01
7:M:33:PHE:HB2	7:M:308:TYR:HA	1.42	1.01
1:A:224:ALA:HB1	1:A:405:ALA:HB3	1.41	1.00
7:M:51:GLY:HA3	7:M:56:ASP:CB	1.91	1.00
7:M:194:LEU:HD11	7:M:268:VAL:CG1	1.89	1.00
1:A:11:GLY:HA2	2:F:50:VAL:N	1.67	1.00
7:M:29:LEU:HD13	7:M:313:ARG:NE	1.76	1.00
3:G:199:GLY:C	3:G:203:ALA:HB2	1.86	1.00
7:M:15:ARG:HH11	7:M:68:LEU:HD21	0.95	1.00
7:M:92:ASP:HA	7:M:124:TRP:CH2	1.97	0.99
1:C:44:GLY:CA	2:F:69:ALA:CB	2.38	0.99
2:E:25:LYS:HA	6:J:161:THR:HG23	1.03	0.99
7:M:89:LEU:HD21	7:M:145:HIS:NE2	1.74	0.99
1:A:25:TYR:O	2:D:65:GLY:HA2	1.62	0.99
7:M:40:LEU:HD23	7:M:49:LEU:HD22	1.42	0.99
1:C:208:GLY:O	1:C:507:CYS:O	1.79	0.99
7:M:89:LEU:HG	7:M:118:THR:HG21	0.99	0.99
7:M:178:LYS:CE	7:M:221:GLY:HA3	1.74	0.99
7:M:214:PRO:HG3	7:M:231:ALA:HA	1.00	0.99
7:M:73:PRO:HG2	7:M:88:LEU:CD1	1.92	0.99
7:M:45:TYR:HE1	7:M:64:THR:HG21	1.23	0.99
1:A:24:MET:CA	2:D:66:LEU:N	2.25	0.98
3:G:199:GLY:O	3:G:203:ALA:HB2	1.63	0.98
7:M:20:LEU:HD21	7:M:24:PHE:CD1	1.95	0.98
7:M:259:LYS:HZ3	7:M:318:GLU:CB	1.75	0.98
1:A:24:MET:CA	2:D:66:LEU:CA	2.18	0.98
7:M:226:ASP:OD2	7:M:229:ARG:HB2	1.64	0.98
1:A:11:GLY:HA2	2:F:50:VAL:H	0.81	0.97
1:A:259:GLY:O	2:F:296:GLU:O	1.82	0.97
1:B:224:ALA:HB1	1:B:405:ALA:HB3	1.41	0.97
1:C:224:ALA:HB2	1:C:405:ALA:HB3	1.46	0.97
7:M:123:VAL:HG12	7:M:139:VAL:CG1	1.92	0.97
1:C:259:GLY:H	2:E:296:GLU:CA	1.51	0.97
7:M:29:LEU:HD12	7:M:313:ARG:CZ	1.93	0.97
7:M:194:LEU:CD1	7:M:268:VAL:CG1	2.43	0.97
1:B:224:ALA:HB2	1:B:405:ALA:HB3	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLY:C	2:E:296:GLU:C	2.33	0.97
2:F:149:LYS:O	2:F:333:THR:HA	1.66	0.96
7:M:85:ARG:NH2	7:M:145:HIS:CD2	2.32	0.96
7:M:155:LEU:O	7:M:159:GLN:NE2	1.97	0.96
7:M:191:TYR:CE1	7:M:269:LEU:HD22	2.00	0.96
1:C:25:TYR:CB	2:F:65:GLY:HA2	1.94	0.96
2:D:334:GLU:CB	2:D:361:LEU:CB	2.44	0.96
7:M:20:LEU:HD21	7:M:24:PHE:CE1	1.98	0.96
7:M:263:ARG:O	7:M:322:CYS:HA	1.66	0.96
7:M:68:LEU:O	7:M:72:LEU:HD11	1.64	0.96
7:M:172:PHE:O	7:M:176:VAL:CG2	2.13	0.95
7:M:166:ALA:O	7:M:170:LYS:N	1.99	0.95
2:E:149:LYS:O	2:E:333:THR:HA	1.66	0.95
7:M:89:LEU:HD11	7:M:145:HIS:NE2	1.79	0.95
7:M:33:PHE:CZ	7:M:308:TYR:CD1	2.54	0.95
7:M:123:VAL:HG13	7:M:139:VAL:HG13	0.96	0.95
2:D:149:LYS:O	2:D:333:THR:HA	1.66	0.95
2:E:150:LEU:HA	2:E:335:GLY:O	1.67	0.95
2:D:150:LEU:HA	2:D:335:GLY:O	1.66	0.95
2:E:25:LYS:CB	6:J:161:THR:CA	2.44	0.95
2:F:150:LEU:HA	2:F:335:GLY:O	1.67	0.94
3:G:135:GLU:C	3:G:137:LEU:N	2.17	0.94
7:M:163:ARG:HB3	7:M:167:LEU:HD12	1.49	0.94
1:A:11:GLY:CA	2:F:50:VAL:CA	2.45	0.94
7:M:312:PRO:HG3	7:M:315:GLN:CD	1.92	0.94
3:G:148:LYS:O	3:G:152:GLU:CB	2.15	0.94
3:G:47:MET:O	3:G:49:ALA:N	2.00	0.94
7:M:45:TYR:CE1	7:M:64:THR:HG21	2.02	0.94
7:M:33:PHE:CD1	7:M:308:TYR:CG	2.55	0.94
7:M:94:HIS:HD2	7:M:95:ASN:OD1	1.50	0.94
7:M:229:ARG:NH2	7:M:243:GLU:CB	2.13	0.94
1:A:224:ALA:HB2	1:A:405:ALA:HB3	1.45	0.93
7:M:226:ASP:OD1	7:M:229:ARG:CD	2.15	0.93
7:M:259:LYS:HZ3	7:M:318:GLU:HB3	1.22	0.93
7:M:57:VAL:HG12	7:M:301:ARG:CZ	1.98	0.93
2:F:149:LYS:O	2:F:333:THR:CA	2.16	0.93
7:M:69:VAL:HA	7:M:72:LEU:CD1	1.99	0.93
1:A:25:TYR:O	2:D:65:GLY:CA	2.17	0.93
2:D:149:LYS:O	2:D:333:THR:CA	2.17	0.93
7:M:29:LEU:HD12	7:M:313:ARG:NH2	1.82	0.93
1:A:70:PRO:CB	1:A:190:ARG:CB	2.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:3:ASP:HB3	7:M:79:GLU:CB	1.89	0.92
7:M:204:ALA:HA	7:M:234:MET:HE2	0.95	0.92
7:M:266:ARG:HB3	7:M:322:CYS:SG	2.09	0.92
2:E:149:LYS:O	2:E:333:THR:CA	2.17	0.92
7:M:266:ARG:CG	7:M:322:CYS:SG	2.58	0.92
7:M:29:LEU:CD1	7:M:313:ARG:NE	2.31	0.92
7:M:88:LEU:CB	7:M:117:GLY:C	2.42	0.92
7:M:220:LYS:CD	7:M:227:ARG:HH22	1.82	0.92
1:C:11:GLY:HA3	2:E:50:VAL:H	1.31	0.92
7:M:57:VAL:CG1	7:M:301:ARG:CZ	2.47	0.92
7:M:223:ARG:NE	7:M:224:PHE:CE2	2.37	0.92
7:M:5:PHE:CE2	7:M:286:VAL:HG11	2.05	0.92
7:M:226:ASP:CG	7:M:229:ARG:HB2	1.95	0.92
7:M:266:ARG:CB	7:M:322:CYS:SG	2.58	0.92
7:M:88:LEU:HD13	7:M:117:GLY:O	1.70	0.92
1:A:267:VAL:N	2:F:124:ARG:CA	2.22	0.91
7:M:109:PHE:HZ	7:M:114:LEU:HD11	1.35	0.91
7:M:29:LEU:HD13	7:M:313:ARG:HG3	1.50	0.91
3:G:174:ALA:O	3:G:175:GLN:C	2.09	0.91
3:G:48:GLU:O	3:G:51:LYS:CB	2.18	0.90
7:M:33:PHE:CD1	7:M:308:TYR:CA	2.53	0.90
1:A:260:ASN:CB	2:F:298:ALA:O	2.18	0.90
7:M:266:ARG:C	7:M:322:CYS:SG	2.54	0.90
1:A:419:PHE:CB	1:A:497:GLN:O	2.20	0.90
1:C:259:GLY:C	2:E:296:GLU:HA	1.81	0.90
7:M:88:LEU:HB3	7:M:117:GLY:CA	2.01	0.90
1:A:25:TYR:CA	2:D:65:GLY:HA2	2.02	0.90
7:M:214:PRO:CG	7:M:231:ALA:HB1	1.91	0.90
3:G:49:ALA:O	3:G:52:ALA:HB3	1.72	0.89
7:M:224:PHE:CD1	7:M:247:THR:HB	2.07	0.89
7:M:89:LEU:CD2	7:M:145:HIS:NE2	2.35	0.89
1:B:24:MET:CB	2:E:66:LEU:HA	2.03	0.89
7:M:127:ALA:HB2	7:M:139:VAL:HG11	1.54	0.89
7:M:41:SER:HA	7:M:46:GLY:CA	2.02	0.89
7:M:54:LEU:HD12	7:M:301:ARG:NH2	1.86	0.89
1:A:25:TYR:CB	2:D:64:THR:O	2.21	0.88
7:M:57:VAL:HG12	7:M:301:ARG:HH11	1.32	0.88
1:B:263:THR:CB	2:D:125:ARG:CA	2.51	0.88
7:M:119:LEU:CD1	7:M:140:LEU:HD23	2.03	0.88
7:M:178:LYS:CE	7:M:221:GLY:HA2	1.71	0.88
1:A:25:TYR:C	2:D:65:GLY:HA2	1.98	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:141:ALA:O	3:G:145:THR:CB	2.20	0.88
7:M:123:VAL:CG1	7:M:139:VAL:HG12	2.02	0.88
7:M:137:ALA:HB1	7:M:152:ARG:HG2	1.53	0.88
7:M:194:LEU:CD1	7:M:268:VAL:HG11	2.01	0.88
3:G:47:MET:O	3:G:48:GLU:C	2.09	0.88
7:M:57:VAL:HG21	7:M:305:ARG:NH1	1.88	0.88
2:F:295:TYR:CB	2:F:332:ILE:CB	2.53	0.87
7:M:119:LEU:HD11	7:M:140:LEU:CD2	2.03	0.87
2:E:295:TYR:CB	2:E:332:ILE:CB	2.52	0.87
1:A:419:PHE:N	1:A:496:GLN:HA	1.89	0.87
2:E:24:ALA:C	6:J:161:THR:CA	2.33	0.87
7:M:33:PHE:CE1	7:M:308:TYR:CD1	2.63	0.87
4:H:75:ALA:C	4:H:75:ALA:HA	1.95	0.87
1:C:259:GLY:C	2:E:296:GLU:CA	2.38	0.87
5:K:110:ALA:HB1	6:L:182:VAL:HG23	1.57	0.87
7:M:48:GLU:OE1	7:M:63:ARG:NE	2.07	0.87
7:M:3:ASP:OD1	7:M:79:GLU:HG2	1.73	0.87
7:M:15:ARG:NH1	7:M:68:LEU:HD23	1.86	0.87
7:M:58:ASP:O	7:M:62:LEU:HB2	1.74	0.87
5:I:110:ALA:HB1	6:J:182:VAL:HG23	1.57	0.87
7:M:223:ARG:CG	7:M:224:PHE:CE2	2.58	0.87
7:M:229:ARG:HH22	7:M:243:GLU:HB3	1.35	0.87
3:G:51:LYS:CB	3:G:136:ALA:HB1	2.04	0.86
7:M:92:ASP:OD1	7:M:124:TRP:CZ2	2.28	0.86
2:D:295:TYR:CB	2:D:332:ILE:CB	2.53	0.86
1:A:217:PRO:O	1:A:431:PHE:CB	2.24	0.86
7:M:29:LEU:O	7:M:306:ARG:NH2	2.09	0.86
7:M:169:ALA:O	7:M:173:PHE:N	2.08	0.86
7:M:194:LEU:CD1	7:M:268:VAL:HG12	2.04	0.86
2:E:25:LYS:H	6:J:161:THR:HA	1.39	0.86
7:M:266:ARG:NE	7:M:295:TRP:HH2	1.67	0.86
2:F:150:LEU:CA	2:F:335:GLY:O	2.24	0.85
7:M:41:SER:HA	7:M:46:GLY:HA3	1.57	0.85
2:D:150:LEU:CA	2:D:335:GLY:O	2.24	0.85
1:A:267:VAL:H	2:F:124:ARG:CA	1.83	0.85
2:E:150:LEU:CA	2:E:335:GLY:O	2.24	0.85
7:M:220:LYS:CD	7:M:227:ARG:NH2	2.39	0.85
7:M:232:ARG:NH1	7:M:243:GLU:OE1	2.08	0.85
1:A:12:PRO:N	2:F:49:GLU:CB	2.39	0.85
2:E:153:PHE:O	2:E:339:LEU:N	2.09	0.85
2:F:8:TYR:CB	6:L:162:GLN:O	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:73:PRO:HG2	7:M:88:LEU:HD11	1.56	0.85
1:B:475:ALA:HB3	4:H:100:PHE:CB	2.05	0.85
2:E:25:LYS:CB	6:J:161:THR:CG2	0.85	0.85
2:F:153:PHE:O	2:F:339:LEU:N	2.09	0.85
7:M:147:LEU:HD12	7:M:172:PHE:HE1	1.42	0.85
7:M:266:ARG:HG2	7:M:322:CYS:SG	2.17	0.85
1:B:263:THR:CB	2:D:125:ARG:N	2.40	0.84
3:G:199:GLY:O	3:G:203:ALA:CB	2.25	0.84
4:H:74:ILE:O	4:H:75:ALA:CA	2.19	0.84
7:M:51:GLY:C	7:M:56:ASP:HB3	2.02	0.84
7:M:266:ARG:HD3	7:M:295:TRP:CD2	2.11	0.84
7:M:61:VAL:CG1	7:M:65:GLN:HG3	2.08	0.84
3:G:167:VAL:O	3:G:168:VAL:C	2.19	0.84
2:E:140:VAL:CB	2:E:435:SER:CB	2.56	0.83
2:E:24:ALA:CB	6:J:159:GLY:C	2.44	0.83
7:M:29:LEU:HD13	7:M:313:ARG:CG	2.08	0.83
1:A:25:TYR:CB	2:D:65:GLY:HA2	2.08	0.83
1:A:352:PRO:CB	2:D:269:GLU:O	2.26	0.83
3:G:158:THR:O	3:G:161:VAL:CB	2.27	0.83
7:M:178:LYS:HE3	7:M:221:GLY:HA2	0.83	0.82
1:A:267:VAL:CA	2:F:124:ARG:CB	2.50	0.82
1:C:18:GLY:O	1:C:19:MET:CB	2.27	0.82
2:D:153:PHE:O	2:D:339:LEU:N	2.08	0.82
7:M:92:ASP:OD1	7:M:124:TRP:HZ2	1.61	0.82
7:M:170:LYS:CG	7:M:174:GLU:CD	2.52	0.82
7:M:190:ASP:HB2	7:M:272:GLU:OE2	1.78	0.82
7:M:191:TYR:HE1	7:M:269:LEU:HB3	1.44	0.82
7:M:109:PHE:CZ	7:M:114:LEU:HD11	2.15	0.82
7:M:187:ALA:O	7:M:272:GLU:OE2	1.98	0.81
1:C:231:GLY:HA2	8:C:600:ADP:H5'1	1.61	0.81
1:A:266:LEU:CA	2:F:124:ARG:CB	2.57	0.81
2:D:134:GLY:HA2	2:D:430:ARG:O	1.81	0.81
3:G:167:VAL:O	3:G:169:ILE:N	2.14	0.81
7:M:9:ASN:ND2	7:M:285:LEU:HG	1.95	0.81
3:G:196:ARG:C	3:G:196:ARG:HA	2.05	0.81
7:M:3:ASP:CB	7:M:79:GLU:HB3	2.11	0.81
7:M:226:ASP:OD2	7:M:229:ARG:CB	2.28	0.81
7:M:137:ALA:HB1	7:M:152:ARG:HD2	1.62	0.80
7:M:3:ASP:CB	7:M:79:GLU:CB	2.58	0.80
7:M:137:ALA:HB1	7:M:152:ARG:CD	2.11	0.80
1:A:71:LEU:CB	1:A:72:ALA:HA	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:H	2:F:124:ARG:CB	1.90	0.80
2:E:25:LYS:CB	6:J:161:THR:HG22	0.52	0.80
7:M:91:ASN:ND2	7:M:116:PRO:O	2.12	0.80
7:M:33:PHE:CB	7:M:308:TYR:HA	2.12	0.80
7:M:73:PRO:HG2	7:M:88:LEU:HD12	1.62	0.80
7:M:93:LEU:CD1	7:M:168:LEU:HD23	2.12	0.80
7:M:170:LYS:HG2	7:M:174:GLU:CD	2.07	0.80
2:F:134:GLY:O	2:F:429:ASN:HA	1.82	0.79
7:M:88:LEU:CB	7:M:118:THR:N	2.44	0.79
1:A:18:GLY:O	1:A:19:MET:CB	2.27	0.79
1:B:224:ALA:HB1	1:B:405:ALA:CB	2.12	0.79
7:M:119:LEU:HD23	7:M:143:PRO:HG3	1.62	0.79
1:C:52:TYR:C	1:C:295:PRO:CB	2.56	0.79
1:A:224:ALA:HB1	1:A:405:ALA:CB	2.12	0.79
1:C:44:GLY:CA	2:F:69:ALA:HB2	2.12	0.79
7:M:259:LYS:HZ1	7:M:318:GLU:HB3	1.48	0.79
2:F:108:PRO:O	6:L:180:SER:CB	2.30	0.79
3:G:132:ARG:C	3:G:134:ALA:N	2.37	0.79
7:M:5:PHE:CD1	7:M:286:VAL:HG21	2.17	0.79
7:M:29:LEU:CD1	7:M:313:ARG:CZ	2.61	0.79
7:M:92:ASP:CA	7:M:124:TRP:CH2	2.66	0.79
1:C:224:ALA:HB1	1:C:405:ALA:CB	2.13	0.78
3:G:199:GLY:C	3:G:203:ALA:CB	2.56	0.78
1:B:18:GLY:O	1:B:19:MET:CB	2.28	0.78
7:M:89:LEU:CD1	7:M:145:HIS:NE2	2.45	0.78
2:E:25:LYS:CA	6:J:161:THR:HA	2.14	0.78
7:M:137:ALA:HB1	7:M:152:ARG:CG	2.14	0.78
3:G:28:LEU:O	3:G:31:LYS:CB	2.32	0.78
6:L:149:ARG:O	6:L:150:LEU:HD13	1.84	0.78
7:M:20:LEU:CD2	7:M:24:PHE:HD1	1.91	0.78
7:M:168:LEU:O	7:M:172:PHE:CB	2.32	0.78
7:M:163:ARG:O	7:M:167:LEU:N	2.16	0.78
3:G:132:ARG:N	3:G:134:ALA:HB3	1.98	0.78
6:J:149:ARG:O	6:J:150:LEU:HD13	1.84	0.78
7:M:90:ARG:NH1	7:M:93:LEU:HD23	1.97	0.78
7:M:312:PRO:HB2	7:M:315:GLN:HB2	1.65	0.77
3:G:45:GLU:O	3:G:46:ALA:C	2.27	0.77
7:M:130:ALA:HB1	7:M:135:GLY:HA3	1.64	0.77
7:M:29:LEU:CD1	7:M:313:ARG:HG3	2.14	0.77
3:G:4:VAL:C	3:G:4:VAL:HA	2.07	0.77
7:M:223:ARG:NE	7:M:224:PHE:HE2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:224:PHE:CE1	7:M:248:PRO:HD2	2.19	0.77
7:M:226:ASP:OD1	7:M:229:ARG:HB2	1.85	0.77
1:C:11:GLY:HA3	2:E:50:VAL:N	2.00	0.77
1:C:44:GLY:HA2	2:F:69:ALA:HB2	1.62	0.77
7:M:226:ASP:OD2	7:M:229:ARG:N	2.17	0.76
7:M:229:ARG:CZ	7:M:243:GLU:HB2	1.89	0.76
3:G:163:ALA:C	3:G:163:ALA:HA	2.04	0.76
7:M:5:PHE:CE2	7:M:283:VAL:HG23	2.19	0.76
7:M:218:PHE:CD2	7:M:227:ARG:HG2	2.20	0.76
3:G:39:PHE:O	3:G:42:LEU:CB	2.34	0.76
7:M:163:ARG:HB3	7:M:167:LEU:HD11	1.68	0.76
7:M:242:ASP:OD1	7:M:254:GLY:N	2.19	0.76
7:M:191:TYR:CE1	7:M:269:LEU:HB3	2.20	0.76
2:D:51:SER:O	2:D:52:GLU:CB	2.33	0.76
7:M:166:ALA:HB1	7:M:170:LYS:CB	2.16	0.75
6:L:41:LEU:HD13	6:L:41:LEU:O	1.86	0.75
7:M:33:PHE:HD1	7:M:308:TYR:HB2	1.44	0.75
2:E:51:SER:O	2:E:52:GLU:CB	2.33	0.75
6:J:41:LEU:HD13	6:J:41:LEU:O	1.86	0.75
1:A:259:GLY:O	2:F:297:ARG:N	2.18	0.75
2:F:51:SER:O	2:F:52:GLU:CB	2.33	0.75
6:J:88:ARG:HA	6:J:171:MET:HE1	1.69	0.75
2:D:149:LYS:CB	2:D:332:ILE:O	2.35	0.75
7:M:99:LEU:CD2	7:M:128:TYR:CD1	2.70	0.75
7:M:283:VAL:HG23	7:M:286:VAL:CG1	2.15	0.75
1:A:24:MET:CB	2:D:66:LEU:N	2.49	0.75
3:G:140:VAL:O	3:G:144:GLU:CB	2.35	0.75
1:B:263:THR:CB	2:D:125:ARG:O	2.35	0.74
1:C:224:ALA:CB	1:C:405:ALA:CB	2.58	0.74
7:M:5:PHE:CD1	7:M:286:VAL:HG11	2.22	0.74
7:M:266:ARG:CZ	7:M:295:TRP:HZ3	1.90	0.74
2:E:149:LYS:CB	2:E:332:ILE:O	2.35	0.74
7:M:72:LEU:HD23	7:M:75:LEU:HD12	1.70	0.74
2:F:149:LYS:CB	2:F:332:ILE:O	2.35	0.74
3:G:135:GLU:O	3:G:136:ALA:C	2.28	0.74
7:M:224:PHE:CE1	7:M:248:PRO:CD	2.69	0.74
2:F:24:ALA:HB3	6:L:161:THR:HG23	1.69	0.74
1:A:24:MET:CB	2:D:66:LEU:CA	2.65	0.74
4:H:75:ALA:C	4:H:75:ALA:CB	2.60	0.74
7:M:266:ARG:HD3	7:M:295:TRP:CH2	2.07	0.74
1:C:44:GLY:CA	2:F:69:ALA:HB3	2.07	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLY:CA	2:F:50:VAL:CB	2.65	0.73
1:B:419:PHE:O	1:B:496:GLN:CB	2.35	0.73
7:M:33:PHE:CE1	7:M:308:TYR:CB	2.55	0.73
7:M:94:HIS:CD2	7:M:95:ASN:OD1	2.40	0.73
2:D:69:ALA:O	2:D:70:THR:CB	2.36	0.73
4:H:65:GLY:CA	4:H:66:ARG:CB	2.65	0.73
1:C:69:LEU:CB	1:C:72:ALA:HB2	2.19	0.73
3:G:142:ASN:O	3:G:146:ARG:CB	2.36	0.73
6:L:88:ARG:HA	6:L:171:MET:HE1	1.69	0.73
1:A:56:SER:CB	2:F:30:GLY:N	2.52	0.73
7:M:33:PHE:CE1	7:M:308:TYR:CG	2.77	0.73
1:A:24:MET:CA	2:D:66:LEU:H	1.92	0.73
7:M:51:GLY:HA3	7:M:56:ASP:CG	2.13	0.73
7:M:93:LEU:HD13	7:M:168:LEU:HD23	1.71	0.73
7:M:167:LEU:HA	7:M:171:ARG:HB3	1.71	0.73
7:M:256:ARG:O	7:M:257:ASP:HB3	1.89	0.73
7:M:61:VAL:HG13	7:M:65:GLN:HG3	1.70	0.72
3:G:150:ILE:O	3:G:151:GLY:O	2.07	0.72
7:M:72:LEU:HB2	7:M:84:VAL:HG11	1.69	0.72
7:M:92:ASP:CA	7:M:124:TRP:CZ2	2.67	0.72
1:A:52:TYR:CB	1:A:297:ALA:HB3	2.19	0.72
2:E:25:LYS:CB	6:J:161:THR:C	2.62	0.72
1:A:224:ALA:CB	1:A:405:ALA:CB	2.58	0.72
2:F:69:ALA:O	2:F:70:THR:CB	2.36	0.72
7:M:3:ASP:HB3	7:M:79:GLU:N	2.01	0.72
1:A:204:PRO:CB	1:A:435:LEU:CB	2.68	0.72
7:M:191:TYR:CZ	7:M:269:LEU:HD22	2.25	0.72
7:M:259:LYS:HZ3	7:M:318:GLU:CG	2.01	0.72
4:H:74:ILE:C	4:H:75:ALA:CA	2.62	0.72
7:M:166:ALA:HB1	7:M:170:LYS:CD	2.20	0.72
7:M:191:TYR:CE1	7:M:269:LEU:CD2	2.72	0.72
7:M:306:ARG:HG3	7:M:311:LEU:HB2	1.70	0.72
2:E:69:ALA:O	2:E:70:THR:CB	2.37	0.72
3:G:48:GLU:C	3:G:51:LYS:H	1.97	0.72
7:M:242:ASP:HA	7:M:253:SER:HA	1.72	0.72
7:M:89:LEU:HD23	7:M:118:THR:OG1	1.90	0.72
7:M:119:LEU:HD13	7:M:123:VAL:HG11	1.72	0.72
7:M:170:LYS:HG3	7:M:174:GLU:CD	2.12	0.72
1:C:259:GLY:H	2:E:296:GLU:CB	2.02	0.71
7:M:92:ASP:HA	7:M:124:TRP:HZ2	1.50	0.71
7:M:10:ALA:HA	7:M:13:ARG:NH1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:29:LEU:HD13	7:M:313:ARG:HE	1.55	0.71
2:F:65:GLY:O	2:F:66:LEU:CB	2.38	0.71
4:H:74:ILE:C	4:H:75:ALA:HA	2.16	0.71
7:M:56:ASP:OD1	7:M:59:ARG:NH2	2.22	0.71
3:G:194:LEU:C	3:G:194:LEU:HA	2.04	0.71
7:M:33:PHE:HD1	7:M:308:TYR:CA	2.01	0.71
7:M:166:ALA:HB1	7:M:170:LYS:HD3	1.71	0.71
7:M:22:GLU:O	7:M:26:GLN:HG2	1.91	0.71
7:M:266:ARG:NH2	7:M:295:TRP:CZ3	2.55	0.71
1:A:259:GLY:C	2:F:296:GLU:O	2.31	0.70
1:B:24:MET:CB	2:E:66:LEU:CA	2.69	0.70
7:M:5:PHE:CE1	7:M:286:VAL:HG21	2.26	0.70
2:D:274:ARG:O	2:D:275:GLU:CB	2.37	0.70
1:B:225:ALA:N	1:B:405:ALA:O	2.25	0.70
2:D:359:SER:C	2:D:361:LEU:N	2.39	0.70
2:F:274:ARG:O	2:F:275:GLU:CB	2.37	0.70
7:M:61:VAL:HG12	7:M:65:GLN:HG3	1.73	0.70
7:M:8:LEU:HG	7:M:12:VAL:CG2	2.22	0.70
7:M:259:LYS:NZ	7:M:318:GLU:CB	2.41	0.70
2:E:25:LYS:CA	6:J:161:THR:CA	2.70	0.70
7:M:51:GLY:C	7:M:56:ASP:CB	2.64	0.70
7:M:232:ARG:NH1	7:M:243:GLU:OE2	2.23	0.70
6:L:87:VAL:HG12	6:L:171:MET:CE	2.12	0.70
7:M:3:ASP:CB	7:M:79:GLU:N	2.52	0.70
1:A:225:ALA:N	1:A:405:ALA:O	2.25	0.70
2:E:65:GLY:O	2:E:66:LEU:CB	2.38	0.70
7:M:3:ASP:HA	7:M:80:ALA:HB3	1.74	0.70
1:C:225:ALA:N	1:C:405:ALA:O	2.25	0.69
1:A:24:MET:HA	2:D:66:LEU:N	1.97	0.69
1:A:25:TYR:H	2:D:65:GLY:C	1.96	0.69
3:G:197:ILE:O	3:G:200:LYS:CB	2.41	0.69
1:A:56:SER:CB	2:F:30:GLY:O	2.40	0.69
2:E:274:ARG:O	2:E:275:GLU:CB	2.37	0.69
2:F:149:LYS:O	2:F:333:THR:C	2.35	0.69
7:M:15:ARG:HH12	7:M:68:LEU:CD2	2.04	0.69
7:M:64:THR:HA	7:M:67:LYS:HD3	1.75	0.69
7:M:166:ALA:C	7:M:170:LYS:HB3	2.16	0.69
1:B:224:ALA:CB	1:B:405:ALA:CB	2.58	0.69
7:M:33:PHE:CD2	7:M:308:TYR:HE1	2.06	0.69
7:M:73:PRO:HG3	7:M:84:VAL:HG12	1.74	0.69
7:M:3:ASP:OD1	7:M:80:ALA:HA	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:33:PHE:CD1	7:M:308:TYR:HA	2.26	0.69
7:M:266:ARG:CD	7:M:295:TRP:CE2	2.35	0.69
2:D:149:LYS:O	2:D:333:THR:C	2.35	0.69
6:L:87:VAL:CG1	6:L:171:MET:HE2	2.13	0.69
7:M:52:GLN:N	7:M:56:ASP:CB	2.56	0.69
7:M:51:GLY:CA	7:M:56:ASP:CB	2.59	0.69
2:F:61:GLU:HA	2:F:229:ILE:CB	2.22	0.69
2:E:149:LYS:O	2:E:333:THR:C	2.35	0.68
7:M:185:GLN:HE22	7:M:282:GLY:CA	2.06	0.68
1:A:5:VAL:CB	1:A:18:GLY:O	2.42	0.68
1:B:419:PHE:C	1:B:496:GLN:HA	2.13	0.68
2:D:65:GLY:O	2:D:66:LEU:CB	2.39	0.68
1:B:10:ALA:O	2:D:49:GLU:HA	1.93	0.68
6:J:87:VAL:HG12	6:J:171:MET:CE	2.12	0.68
7:M:69:VAL:HA	7:M:72:LEU:HD12	1.72	0.68
1:B:5:VAL:CB	1:B:18:GLY:O	2.42	0.68
4:H:75:ALA:HB2	4:H:85:ASP:CB	2.19	0.68
7:M:16:ARG:NH2	7:M:19:LEU:CD1	2.57	0.68
1:A:11:GLY:HA3	2:F:50:VAL:CB	2.23	0.68
3:G:151:GLY:O	3:G:152:GLU:C	2.37	0.67
7:M:68:LEU:O	7:M:72:LEU:HD21	1.94	0.67
1:A:25:TYR:O	2:D:65:GLY:HA3	1.93	0.67
7:M:76:VAL:HG23	7:M:81:ARG:HA	1.77	0.67
7:M:95:ASN:ND2	7:M:114:LEU:HD22	2.09	0.67
7:M:185:GLN:OE1	7:M:283:VAL:HG12	1.94	0.67
7:M:145:HIS:CE1	7:M:147:LEU:HB2	2.30	0.67
7:M:137:ALA:HB3	7:M:152:ARG:HD2	0.70	0.67
1:C:5:VAL:CB	1:C:18:GLY:O	2.42	0.67
1:C:189:VAL:O	1:C:304:TYR:CB	2.42	0.67
7:M:9:ASN:ND2	7:M:285:LEU:CG	2.57	0.67
7:M:89:LEU:N	7:M:118:THR:CG2	2.55	0.67
7:M:103:LYS:HD3	7:M:128:TYR:CE1	2.30	0.67
7:M:306:ARG:HD2	7:M:311:LEU:O	1.93	0.67
1:B:24:MET:CA	2:E:67:ASP:O	2.38	0.67
3:G:151:GLY:HA2	3:G:155:LYS:CB	2.26	0.67
6:J:139:GLY:O	6:J:140:VAL:HG12	1.96	0.66
7:M:283:VAL:CG2	7:M:286:VAL:CG1	2.72	0.66
7:M:23:SER:HA	7:M:26:GLN:CG	2.25	0.66
7:M:54:LEU:HD12	7:M:301:ARG:HH22	1.58	0.66
7:M:224:PHE:CD2	7:M:249:PHE:HE2	2.14	0.66
3:G:156:LYS:C	3:G:158:THR:N	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:40:LEU:CD2	7:M:49:LEU:HD22	2.21	0.66
6:J:150:LEU:HD23	6:J:168:LEU:HD21	1.78	0.66
7:M:256:ARG:O	7:M:257:ASP:CB	2.44	0.66
1:C:429:SER:C	1:C:431:PHE:H	2.03	0.66
7:M:208:GLN:HA	7:M:234:MET:O	1.95	0.66
1:A:419:PHE:H	1:A:496:GLN:HA	1.59	0.66
1:C:56:SER:CB	2:E:30:GLY:O	2.44	0.66
7:M:119:LEU:HD13	7:M:123:VAL:CG1	2.26	0.66
3:G:31:LYS:N	3:G:31:LYS:HA	2.02	0.66
7:M:90:ARG:HH12	7:M:93:LEU:HD23	1.58	0.65
2:E:61:GLU:O	2:E:227:PRO:CB	2.44	0.65
1:A:260:ASN:N	2:F:296:GLU:HA	1.99	0.65
2:D:334:GLU:O	2:D:361:LEU:CB	2.45	0.65
3:G:3:GLN:O	3:G:5:SER:N	2.29	0.65
3:G:41:GLY:O	3:G:42:LEU:C	2.38	0.65
6:L:150:LEU:HD23	6:L:168:LEU:HD21	1.78	0.65
7:M:52:GLN:NE2	7:M:308:TYR:OH	2.30	0.65
6:L:139:GLY:O	6:L:140:VAL:HG12	1.96	0.65
2:D:334:GLU:CA	2:D:361:LEU:CB	2.75	0.65
3:G:156:LYS:O	3:G:157:THR:C	2.33	0.65
1:C:27:ILE:HA	1:C:71:LEU:H	1.61	0.65
3:G:141:ALA:HA	3:G:144:GLU:CB	2.26	0.65
7:M:88:LEU:CB	7:M:117:GLY:HA2	2.27	0.65
7:M:57:VAL:HG11	7:M:301:ARG:CZ	2.25	0.64
7:M:152:ARG:NE	7:M:156:ARG:NH1	2.44	0.64
4:H:75:ALA:N	4:H:75:ALA:CB	2.56	0.64
3:G:132:ARG:O	3:G:133:TYR:C	2.37	0.64
4:H:65:GLY:HA2	4:H:66:ARG:CB	2.27	0.64
7:M:20:LEU:CG	7:M:24:PHE:CD1	2.77	0.64
7:M:137:ALA:CB	7:M:152:ARG:CG	2.73	0.64
7:M:312:PRO:CG	7:M:315:GLN:CD	2.62	0.64
7:M:54:LEU:HB3	7:M:55:PRO:HD3	1.80	0.64
7:M:64:THR:O	7:M:67:LYS:HG2	1.97	0.64
3:G:150:ILE:C	3:G:151:GLY:O	2.39	0.64
3:G:158:THR:C	3:G:161:VAL:CB	2.70	0.64
3:G:172:ILE:O	3:G:176:ILE:CB	2.45	0.64
7:M:229:ARG:HG2	7:M:229:ARG:HH11	1.63	0.64
3:G:135:GLU:C	3:G:137:LEU:H	2.03	0.64
2:E:212:GLY:N	6:J:59:ARG:NH1	2.44	0.64
6:L:67:LEU:HD23	6:L:67:LEU:O	1.98	0.64
7:M:4:ASP:OD1	7:M:282:GLY:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:223:ARG:CD	7:M:224:PHE:CE2	2.81	0.63
7:M:263:ARG:O	7:M:322:CYS:CA	2.44	0.63
7:M:238:TYR:HB3	7:M:256:ARG:NE	2.14	0.63
1:C:11:GLY:CA	2:E:49:GLU:HA	2.28	0.63
7:M:5:PHE:CD2	7:M:283:VAL:HG23	2.34	0.63
7:M:109:PHE:HZ	7:M:114:LEU:CD1	2.09	0.63
7:M:134:ALA:O	7:M:138:GLN:HG3	1.98	0.63
7:M:263:ARG:HG2	7:M:322:CYS:C	2.23	0.63
3:G:148:LYS:O	3:G:149:LYS:O	2.17	0.63
7:M:89:LEU:CD2	7:M:145:HIS:CD2	2.67	0.63
3:G:18:LEU:O	3:G:21:ALA:HB3	1.99	0.63
7:M:193:ALA:HB1	7:M:222:GLY:C	2.24	0.63
7:M:41:SER:HA	7:M:46:GLY:HA2	1.79	0.63
7:M:306:ARG:CG	7:M:311:LEU:HB2	2.29	0.63
2:D:359:SER:C	2:D:361:LEU:H	2.07	0.63
3:G:141:ALA:HA	3:G:145:THR:H	1.62	0.63
6:J:67:LEU:O	6:J:67:LEU:HD23	1.98	0.63
6:J:101:PRO:O	6:J:104:VAL:HG22	1.99	0.63
7:M:3:ASP:HA	7:M:80:ALA:CB	2.29	0.63
7:M:191:TYR:HB2	7:M:272:GLU:HG2	1.81	0.63
1:C:259:GLY:C	2:E:296:GLU:O	2.35	0.62
7:M:283:VAL:CG2	7:M:286:VAL:HG13	2.29	0.62
3:G:156:LYS:HA	3:G:159:ARG:H	1.64	0.62
7:M:54:LEU:CD1	7:M:301:ARG:NH2	2.61	0.62
7:M:267:CYS:SG	7:M:322:CYS:O	2.51	0.62
2:E:76:VAL:O	2:E:77:GLU:CB	2.47	0.62
7:M:31:LEU:HB3	7:M:35:ASP:CB	2.29	0.62
7:M:88:LEU:HD22	7:M:117:GLY:CA	2.29	0.62
7:M:152:ARG:NE	7:M:156:ARG:HH12	1.98	0.62
1:C:25:TYR:CB	2:F:65:GLY:CA	2.75	0.62
7:M:99:LEU:O	7:M:103:LYS:HB2	1.98	0.62
6:L:101:PRO:O	6:L:104:VAL:HG22	1.99	0.62
1:A:419:PHE:HA	1:A:420:PRO:C	2.25	0.62
2:F:76:VAL:O	2:F:77:GLU:CB	2.47	0.62
7:M:167:LEU:O	7:M:171:ARG:HB3	1.99	0.61
6:J:149:ARG:HB3	6:J:150:LEU:HD22	1.82	0.61
7:M:145:HIS:HE1	7:M:147:LEU:HB2	1.64	0.61
7:M:193:ALA:HB3	7:M:223:ARG:HB2	1.81	0.61
7:M:8:LEU:CD1	7:M:12:VAL:HG23	2.30	0.61
6:J:88:ARG:CA	6:J:171:MET:HE1	2.31	0.61
7:M:31:LEU:HD22	7:M:35:ASP:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLY:O	1:A:507:CYS:O	2.18	0.61
6:L:88:ARG:CA	6:L:171:MET:HE1	2.31	0.61
7:M:68:LEU:O	7:M:72:LEU:CD1	2.44	0.61
7:M:8:LEU:HG	7:M:12:VAL:HG21	1.83	0.61
3:G:47:MET:C	3:G:49:ALA:N	2.57	0.61
7:M:31:LEU:HB3	7:M:35:ASP:HB2	1.82	0.61
7:M:238:TYR:HB3	7:M:256:ARG:CD	2.31	0.61
1:B:9:ILE:CA	2:D:50:VAL:O	2.48	0.61
2:D:134:GLY:O	2:D:430:ARG:N	2.34	0.61
7:M:72:LEU:CB	7:M:84:VAL:HG11	2.31	0.61
7:M:92:ASP:CA	7:M:124:TRP:HH2	2.14	0.61
1:C:419:PHE:HA	1:C:420:PRO:C	2.25	0.60
3:G:47:MET:C	3:G:49:ALA:H	2.09	0.60
3:G:170:PRO:O	3:G:174:ALA:HB2	2.00	0.60
7:M:169:ALA:O	7:M:170:LYS:C	2.44	0.60
7:M:266:ARG:HD2	7:M:322:CYS:SG	2.41	0.60
7:M:29:LEU:CD1	7:M:313:ARG:HE	2.12	0.60
1:B:419:PHE:HA	1:B:420:PRO:C	2.25	0.60
7:M:152:ARG:HE	7:M:156:ARG:NH1	1.98	0.60
2:F:25:LYS:CB	6:L:115:LEU:CB	2.79	0.60
7:M:154:VAL:O	7:M:158:THR:HG22	2.01	0.60
3:G:135:GLU:HA	3:G:138:ILE:N	2.17	0.60
7:M:238:TYR:CB	7:M:256:ARG:NE	2.64	0.60
7:M:88:LEU:HD22	7:M:117:GLY:HA2	1.83	0.60
7:M:99:LEU:O	7:M:103:LYS:CB	2.50	0.60
7:M:267:CYS:CA	7:M:322:CYS:SG	2.89	0.60
5:K:95:GLU:O	5:K:99:VAL:HG13	2.02	0.60
5:I:95:GLU:O	5:I:99:VAL:HG13	2.02	0.60
6:L:149:ARG:HB3	6:L:150:LEU:HD22	1.82	0.60
1:A:12:PRO:O	1:A:13:ALA:HB3	2.01	0.59
7:M:39:LEU:O	7:M:42:GLU:HG2	2.02	0.59
2:D:76:VAL:O	2:D:77:GLU:CB	2.47	0.59
7:M:88:LEU:CB	7:M:117:GLY:CA	2.77	0.59
5:I:37:LEU:HD23	6:J:16:ILE:HG22	1.84	0.59
7:M:224:PHE:CE1	7:M:248:PRO:HD3	2.35	0.59
1:C:12:PRO:O	1:C:13:ALA:HB3	2.02	0.59
3:G:160:ARG:O	3:G:164:LEU:CB	2.50	0.59
5:K:37:LEU:HD23	6:L:16:ILE:HG22	1.84	0.59
7:M:51:GLY:CA	7:M:56:ASP:CG	2.75	0.59
7:M:166:ALA:O	7:M:170:LYS:HB3	2.03	0.59
1:A:429:SER:CB	1:A:431:PHE:H	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:PRO:O	1:B:13:ALA:HB3	2.02	0.59
7:M:119:LEU:HB3	7:M:123:VAL:HB	1.85	0.59
7:M:229:ARG:HB3	7:M:240:VAL:HG13	1.85	0.59
7:M:246:GLY:O	7:M:247:THR:HG22	2.03	0.59
7:M:263:ARG:CG	7:M:321:VAL:O	2.43	0.59
3:G:189:GLU:CB	3:G:189:GLU:HA	2.18	0.58
3:G:194:LEU:C	3:G:194:LEU:CB	2.73	0.58
7:M:71:ASP:C	7:M:73:PRO:HD2	2.28	0.58
7:M:266:ARG:HG2	7:M:322:CYS:HG	1.67	0.58
2:D:134:GLY:CA	2:D:430:ARG:O	2.51	0.58
7:M:215:ASP:OD1	7:M:228:VAL:HA	2.04	0.58
7:M:119:LEU:CD2	7:M:143:PRO:HG3	2.31	0.58
7:M:33:PHE:CG	7:M:308:TYR:HA	2.38	0.58
7:M:57:VAL:CG1	7:M:301:ARG:HG2	2.34	0.58
7:M:85:ARG:NH2	7:M:145:HIS:CG	2.71	0.58
7:M:147:LEU:HD11	7:M:172:PHE:CE1	2.34	0.58
3:G:167:VAL:C	3:G:167:VAL:HA	2.16	0.58
7:M:58:ASP:N	7:M:301:ARG:HH12	2.01	0.58
7:M:193:ALA:CB	7:M:223:ARG:HB2	2.33	0.58
1:A:189:VAL:HA	1:A:308:THR:CB	2.34	0.58
3:G:165:GLU:O	3:G:166:GLN:C	2.47	0.58
7:M:8:LEU:HG	7:M:12:VAL:HG23	1.85	0.58
7:M:12:VAL:O	7:M:13:ARG:C	2.45	0.58
7:M:20:LEU:HB3	7:M:24:PHE:CB	2.33	0.58
7:M:54:LEU:HD12	7:M:301:ARG:HH21	1.68	0.58
1:A:241:LEU:O	1:A:245:SER:N	2.31	0.58
1:C:241:LEU:O	1:C:245:SER:N	2.31	0.58
3:G:45:GLU:C	3:G:47:MET:N	2.58	0.57
6:J:87:VAL:CG1	6:J:171:MET:HE2	2.13	0.57
2:F:8:TYR:CB	6:L:162:GLN:HB2	2.34	0.57
7:M:263:ARG:HH21	7:M:318:GLU:HG2	1.69	0.57
1:C:260:ASN:CB	2:E:298:ALA:O	2.53	0.57
7:M:174:GLU:HG2	7:M:219:LEU:HD21	1.86	0.57
7:M:199:GLU:OE1	7:M:202:ARG:NH1	2.38	0.57
3:G:142:ASN:CB	3:G:142:ASN:HA	2.16	0.57
7:M:72:LEU:HB2	7:M:84:VAL:CG1	2.34	0.57
1:A:25:TYR:N	2:D:65:GLY:HA2	2.18	0.57
3:G:167:VAL:C	3:G:169:ILE:N	2.61	0.57
6:L:135:ALA:HA	6:L:140:VAL:H	1.70	0.57
7:M:16:ARG:CZ	7:M:19:LEU:CD1	2.82	0.57
7:M:266:ARG:CD	7:M:322:CYS:SG	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:135:GLU:O	3:G:137:LEU:N	2.33	0.57
7:M:52:GLN:N	7:M:56:ASP:HB2	2.20	0.57
7:M:185:GLN:HE22	7:M:282:GLY:HA3	1.69	0.57
1:A:132:GLY:HA3	1:A:371:LEU:C	2.30	0.57
7:M:15:ARG:HH12	7:M:68:LEU:HD23	1.67	0.57
7:M:226:ASP:OD1	7:M:229:ARG:CB	2.51	0.57
1:C:429:SER:C	1:C:431:PHE:N	2.60	0.57
3:G:132:ARG:C	3:G:134:ALA:H	2.13	0.56
7:M:259:LYS:HE2	7:M:319:GLU:CA	2.35	0.56
1:B:23:ARG:O	2:E:68:LEU:HA	2.05	0.56
3:G:44:ARG:C	3:G:47:MET:CB	2.72	0.56
1:B:263:THR:CB	2:D:124:ARG:C	2.78	0.56
2:D:334:GLU:O	2:D:361:LEU:CA	2.53	0.56
3:G:48:GLU:O	3:G:51:LYS:N	2.38	0.56
3:G:186:ARG:O	3:G:190:ASP:CB	2.53	0.56
4:H:84:HIS:O	4:H:85:ASP:C	2.48	0.56
7:M:3:ASP:OD1	7:M:80:ALA:CA	2.40	0.56
7:M:95:ASN:O	7:M:99:LEU:HD12	2.05	0.56
7:M:194:LEU:HD13	7:M:268:VAL:CG1	2.34	0.56
3:G:137:LEU:O	3:G:140:VAL:CB	2.54	0.56
6:J:135:ALA:HA	6:J:140:VAL:H	1.70	0.56
7:M:58:ASP:O	7:M:62:LEU:N	2.26	0.56
7:M:263:ARG:NH2	7:M:318:GLU:HG2	2.20	0.56
1:C:11:GLY:HA3	2:E:49:GLU:CA	2.35	0.56
7:M:140:LEU:HB2	7:M:148:ALA:HB1	1.87	0.56
7:M:52:GLN:H	7:M:56:ASP:CG	2.13	0.56
7:M:88:LEU:CA	7:M:117:GLY:HA2	2.35	0.56
1:A:71:LEU:CB	1:A:72:ALA:CA	2.83	0.56
7:M:57:VAL:C	7:M:301:ARG:HH12	2.13	0.56
7:M:89:LEU:H	7:M:118:THR:HG23	1.68	0.56
7:M:218:PHE:CD1	7:M:227:ARG:HA	2.40	0.56
7:M:259:LYS:NZ	7:M:318:GLU:CG	2.68	0.56
3:G:158:THR:HA	3:G:161:VAL:CB	2.37	0.56
1:C:419:PHE:CB	1:C:497:GLN:O	2.54	0.55
7:M:224:PHE:CZ	7:M:248:PRO:HD2	2.41	0.55
7:M:246:GLY:O	7:M:247:THR:CG2	2.54	0.55
3:G:132:ARG:N	3:G:134:ALA:CB	2.68	0.55
7:M:200:ASN:HB3	7:M:230:PHE:CE1	2.41	0.55
1:A:25:TYR:N	2:D:65:GLY:C	2.60	0.55
7:M:69:VAL:HA	7:M:72:LEU:HD11	1.86	0.55
7:M:211:GLY:C	7:M:235:GLU:OE1	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:TYR:O	6:L:161:THR:O	2.24	0.55
3:G:55:GLN:CB	3:G:133:TYR:CB	2.85	0.55
3:G:52:ALA:CB	3:G:52:ALA:C	2.74	0.55
7:M:194:LEU:HD21	7:M:249:PHE:CZ	2.41	0.55
7:M:224:PHE:CD2	7:M:249:PHE:CE2	2.94	0.55
7:M:259:LYS:HE2	7:M:319:GLU:N	2.21	0.55
7:M:89:LEU:CD2	7:M:118:THR:HG21	2.36	0.55
7:M:283:VAL:HG22	7:M:286:VAL:HG13	1.88	0.55
1:A:71:LEU:HA	1:A:189:VAL:H	1.72	0.55
7:M:5:PHE:CG	7:M:286:VAL:CB	2.90	0.55
1:A:225:ALA:O	1:A:406:PHE:HA	2.07	0.54
1:B:241:LEU:O	1:B:245:SER:N	2.32	0.54
7:M:71:ASP:C	7:M:73:PRO:CD	2.80	0.54
3:G:137:LEU:O	3:G:140:VAL:N	2.40	0.54
3:G:146:ARG:O	3:G:147:LEU:C	2.50	0.54
7:M:266:ARG:NE	7:M:295:TRP:CZ2	2.25	0.54
7:M:167:LEU:HA	7:M:171:ARG:CB	2.37	0.54
6:L:42:LEU:O	6:L:42:LEU:HD23	2.07	0.54
7:M:9:ASN:ND2	7:M:285:LEU:HB3	2.23	0.54
7:M:232:ARG:NH2	7:M:239:ALA:HB3	2.22	0.54
6:L:108:ALA:O	6:L:112:LEU:HD23	2.07	0.54
7:M:88:LEU:HA	7:M:117:GLY:HA2	1.89	0.54
7:M:191:TYR:HE1	7:M:269:LEU:CB	2.18	0.54
7:M:214:PRO:CG	7:M:231:ALA:HB2	2.13	0.54
7:M:5:PHE:HB3	7:M:286:VAL:HB	1.90	0.54
7:M:166:ALA:HB1	7:M:170:LYS:HB3	1.89	0.54
1:A:557:GLU:C	1:A:559:PHE:N	2.66	0.54
7:M:12:VAL:O	7:M:15:ARG:N	2.38	0.54
7:M:166:ALA:O	7:M:170:LYS:CA	2.56	0.54
7:M:33:PHE:CE2	7:M:308:TYR:HE1	2.17	0.54
7:M:242:ASP:OD1	7:M:254:GLY:CA	2.56	0.54
1:A:404:GLY:O	1:A:430:LEU:CB	2.56	0.54
1:C:259:GLY:CA	2:E:296:GLU:C	2.60	0.54
1:C:296:VAL:HA	1:C:333:ALA:HB1	1.90	0.54
3:G:136:ALA:O	3:G:140:VAL:CB	2.55	0.54
6:J:42:LEU:O	6:J:42:LEU:HD23	2.07	0.54
1:B:296:VAL:HA	1:B:333:ALA:HB1	1.90	0.54
3:G:205:GLU:CB	3:G:205:GLU:N	2.67	0.54
7:M:95:ASN:ND2	7:M:114:LEU:CD2	2.71	0.54
7:M:152:ARG:HB3	7:M:156:ARG:NH1	2.23	0.54
7:M:166:ALA:HB1	7:M:170:LYS:HB2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:170:LYS:O	7:M:174:GLU:N	2.30	0.54
1:C:557:GLU:C	1:C:559:PHE:N	2.66	0.53
7:M:16:ARG:CZ	7:M:19:LEU:HD11	2.38	0.53
7:M:152:ARG:CZ	7:M:156:ARG:HH12	2.21	0.53
7:M:175:ASP:O	7:M:179:ALA:CB	2.56	0.53
1:B:225:ALA:O	1:B:406:PHE:HA	2.08	0.53
1:B:557:GLU:C	1:B:559:PHE:N	2.66	0.53
5:K:119:LEU:HD12	5:K:120:PRO:HD3	1.90	0.53
7:M:138:GLN:HG2	7:M:152:ARG:NH1	2.23	0.53
7:M:177:ALA:HB1	7:M:196:VAL:HG21	1.88	0.53
7:M:312:PRO:CB	7:M:315:GLN:HB2	2.37	0.53
1:A:25:TYR:CB	2:D:65:GLY:CA	2.84	0.53
3:G:49:ALA:O	3:G:52:ALA:CB	2.53	0.53
1:C:11:GLY:HA2	2:E:49:GLU:HA	1.89	0.53
1:C:225:ALA:O	1:C:406:PHE:HA	2.07	0.53
6:J:108:ALA:O	6:J:112:LEU:HD23	2.07	0.53
7:M:224:PHE:CZ	7:M:248:PRO:CD	2.91	0.53
2:D:153:PHE:CB	2:D:338:GLN:HA	2.39	0.53
7:M:242:ASP:OD1	7:M:254:GLY:HA2	2.09	0.53
7:M:170:LYS:HG2	7:M:174:GLU:OE2	1.90	0.53
1:B:227:PRO:HA	1:B:384:VAL:CB	2.39	0.53
1:C:224:ALA:CA	1:C:405:ALA:HB3	2.37	0.53
1:B:224:ALA:CA	1:B:405:ALA:HB3	2.37	0.53
2:F:153:PHE:CB	2:F:338:GLN:HA	2.39	0.53
3:G:138:ILE:O	3:G:139:ARG:O	2.27	0.53
3:G:141:ALA:CA	3:G:145:THR:H	2.22	0.53
7:M:29:LEU:HD13	7:M:313:ARG:CD	2.39	0.53
2:E:153:PHE:CB	2:E:338:GLN:HA	2.39	0.53
3:G:43:VAL:O	3:G:44:ARG:C	2.51	0.52
5:K:65:LYS:HG3	6:L:42:LEU:HD11	1.91	0.52
7:M:88:LEU:C	7:M:118:THR:HG23	2.31	0.52
7:M:152:ARG:HB3	7:M:156:ARG:CZ	2.40	0.52
7:M:226:ASP:CG	7:M:229:ARG:CB	2.78	0.52
7:M:229:ARG:O	7:M:240:VAL:HG21	2.09	0.52
1:A:352:PRO:CB	2:D:272:ALA:HB3	2.39	0.52
3:G:138:ILE:C	3:G:139:ARG:O	2.45	0.52
3:G:145:THR:O	3:G:149:LYS:CB	2.57	0.52
3:G:167:VAL:C	3:G:169:ILE:H	2.18	0.52
7:M:107:ARG:NH1	7:M:111:GLU:OE1	2.40	0.52
7:M:263:ARG:HG3	7:M:321:VAL:C	2.33	0.52
3:G:42:LEU:O	3:G:45:GLU:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:198:LYS:O	3:G:199:GLY:C	2.52	0.52
5:I:119:LEU:HD12	5:I:120:PRO:HD3	1.90	0.52
7:M:37:LEU:HD23	7:M:49:LEU:HD21	1.90	0.52
1:A:227:PRO:HA	1:A:384:VAL:CB	2.39	0.52
1:A:259:GLY:O	2:F:298:ALA:N	2.42	0.52
1:A:346:ALA:HB2	2:D:272:ALA:CB	2.40	0.52
1:B:429:SER:C	1:B:431:PHE:H	2.17	0.52
2:D:359:SER:CA	2:D:362:MET:H	2.22	0.52
6:J:100:TRP:N	6:J:101:PRO:HD2	2.24	0.52
2:F:62:GLU:HA	2:F:227:PRO:CB	2.39	0.52
7:M:73:PRO:CG	7:M:88:LEU:HD11	2.36	0.52
7:M:226:ASP:OD1	7:M:229:ARG:CG	2.57	0.52
1:B:24:MET:CB	2:E:66:LEU:C	2.83	0.52
5:I:80:GLU:OE1	6:J:57:LEU:HD11	2.10	0.52
1:A:263:THR:O	2:F:124:ARG:HA	2.10	0.52
5:K:80:GLU:OE1	6:L:57:LEU:HD11	2.10	0.52
6:L:100:TRP:N	6:L:101:PRO:HD2	2.25	0.52
7:M:88:LEU:CD2	7:M:117:GLY:HA2	2.39	0.52
1:C:227:PRO:HA	1:C:384:VAL:CB	2.40	0.52
3:G:166:GLN:O	3:G:169:ILE:CB	2.58	0.52
4:H:62:LEU:O	4:H:63:MET:CB	2.46	0.52
5:I:65:LYS:HG3	6:J:42:LEU:HD11	1.91	0.52
7:M:76:VAL:CG2	7:M:81:ARG:HA	2.38	0.52
7:M:123:VAL:HG12	7:M:139:VAL:HG12	1.74	0.52
7:M:138:GLN:CG	7:M:152:ARG:NH1	2.72	0.52
7:M:166:ALA:O	7:M:170:LYS:CB	2.58	0.52
1:C:11:GLY:CA	2:E:50:VAL:H	2.14	0.52
5:I:28:GLU:O	5:I:32:GLN:HG3	2.10	0.51
7:M:69:VAL:HA	7:M:72:LEU:CG	2.40	0.51
1:A:52:TYR:O	1:A:53:GLU:CB	2.58	0.51
1:C:69:LEU:CA	1:C:72:ALA:HB2	2.40	0.51
2:E:150:LEU:C	2:E:335:GLY:O	2.53	0.51
7:M:61:VAL:HG21	7:M:301:ARG:HD2	1.92	0.51
2:D:150:LEU:C	2:D:335:GLY:O	2.52	0.51
5:I:114:VAL:HG11	6:J:87:VAL:HG11	1.93	0.51
1:A:296:VAL:HA	1:A:333:ALA:HB1	1.91	0.51
2:F:150:LEU:C	2:F:335:GLY:O	2.53	0.51
3:G:7:THR:O	3:G:9:MET:N	2.42	0.51
7:M:259:LYS:HZ3	7:M:318:GLU:HG2	1.72	0.51
1:A:24:MET:C	2:D:66:LEU:N	2.32	0.51
7:M:33:PHE:CG	7:M:308:TYR:CG	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:312:PRO:HG2	7:M:315:GLN:CB	2.41	0.51
2:D:134:GLY:C	2:D:430:ARG:O	2.54	0.51
2:E:359:SER:CB	2:E:362:MET:CB	2.88	0.51
3:G:171:GLY:O	3:G:174:ALA:HB3	2.11	0.51
7:M:103:LYS:HD3	7:M:128:TYR:CZ	2.45	0.51
1:B:52:TYR:O	1:B:53:GLU:CB	2.58	0.51
3:G:173:ARG:O	3:G:177:ARG:CB	2.58	0.51
5:K:114:VAL:HG11	6:L:87:VAL:HG11	1.92	0.51
5:K:28:GLU:O	5:K:32:GLN:HG3	2.10	0.51
6:L:116:PRO:HG2	6:L:163:VAL:HG21	1.93	0.51
7:M:8:LEU:O	7:M:12:VAL:HG23	2.10	0.51
7:M:93:LEU:CD1	7:M:168:LEU:CD2	2.88	0.51
1:A:224:ALA:CA	1:A:405:ALA:HB3	2.37	0.51
5:I:65:LYS:CG	6:J:42:LEU:HD11	2.41	0.51
1:C:52:TYR:O	1:C:53:GLU:CB	2.58	0.50
2:E:25:LYS:CB	6:J:161:THR:HG23	1.19	0.50
6:L:98:PRO:C	6:L:100:TRP:H	2.20	0.50
6:L:12:VAL:O	6:L:14:ALA:N	2.44	0.50
1:A:24:MET:CB	2:D:66:LEU:HA	2.29	0.50
2:D:130:PHE:CB	2:D:370:LYS:O	2.60	0.50
3:G:148:LYS:O	3:G:152:GLU:CA	2.59	0.50
6:J:12:VAL:O	6:J:14:ALA:N	2.44	0.50
5:K:65:LYS:CG	6:L:42:LEU:HD11	2.41	0.50
7:M:69:VAL:HA	7:M:72:LEU:HG	1.92	0.50
1:B:70:PRO:O	1:B:71:LEU:C	2.55	0.50
2:D:149:LYS:O	2:D:333:THR:CB	2.60	0.50
1:B:73:VAL:O	1:B:186:THR:HA	2.12	0.50
7:M:204:ALA:CB	7:M:234:MET:CE	2.90	0.50
1:A:418:HIS:HA	1:A:496:GLN:CB	2.42	0.50
2:F:149:LYS:O	2:F:333:THR:CB	2.59	0.50
6:J:159:GLY:O	6:J:161:THR:N	2.45	0.50
7:M:9:ASN:HD22	7:M:285:LEU:CG	2.24	0.50
7:M:257:ASP:OD2	7:M:260:ALA:CB	2.59	0.50
3:G:183:LEU:O	3:G:186:ARG:CB	2.59	0.50
6:J:4:LEU:O	6:J:5:GLU:HB3	2.12	0.50
1:A:11:GLY:C	2:F:50:VAL:O	2.54	0.50
7:M:3:ASP:OD1	7:M:79:GLU:C	2.44	0.50
7:M:197:ASP:OD1	7:M:222:GLY:HA3	2.12	0.49
7:M:263:ARG:NH2	7:M:318:GLU:CG	2.74	0.49
1:A:73:VAL:O	1:A:186:THR:HA	2.12	0.49
1:B:9:ILE:HA	2:D:50:VAL:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:116:PRO:HG2	6:J:163:VAL:HG21	1.93	0.49
7:M:89:LEU:CA	7:M:118:THR:HG23	2.42	0.49
7:M:224:PHE:CE1	7:M:247:THR:HB	2.46	0.49
3:G:146:ARG:O	3:G:149:LYS:N	2.45	0.49
7:M:220:LYS:HD3	7:M:227:ARG:CZ	2.34	0.49
1:A:217:PRO:C	1:A:431:PHE:CB	2.84	0.49
2:D:150:LEU:CB	2:D:335:GLY:O	2.60	0.49
6:L:4:LEU:O	6:L:5:GLU:HB3	2.12	0.49
6:L:159:GLY:O	6:L:161:THR:N	2.44	0.49
7:M:79:GLU:OE2	7:M:185:GLN:CG	2.60	0.49
6:J:99:GLU:O	6:J:103:VAL:HG23	2.13	0.49
1:C:73:VAL:O	1:C:186:THR:HA	2.12	0.49
6:J:98:PRO:C	6:J:100:TRP:H	2.20	0.49
5:K:91:ARG:HD3	6:L:68:VAL:HG21	1.95	0.49
7:M:5:PHE:CB	7:M:286:VAL:HB	2.43	0.49
7:M:29:LEU:HD23	7:M:306:ARG:HE	1.77	0.49
7:M:85:ARG:HH22	7:M:145:HIS:CD2	2.28	0.49
7:M:120:ARG:O	7:M:123:VAL:N	2.42	0.49
7:M:141:ALA:C	7:M:143:PRO:HD2	2.38	0.49
7:M:10:ALA:HB2	7:M:13:ARG:HH12	1.78	0.49
1:B:471:VAL:CB	4:H:98:ILE:O	2.61	0.49
1:C:216:PHE:HA	1:C:429:SER:CB	2.43	0.49
2:E:149:LYS:O	2:E:333:THR:CB	2.60	0.49
5:I:45:GLU:HA	5:I:48:VAL:HG12	1.95	0.49
6:L:12:VAL:HG23	6:L:13:GLU:N	2.27	0.49
7:M:204:ALA:O	7:M:234:MET:HG3	2.13	0.49
7:M:205:PHE:CE2	7:M:258:LEU:HB2	2.47	0.49
7:M:214:PRO:CD	7:M:231:ALA:HB1	2.42	0.49
6:L:99:GLU:O	6:L:103:VAL:HG23	2.13	0.49
7:M:45:TYR:CE1	7:M:64:THR:CG2	2.88	0.49
7:M:54:LEU:CD1	7:M:301:ARG:HH21	2.23	0.49
7:M:79:GLU:CD	7:M:185:GLN:HE21	2.21	0.49
7:M:223:ARG:NE	7:M:224:PHE:CZ	2.78	0.49
1:C:11:GLY:HA3	2:E:49:GLU:HA	1.94	0.48
3:G:7:THR:O	3:G:8:ARG:O	2.30	0.48
7:M:8:LEU:O	7:M:12:VAL:N	2.45	0.48
7:M:25:PHE:HD1	7:M:303:LEU:CD1	2.26	0.48
7:M:125:ARG:O	7:M:129:GLU:HG3	2.13	0.48
7:M:286:VAL:O	7:M:287:LEU:C	2.54	0.48
1:B:224:ALA:HB2	1:B:405:ALA:CB	2.31	0.48
3:G:142:ASN:CB	3:G:142:ASN:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:12:VAL:HG23	6:J:13:GLU:N	2.27	0.48
6:L:125:PRO:HD3	6:L:145:GLU:HB3	1.95	0.48
7:M:103:LYS:NZ	7:M:128:TYR:O	2.27	0.48
3:G:198:LYS:O	3:G:199:GLY:O	2.31	0.48
7:M:12:VAL:C	7:M:14:VAL:N	2.72	0.48
7:M:92:ASP:CB	7:M:124:TRP:CH2	2.96	0.48
7:M:141:ALA:O	7:M:142:VAL:C	2.55	0.48
7:M:232:ARG:NH1	7:M:243:GLU:CD	2.46	0.48
7:M:252:LEU:O	7:M:253:SER:C	2.55	0.48
3:G:134:ALA:O	3:G:137:LEU:CB	2.61	0.48
3:G:138:ILE:O	3:G:142:ASN:CB	2.62	0.48
3:G:179:ILE:O	3:G:180:GLN:C	2.55	0.48
3:G:200:LYS:HA	3:G:203:ALA:HB3	1.96	0.48
4:H:77:LEU:O	4:H:78:LYS:C	2.37	0.48
7:M:88:LEU:HB3	7:M:117:GLY:HA2	1.80	0.48
1:A:475:ALA:HB1	2:D:398:ILE:O	2.13	0.48
3:G:134:ALA:O	4:H:16:ALA:HB2	2.13	0.48
6:L:95:PRO:HA	6:L:100:TRP:CG	2.49	0.48
7:M:167:LEU:CA	7:M:171:ARG:HB3	2.42	0.48
2:F:150:LEU:CB	2:F:335:GLY:O	2.61	0.48
3:G:153:GLU:O	3:G:154:ILE:O	2.32	0.48
6:J:95:PRO:HA	6:J:100:TRP:CG	2.49	0.48
7:M:224:PHE:HD2	7:M:249:PHE:HE2	1.61	0.48
7:M:317:GLU:HA	7:M:320:VAL:HG22	1.96	0.48
1:C:231:GLY:CA	8:C:600:ADP:H5'1	2.37	0.48
3:G:3:GLN:O	3:G:6:PRO:N	2.46	0.48
5:I:91:ARG:HD3	6:J:68:VAL:HG21	1.95	0.48
7:M:119:LEU:HB3	7:M:123:VAL:CB	2.43	0.48
1:A:24:MET:CB	2:D:66:LEU:CB	2.92	0.48
1:B:440:ARG:HA	1:B:444:ALA:O	2.14	0.48
2:E:349:TYR:HA	2:E:350:PRO:C	2.39	0.48
7:M:9:ASN:HD22	7:M:285:LEU:HD23	1.79	0.48
7:M:93:LEU:HD13	7:M:168:LEU:CD2	2.42	0.48
7:M:103:LYS:CD	7:M:128:TYR:CZ	2.97	0.48
7:M:266:ARG:HD2	7:M:295:TRP:HZ2	1.62	0.48
1:A:404:GLY:O	1:A:430:LEU:N	2.47	0.47
6:J:125:PRO:HD3	6:J:145:GLU:HB3	1.95	0.47
1:A:419:PHE:H	1:A:496:GLN:CA	2.27	0.47
2:D:349:TYR:HA	2:D:350:PRO:C	2.38	0.47
3:G:4:VAL:C	3:G:6:PRO:N	2.71	0.47
6:J:107:LEU:HD23	6:J:165:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:HA	1:A:444:ALA:O	2.14	0.47
5:I:37:LEU:HD23	6:J:16:ILE:CG2	2.44	0.47
7:M:8:LEU:CD1	7:M:12:VAL:CG2	2.92	0.47
7:M:16:ARG:NH2	7:M:19:LEU:HD11	2.29	0.47
7:M:119:LEU:HD22	7:M:123:VAL:HG11	1.96	0.47
7:M:266:ARG:NH2	7:M:295:TRP:CH2	2.74	0.47
2:E:61:GLU:HA	2:E:229:ILE:CB	2.44	0.47
2:E:150:LEU:CB	2:E:335:GLY:O	2.61	0.47
3:G:48:GLU:CB	3:G:51:LYS:CB	2.92	0.47
5:K:37:LEU:HD23	6:L:16:ILE:CG2	2.44	0.47
5:K:45:GLU:HA	5:K:48:VAL:HG12	1.95	0.47
7:M:163:ARG:CB	7:M:167:LEU:HD12	2.33	0.47
7:M:154:VAL:CG1	7:M:167:LEU:HD13	2.44	0.47
2:F:349:TYR:HA	2:F:350:PRO:C	2.38	0.47
7:M:8:LEU:CG	7:M:12:VAL:CG2	2.93	0.47
7:M:25:PHE:CE1	7:M:300:LEU:CD2	2.98	0.47
7:M:312:PRO:HG2	7:M:315:GLN:HB3	1.95	0.47
1:A:24:MET:HA	2:D:66:LEU:HA	0.56	0.47
1:B:71:LEU:O	1:B:188:PRO:HA	2.15	0.47
1:C:233:GLY:CA	8:C:600:ADP:C8	2.97	0.47
6:L:107:LEU:HD23	6:L:165:ASN:OD1	2.15	0.47
7:M:193:ALA:HB1	7:M:222:GLY:O	2.14	0.47
1:C:440:ARG:HA	1:C:444:ALA:O	2.14	0.47
7:M:152:ARG:NH2	7:M:156:ARG:NH1	2.63	0.47
5:K:119:LEU:N	5:K:120:PRO:CD	2.78	0.47
7:M:96:LEU:HD23	7:M:168:LEU:HD21	1.95	0.47
7:M:152:ARG:CZ	7:M:156:ARG:NH1	2.77	0.47
3:G:189:GLU:CB	3:G:189:GLU:N	2.69	0.47
7:M:88:LEU:HD13	7:M:117:GLY:C	2.39	0.47
7:M:257:ASP:OD2	7:M:260:ALA:HB2	2.14	0.47
1:A:11:GLY:N	2:F:50:VAL:O	2.47	0.46
7:M:191:TYR:CE1	7:M:269:LEU:CB	2.94	0.46
1:A:25:TYR:N	2:D:65:GLY:CA	2.77	0.46
7:M:238:TYR:HB2	7:M:256:ARG:NE	2.29	0.46
1:A:71:LEU:CB	1:A:188:PRO:CB	2.87	0.46
7:M:8:LEU:CG	7:M:12:VAL:HG23	2.45	0.46
1:C:208:GLY:C	1:C:507:CYS:O	2.57	0.46
3:G:200:LYS:CA	3:G:203:ALA:HB3	2.45	0.46
7:M:194:LEU:HD21	7:M:249:PHE:HZ	1.81	0.46
7:M:89:LEU:H	7:M:118:THR:CG2	2.25	0.46
3:G:135:GLU:HA	3:G:138:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:283:VAL:O	7:M:284:GLY:C	2.59	0.46
1:C:419:PHE:N	1:C:496:GLN:HA	2.31	0.46
7:M:238:TYR:CB	7:M:256:ARG:CD	2.93	0.46
7:M:256:ARG:O	7:M:257:ASP:OD1	2.34	0.46
1:A:132:GLY:HA3	1:A:371:LEU:O	2.16	0.46
7:M:172:PHE:O	7:M:176:VAL:CB	2.64	0.46
3:G:21:ALA:HB3	3:G:22:GLN:H	1.47	0.46
5:I:119:LEU:N	5:I:120:PRO:CD	2.78	0.46
6:J:91:LEU:HD13	6:J:167:LEU:HB2	1.98	0.46
7:M:12:VAL:O	7:M:14:VAL:N	2.48	0.46
7:M:137:ALA:CB	7:M:152:ARG:HG2	2.33	0.46
7:M:266:ARG:NH2	7:M:295:TRP:HZ3	2.06	0.46
6:L:124:ASN:OD1	6:L:148:LEU:N	2.49	0.45
7:M:5:PHE:CZ	7:M:286:VAL:HG11	2.49	0.45
1:A:346:ALA:HB2	2:D:272:ALA:HB2	1.98	0.45
6:J:124:ASN:OD1	6:J:148:LEU:N	2.49	0.45
7:M:23:SER:HA	7:M:26:GLN:HG2	1.98	0.45
7:M:210:SER:OG	7:M:212:LEU:HG	2.16	0.45
7:M:241:LEU:O	7:M:253:SER:HA	2.17	0.45
2:D:334:GLU:C	2:D:361:LEU:CB	2.88	0.45
5:K:96:ALA:O	5:K:99:VAL:HG22	2.17	0.45
6:L:91:LEU:HD13	6:L:167:LEU:HB2	1.98	0.45
6:L:94:LEU:HD22	6:L:100:TRP:CE3	2.52	0.45
7:M:170:LYS:O	7:M:174:GLU:CB	2.64	0.45
1:B:25:TYR:O	2:E:65:GLY:HA2	2.17	0.45
2:F:360:ARG:C	2:F:362:MET:N	2.38	0.45
3:G:141:ALA:HB1	3:G:145:THR:CB	2.47	0.45
6:J:94:LEU:HD22	6:J:100:TRP:CE3	2.52	0.45
7:M:10:ALA:CA	7:M:13:ARG:NH1	2.78	0.45
7:M:52:GLN:H	7:M:56:ASP:CB	2.30	0.45
7:M:167:LEU:HD23	7:M:171:ARG:HB2	1.99	0.45
7:M:204:ALA:CB	7:M:234:MET:HE3	2.47	0.45
7:M:218:PHE:CE1	7:M:226:ASP:O	2.69	0.45
1:C:26:ASP:O	1:C:71:LEU:N	2.50	0.45
6:L:128:LEU:HD21	6:L:142:LEU:O	2.17	0.45
7:M:25:PHE:HE1	7:M:300:LEU:CD2	2.29	0.45
3:G:35:LEU:O	3:G:38:GLU:CB	2.65	0.45
7:M:72:LEU:N	7:M:73:PRO:CD	2.80	0.45
7:M:99:LEU:O	7:M:103:LYS:N	2.40	0.45
7:M:120:ARG:NH1	7:M:122:GLU:HG3	2.31	0.45
1:A:224:ALA:HB2	1:A:405:ALA:CB	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:O	1:A:495:LEU:O	2.34	0.45
7:M:188:LEU:HD11	7:M:192:LEU:HD11	1.99	0.45
7:M:204:ALA:CA	7:M:234:MET:CE	2.69	0.45
1:A:56:SER:CB	2:F:30:GLY:CA	2.95	0.45
2:E:8:TYR:O	6:J:162:GLN:HG3	2.17	0.45
2:E:25:LYS:CA	6:J:161:THR:CB	2.70	0.45
5:I:96:ALA:O	5:I:99:VAL:HG22	2.17	0.45
7:M:170:LYS:CE	7:M:174:GLU:OE2	2.64	0.45
7:M:185:GLN:HE22	7:M:282:GLY:HA2	1.80	0.45
1:C:296:VAL:CA	1:C:333:ALA:HB1	2.47	0.45
7:M:45:TYR:HE1	7:M:64:THR:CG2	2.10	0.45
7:M:175:ASP:O	7:M:179:ALA:HB3	2.17	0.45
1:B:208:GLY:O	1:B:507:CYS:CB	2.65	0.45
7:M:3:ASP:C	7:M:3:ASP:OD2	2.60	0.45
7:M:74:ARG:O	7:M:74:ARG:HG3	2.17	0.45
7:M:134:ALA:HA	7:M:152:ARG:NE	2.32	0.45
7:M:321:VAL:HG12	7:M:322:CYS:N	2.32	0.45
1:B:296:VAL:CA	1:B:333:ALA:HB1	2.47	0.44
3:G:52:ALA:O	3:G:55:GLN:O	2.34	0.44
7:M:130:ALA:CB	7:M:135:GLY:HA3	2.41	0.44
1:C:44:GLY:N	2:F:69:ALA:HB2	2.32	0.44
7:M:229:ARG:HH22	7:M:243:GLU:CB	2.08	0.44
1:A:314:ARG:HA	1:A:318:PHE:O	2.18	0.44
1:C:314:ARG:HA	1:C:318:PHE:O	2.18	0.44
3:G:45:GLU:O	3:G:47:MET:N	2.50	0.44
7:M:20:LEU:HB3	7:M:24:PHE:HB3	2.00	0.44
7:M:90:ARG:O	7:M:93:LEU:HB3	2.17	0.44
7:M:246:GLY:C	7:M:247:THR:CG2	2.91	0.44
1:B:314:ARG:HA	1:B:318:PHE:O	2.18	0.44
7:M:170:LYS:O	7:M:174:GLU:HG3	2.16	0.44
7:M:252:LEU:HD22	7:M:255:VAL:HG21	1.99	0.44
2:D:153:PHE:O	2:D:338:GLN:HA	2.18	0.44
4:H:94:VAL:O	4:H:95:ARG:C	2.58	0.44
7:M:5:PHE:CD1	7:M:286:VAL:CG2	2.95	0.44
7:M:202:ARG:O	7:M:206:LYS:HG3	2.18	0.44
1:B:388:GLY:C	1:B:390:ASP:H	2.26	0.44
1:C:233:GLY:HA2	8:C:600:ADP:C8	2.52	0.44
2:E:24:ALA:CB	6:J:160:LYS:N	2.79	0.44
6:J:128:LEU:HD21	6:J:142:LEU:O	2.17	0.44
7:M:36:PHE:CZ	7:M:304:ALA:HB2	2.51	0.44
7:M:147:LEU:HD13	7:M:172:PHE:HD1	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:VAL:CA	1:A:333:ALA:HB1	2.47	0.44
5:I:66:ALA:HB1	6:J:45:ARG:CZ	2.48	0.44
1:A:86:GLY:O	1:A:305:VAL:CB	2.66	0.44
1:C:388:GLY:C	1:C:390:ASP:H	2.25	0.44
2:E:153:PHE:O	2:E:338:GLN:HA	2.18	0.44
3:G:4:VAL:CA	3:G:5:SER:N	2.68	0.44
6:J:171:MET:O	6:J:174:ALA:HB3	2.17	0.44
7:M:3:ASP:CG	7:M:79:GLU:HG2	2.40	0.44
1:A:56:SER:CB	2:F:30:GLY:H	2.29	0.43
2:F:153:PHE:O	2:F:338:GLN:HA	2.18	0.43
3:G:151:GLY:O	3:G:152:GLU:O	2.35	0.43
6:L:171:MET:O	6:L:174:ALA:HB3	2.18	0.43
1:B:80:LEU:C	1:B:82:GLY:H	2.26	0.43
7:M:3:ASP:CG	7:M:79:GLU:HB3	2.42	0.43
7:M:283:VAL:HG22	7:M:286:VAL:CG1	2.46	0.43
2:D:359:SER:C	2:D:362:MET:H	2.26	0.43
7:M:138:GLN:O	7:M:142:VAL:HG13	2.19	0.43
1:A:75:LEU:O	1:A:184:TYR:HA	2.19	0.43
1:A:80:LEU:C	1:A:82:GLY:H	2.27	0.43
1:C:259:GLY:HA2	2:E:296:GLU:C	2.22	0.43
5:K:66:ALA:HB1	6:L:45:ARG:CZ	2.48	0.43
7:M:5:PHE:CE2	7:M:286:VAL:CG1	2.89	0.43
7:M:9:ASN:ND2	7:M:285:LEU:CB	2.80	0.43
7:M:95:ASN:CG	7:M:114:LEU:HD23	2.44	0.43
7:M:154:VAL:O	7:M:158:THR:N	2.49	0.43
7:M:173:PHE:HA	7:M:176:VAL:HB	2.00	0.43
1:A:388:GLY:C	1:A:390:ASP:H	2.25	0.43
4:H:59:VAL:O	4:H:60:GLU:C	2.61	0.43
7:M:127:ALA:HB2	7:M:139:VAL:CG1	2.37	0.43
2:E:334:GLU:O	2:E:360:ARG:N	2.49	0.43
3:G:159:ARG:C	3:G:161:VAL:N	2.77	0.43
6:J:116:PRO:CG	6:J:163:VAL:HG21	2.48	0.43
7:M:266:ARG:CA	7:M:322:CYS:SG	3.06	0.43
5:I:85:LEU:O	5:I:88:TYR:N	2.52	0.43
6:L:111:ALA:HB1	6:L:154:ALA:CB	2.49	0.43
6:L:116:PRO:CG	6:L:163:VAL:HG21	2.48	0.43
7:M:9:ASN:HD22	7:M:285:LEU:HB3	1.83	0.43
7:M:214:PRO:O	7:M:216:ALA:N	2.51	0.43
1:C:189:VAL:CB	1:C:304:TYR:CB	2.97	0.43
3:G:27:LEU:CB	3:G:27:LEU:C	2.80	0.43
3:G:175:GLN:O	3:G:177:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:92:ASP:CA	7:M:124:TRP:HZ2	2.21	0.43
3:G:135:GLU:O	3:G:139:ARG:CB	2.67	0.43
3:G:148:LYS:C	3:G:149:LYS:O	2.59	0.43
4:H:75:ALA:C	4:H:75:ALA:HB1	2.42	0.43
7:M:69:VAL:CA	7:M:72:LEU:HG	2.49	0.43
7:M:79:GLU:OE2	7:M:185:GLN:HG2	2.19	0.43
7:M:229:ARG:HH11	7:M:229:ARG:CG	2.26	0.43
1:A:241:LEU:O	1:A:245:SER:CB	2.67	0.43
1:C:75:LEU:O	1:C:184:TYR:HA	2.19	0.43
7:M:25:PHE:HE1	7:M:300:LEU:HD23	1.84	0.43
6:J:111:ALA:HB1	6:J:154:ALA:HB2	2.01	0.42
6:J:111:ALA:HB1	6:J:154:ALA:CB	2.49	0.42
7:M:140:LEU:CB	7:M:148:ALA:HB1	2.49	0.42
7:M:188:LEU:HG	7:M:192:LEU:HD13	2.00	0.42
1:C:224:ALA:HB2	1:C:405:ALA:CB	2.32	0.42
6:J:66:LEU:HD12	6:J:70:THR:HG23	2.01	0.42
1:A:255:CYS:HA	1:A:290:ASN:CB	2.49	0.42
1:B:241:LEU:O	1:B:245:SER:CB	2.67	0.42
1:B:255:CYS:HA	1:B:290:ASN:CB	2.49	0.42
1:C:241:LEU:O	1:C:245:SER:CB	2.67	0.42
6:J:101:PRO:HA	6:J:104:VAL:HG22	2.01	0.42
7:M:16:ARG:C	7:M:18:THR:N	2.77	0.42
7:M:85:ARG:NH2	7:M:145:HIS:HA	2.34	0.42
1:B:75:LEU:O	1:B:184:TYR:HA	2.19	0.42
2:D:258:THR:HA	2:D:259:ASP:HA	1.85	0.42
6:J:100:TRP:O	6:J:104:VAL:HG13	2.19	0.42
6:J:149:ARG:C	6:J:150:LEU:HD13	2.44	0.42
6:L:100:TRP:CH2	6:L:104:VAL:HG12	2.54	0.42
7:M:3:ASP:CA	7:M:80:ALA:CB	2.97	0.42
7:M:5:PHE:CE2	7:M:80:ALA:HB1	2.54	0.42
1:A:25:TYR:CB	2:D:64:THR:C	2.90	0.42
1:C:12:PRO:N	2:E:49:GLU:CB	2.83	0.42
1:C:80:LEU:C	1:C:82:GLY:H	2.27	0.42
5:K:85:LEU:O	5:K:88:TYR:N	2.52	0.42
7:M:142:VAL:HG23	7:M:143:PRO:HD3	2.01	0.42
7:M:223:ARG:CD	7:M:224:PHE:HE2	2.30	0.42
7:M:266:ARG:HD3	7:M:295:TRP:CZ3	2.53	0.42
6:J:119:LYS:HB2	6:J:155:VAL:O	2.20	0.42
6:L:100:TRP:O	6:L:104:VAL:HG13	2.19	0.42
2:D:189:VAL:O	2:D:217:SER:HA	2.20	0.42
2:F:189:VAL:O	2:F:217:SER:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:88:LEU:HD22	7:M:117:GLY:N	2.34	0.42
7:M:92:ASP:CB	7:M:124:TRP:HH2	2.32	0.42
7:M:292:GLU:O	7:M:296:GLU:HB2	2.20	0.42
1:C:255:CYS:HA	1:C:290:ASN:CB	2.49	0.42
3:G:48:GLU:O	3:G:51:LYS:CA	2.67	0.42
6:J:95:PRO:HG3	6:J:150:LEU:HD12	2.02	0.42
7:M:16:ARG:NE	7:M:19:LEU:HD11	2.34	0.42
7:M:38:ARG:O	7:M:39:LEU:C	2.63	0.42
7:M:170:LYS:O	7:M:174:GLU:CG	2.68	0.42
1:B:221:GLY:O	1:B:366:GLY:HA2	2.20	0.42
2:F:149:LYS:C	2:F:334:GLU:H	2.14	0.42
7:M:166:ALA:C	7:M:170:LYS:CB	2.91	0.42
3:G:17:GLN:O	3:G:18:LEU:C	2.63	0.42
6:L:111:ALA:HB1	6:L:154:ALA:HB2	2.01	0.42
7:M:145:HIS:HD1	7:M:148:ALA:H	1.68	0.42
7:M:229:ARG:NH1	7:M:229:ARG:HG2	2.33	0.42
3:G:175:GLN:O	3:G:178:PHE:N	2.51	0.41
6:L:101:PRO:HA	6:L:104:VAL:HG22	2.00	0.41
6:L:119:LYS:HB2	6:L:155:VAL:O	2.19	0.41
7:M:3:ASP:CG	7:M:79:GLU:CB	2.93	0.41
7:M:5:PHE:CD2	7:M:286:VAL:HG12	2.45	0.41
7:M:73:PRO:CG	7:M:84:VAL:HG12	2.47	0.41
2:D:359:SER:O	2:D:360:ARG:C	2.60	0.41
6:J:100:TRP:CH2	6:J:104:VAL:HG12	2.54	0.41
6:L:95:PRO:HG3	6:L:150:LEU:HD12	2.02	0.41
7:M:72:LEU:C	7:M:84:VAL:HG11	2.44	0.41
7:M:119:LEU:CD1	7:M:140:LEU:CD2	2.82	0.41
7:M:211:GLY:HA2	7:M:235:GLU:OE1	2.20	0.41
1:B:10:ALA:O	2:D:50:VAL:N	2.47	0.41
2:E:189:VAL:O	2:E:217:SER:HA	2.20	0.41
3:G:11:LEU:O	3:G:12:LEU:C	2.64	0.41
7:M:92:ASP:CG	7:M:124:TRP:CZ2	2.97	0.41
7:M:133:PRO:HB3	7:M:155:LEU:HB3	2.01	0.41
7:M:93:LEU:HD12	7:M:168:LEU:HD23	1.95	0.41
7:M:166:ALA:CB	7:M:170:LYS:CB	2.94	0.41
7:M:205:PHE:CZ	7:M:258:LEU:HB2	2.55	0.41
3:G:149:LYS:O	3:G:150:ILE:C	2.64	0.41
5:K:107:LEU:HD23	5:K:107:LEU:C	2.46	0.41
6:L:66:LEU:HD12	6:L:70:THR:HG23	2.02	0.41
7:M:88:LEU:HB2	7:M:118:THR:HG22	2.01	0.41
3:G:146:ARG:O	3:G:149:LYS:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:104:MET:HA	5:I:107:LEU:HD12	2.03	0.41
7:M:25:PHE:HD1	7:M:303:LEU:HD12	1.86	0.41
1:B:10:ALA:O	2:D:49:GLU:CA	2.65	0.41
1:C:11:GLY:CA	2:E:49:GLU:CA	2.95	0.41
1:C:133:MET:O	1:C:148:LEU:HA	2.21	0.41
2:D:149:LYS:CB	2:D:333:THR:HA	2.51	0.41
3:G:3:GLN:O	3:G:4:VAL:C	2.63	0.41
7:M:141:ALA:O	7:M:144:GLY:N	2.54	0.41
5:I:107:LEU:HD21	6:J:83:VAL:HG22	2.02	0.41
7:M:5:PHE:CE1	7:M:286:VAL:HG11	2.54	0.41
7:M:31:LEU:HB3	7:M:35:ASP:HB3	2.00	0.41
7:M:188:LEU:CD1	7:M:192:LEU:HD11	2.51	0.41
1:A:227:PRO:CB	1:A:384:VAL:CB	2.99	0.41
1:A:346:ALA:HB2	2:D:272:ALA:HB1	2.03	0.41
1:C:141:PHE:O	1:C:143:PHE:O	2.39	0.41
1:C:227:PRO:CB	1:C:384:VAL:CB	2.99	0.41
3:G:43:VAL:O	3:G:45:GLU:N	2.54	0.41
3:G:163:ALA:C	3:G:163:ALA:CB	2.79	0.41
5:I:36:ARG:NH1	6:J:16:ILE:HD11	2.36	0.41
5:I:41:LYS:O	5:I:44:ALA:HB3	2.21	0.41
5:I:107:LEU:C	5:I:107:LEU:HD23	2.46	0.41
7:M:52:GLN:N	7:M:56:ASP:CG	2.79	0.41
7:M:57:VAL:HG11	7:M:301:ARG:HG2	2.03	0.41
7:M:175:ASP:O	7:M:176:VAL:C	2.63	0.41
1:A:141:PHE:O	1:A:143:PHE:O	2.39	0.41
1:B:133:MET:O	1:B:148:LEU:HA	2.20	0.41
3:G:20:LEU:O	3:G:21:ALA:C	2.64	0.41
7:M:170:LYS:O	7:M:174:GLU:HB2	2.21	0.41
1:B:227:PRO:CB	1:B:384:VAL:CB	2.99	0.40
1:C:226:ILE:O	1:C:384:VAL:N	2.54	0.40
3:G:174:ALA:O	3:G:175:GLN:O	2.37	0.40
7:M:25:PHE:CE1	7:M:300:LEU:HD23	2.56	0.40
7:M:286:VAL:O	7:M:289:TYR:N	2.53	0.40
2:F:149:LYS:CB	2:F:333:THR:HA	2.51	0.40
7:M:3:ASP:OD2	7:M:4:ASP:HA	2.21	0.40
7:M:33:PHE:HD1	7:M:308:TYR:N	2.19	0.40
1:A:133:MET:O	1:A:148:LEU:HA	2.21	0.40
2:E:149:LYS:CB	2:E:333:THR:HA	2.51	0.40
4:H:25:SER:O	4:H:26:ALA:C	2.65	0.40
5:I:95:GLU:HA	5:I:98:ALA:HB3	2.04	0.40
5:K:36:ARG:NH1	6:L:16:ILE:HD11	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:107:LEU:HD21	6:L:83:VAL:HG22	2.02	0.40
7:M:96:LEU:HD23	7:M:168:LEU:CD2	2.51	0.40
7:M:246:GLY:C	7:M:247:THR:HG23	2.47	0.40
7:M:312:PRO:CG	7:M:315:GLN:CB	2.99	0.40
1:A:221:GLY:O	1:A:366:GLY:HA2	2.21	0.40
1:C:221:GLY:O	1:C:366:GLY:HA2	2.21	0.40
2:F:258:THR:HA	2:F:259:ASP:HA	1.85	0.40
3:G:40:PHE:O	3:G:43:VAL:CB	2.69	0.40
3:G:189:GLU:O	3:G:190:ASP:C	2.62	0.40
6:L:149:ARG:C	6:L:150:LEU:HD13	2.44	0.40
7:M:16:ARG:HH11	7:M:16:ARG:HD3	1.63	0.40
1:B:226:ILE:O	1:B:384:VAL:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	3	23
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	3	21
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	3	22
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	6	31
2	E	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	6	31
2	F	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	5	29
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	6	31
5	I	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	6	31
5	K	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	J	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	1	14
6	L	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	1	14
7	M	318/323 (98%)	281 (88%)	32 (10%)	5 (2%)	7	38
All	All	4110/4402 (93%)	3678 (90%)	293 (7%)	139 (3%)	4	21

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO
1	A	256	GLY
1	A	260	ASN
1	A	325	ASP
1	A	394	PRO
1	A	395	VAL
1	A	558	GLU
1	B	12	PRO
1	B	19	MET
1	B	53	GLU
1	B	143	PHE
1	B	227	PRO
1	B	256	GLY
1	B	260	ASN
1	B	325	ASP
1	B	394	PRO
1	B	395	VAL
1	B	558	GLU
1	C	12	PRO
1	C	19	MET
1	C	53	GLU
1	C	71	LEU
1	C	143	PHE
1	C	227	PRO
1	C	256	GLY
1	C	260	ASN
1	C	325	ASP
1	C	394	PRO
1	C	395	VAL

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Mol	Chain	Res	Type
1	C	558	GLU
2	D	52	GLU
2	D	79	VAL
2	D	316	MET
2	D	356	PRO
2	D	427	GLN
2	E	52	GLU
2	E	316	MET
2	E	356	PRO
2	E	427	GLN
2	F	52	GLU
2	F	316	MET
2	F	356	PRO
2	F	361	LEU
2	F	427	GLN
3	G	3	GLN
3	G	4	VAL
3	G	43	VAL
3	G	47	MET
3	G	48	GLU
3	G	140	VAL
3	G	149	LYS
3	G	152	GLU
3	G	161	VAL
3	G	172	ILE
3	G	174	ALA
3	G	200	LYS
4	H	85	ASP
4	H	100	PHE
5	I	22	LEU
6	J	160	LYS
5	K	22	LEU
6	L	160	LYS
7	M	257	ASP
1	A	88	GLN
1	A	255	CYS
1	B	71	LEU
1	B	88	GLN
1	B	255	CYS
1	B	430	LEU
1	C	88	GLN
1	C	255	CYS

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Mol	Chain	Res	Type
2	D	26	ASP
2	D	428	GLN
2	E	26	ASP
2	E	79	VAL
2	E	428	GLN
2	F	26	ASP
2	F	428	GLN
3	G	2	SER
3	G	6	PRO
3	G	13	GLN
3	G	150	ILE
3	G	151	GLY
3	G	185	GLN
6	J	5	GLU
6	J	14	ALA
6	J	140	VAL
6	J	174	ALA
6	L	5	GLU
6	L	14	ALA
6	L	140	VAL
6	L	174	ALA
7	M	50	ALA
1	A	109	HIS
1	B	109	HIS
1	C	109	HIS
2	F	79	VAL
3	G	139	ARG
3	G	155	LYS
3	G	162	ASN
3	G	165	GLU
6	J	99	GLU
6	J	139	GLY
6	J	149	ARG
6	L	99	GLU
6	L	139	GLY
6	L	149	ARG
7	M	104	ALA
7	M	215	ASP
3	G	45	GLU
3	G	137	LEU
3	G	186	ARG
6	J	13	GLU

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Mol	Chain	Res	Type
6	J	119	LYS
6	L	13	GLU
6	L	119	LYS
7	M	110	GLU
1	A	374	GLU
1	B	374	GLU
1	C	374	GLU
2	D	317	PRO
2	E	317	PRO
2	F	317	PRO
3	G	53	LEU
3	G	197	ILE
2	D	355	LEU
2	E	355	LEU
2	F	355	LEU
1	A	388	GLY
1	B	388	GLY
1	C	388	GLY
3	G	179	ILE
5	I	119	LEU
5	K	119	LEU
3	G	168	VAL

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	
5	I	62/76 (82%)	57 (92%)	5 (8%)	11	31
5	K	62/76 (82%)	57 (92%)	5 (8%)	11	31
6	J	108/141 (77%)	92 (85%)	16 (15%)	3	13
6	L	108/141 (77%)	92 (85%)	16 (15%)	3	13
7	M	254/256 (99%)	247 (97%)	7 (3%)	38	60
All	All	594/690 (86%)	545 (92%)	49 (8%)	13	31

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	54	GLU
5	I	69	LEU
5	I	82	GLU
5	I	118	VAL
5	I	119	LEU
6	J	16	ILE
6	J	28	GLU
6	J	33	GLU
6	J	36	GLU
6	J	66	LEU
6	J	79	VAL
6	J	88	ARG
6	J	99	GLU
6	J	132	GLU
6	J	140	VAL
6	J	142	LEU
6	J	149	ARG
6	J	150	LEU
6	J	165	ASN
6	J	168	LEU
6	J	184	GLN
5	K	54	GLU
5	K	69	LEU
5	K	82	GLU
5	K	118	VAL
5	K	119	LEU
6	L	16	ILE
6	L	28	GLU
6	L	33	GLU
6	L	36	GLU
6	L	66	LEU
6	L	79	VAL
6	L	88	ARG
6	L	99	GLU
6	L	132	GLU
6	L	140	VAL
6	L	142	LEU
6	L	149	ARG
6	L	150	LEU
6	L	165	ASN
6	L	168	LEU
6	L	184	GLN
7	M	3	ASP

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Mol	Chain	Res	Type
7	M	4	ASP
7	M	26	GLN
7	M	62	LEU
7	M	65	GLN
7	M	74	ARG
7	M	76	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	M	9	ASN
7	M	52	GLN
7	M	65	GLN
7	M	94	HIS
7	M	185	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
8	ADP	C	600	-	28,29,29	1.03	2 (7%)	43,45,45	0.80	3 (6%)
8	ADP	A	600	-	28,29,29	1.22	3 (10%)	43,45,45	0.69	1 (2%)

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
8	ADP	C	600	-	-	0/16/32/32	0/3/3/3
8	ADP	A	600	-	-	2/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ADP	PA-O3A	4.05	1.63	1.59
8	C	600	ADP	PB-O2B	-2.52	1.45	1.54
8	A	600	ADP	PB-O2B	-2.42	1.45	1.54
8	C	600	ADP	PA-O1A	-2.35	1.42	1.50
8	A	600	ADP	PB-O3B	-2.01	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	600	ADP	O3B-PB-O2B	2.38	116.74	107.80
8	A	600	ADP	O3A-PA-O1A	2.09	116.99	110.70
8	C	600	ADP	O4'-C4'-C3'	-2.06	101.06	105.15
8	C	600	ADP	O5'-PA-O1A	2.06	117.09	108.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

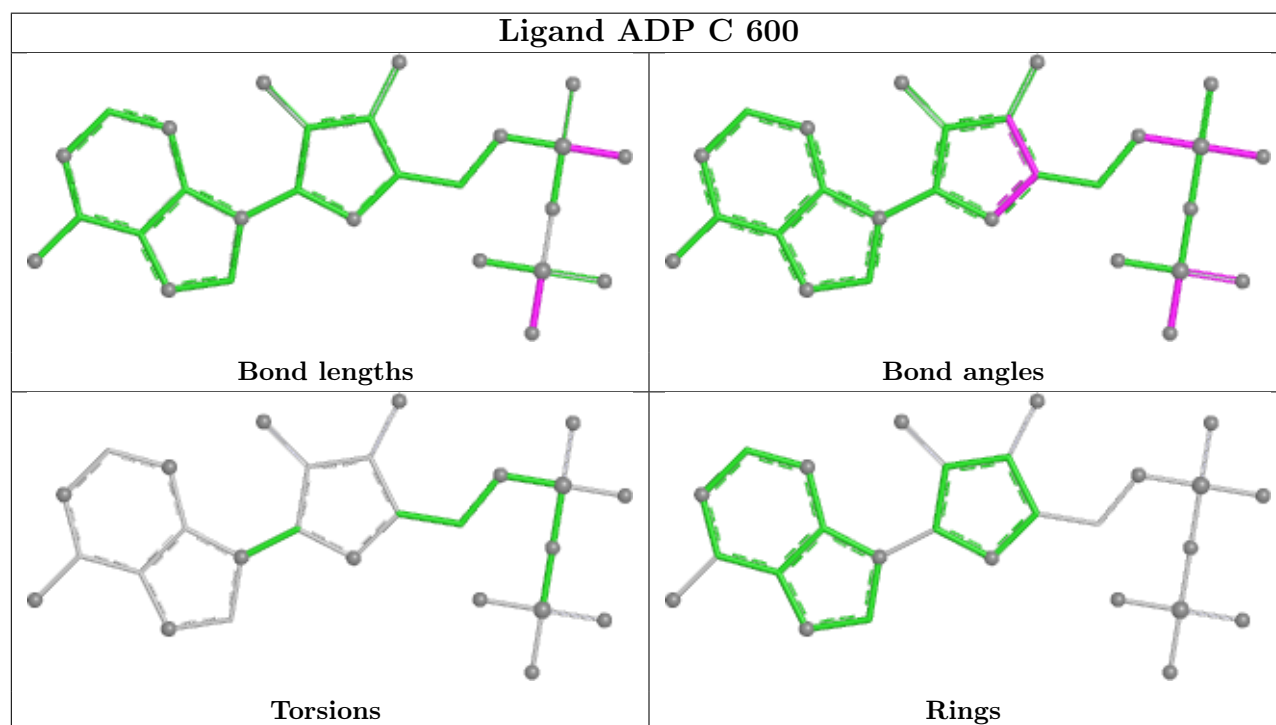
Mol	Chain	Res	Type	Atoms
8	A	600	ADP	PA-O3A-PB-O2B
8	A	600	ADP	PA-O3A-PB-O3B

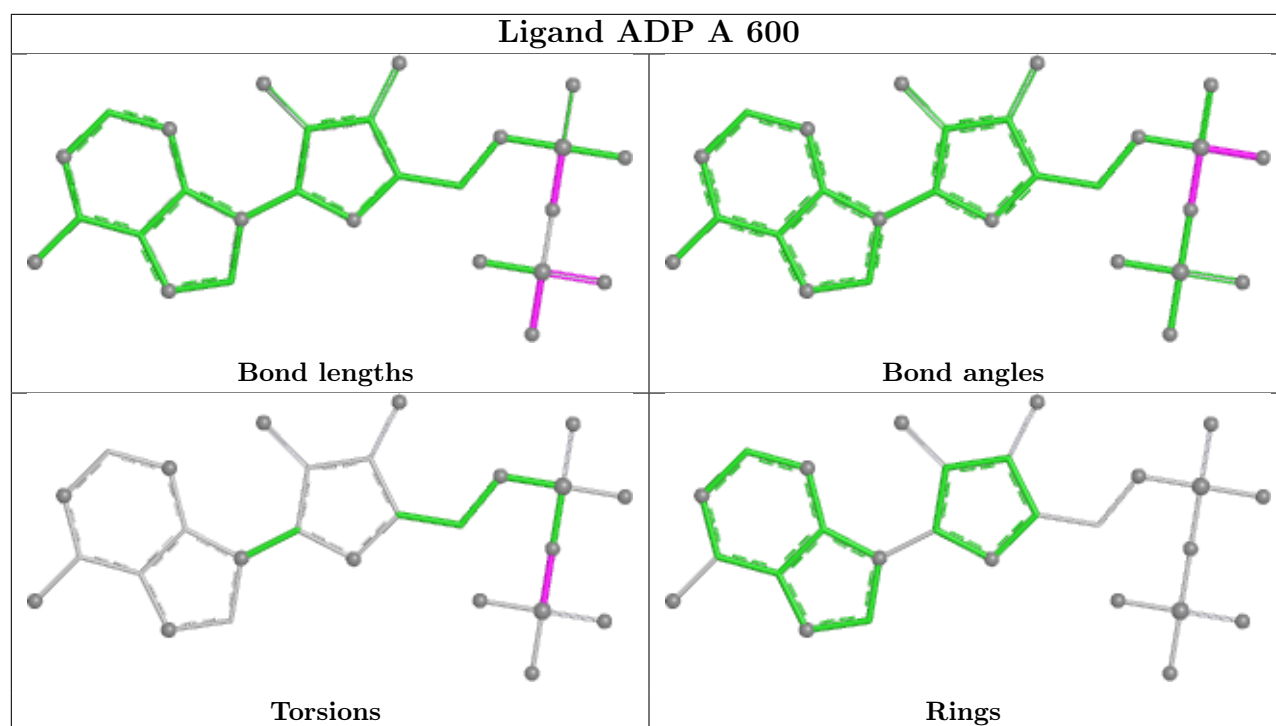
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	600	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

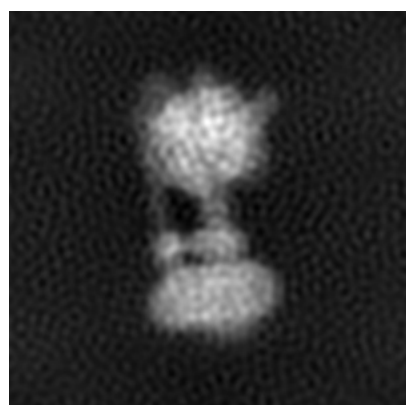
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5335. These allow visual inspection of the internal detail of the map and identification of artifacts.

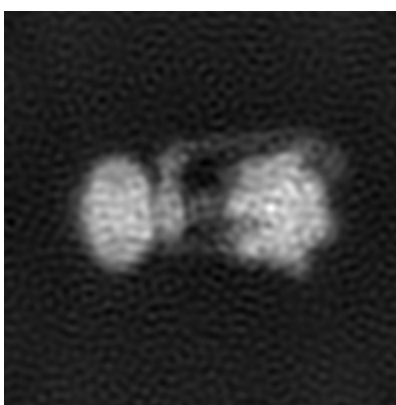
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

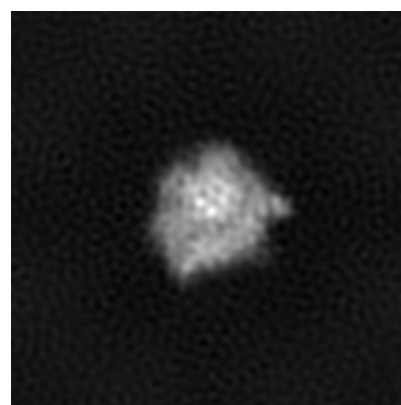
6.1.1 Primary map



X



Y

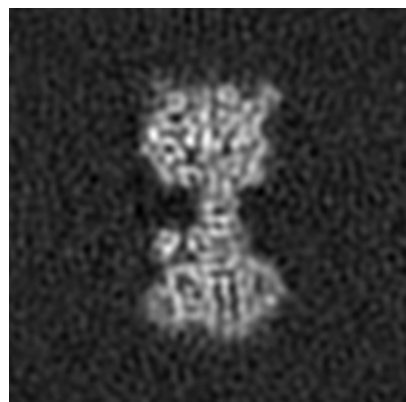


Z

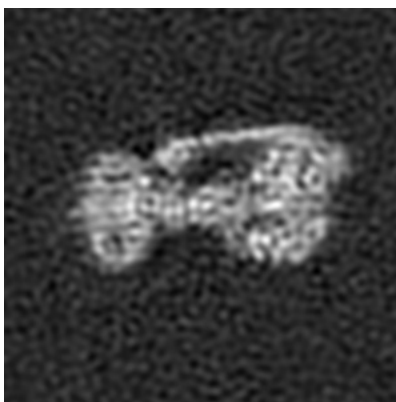
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

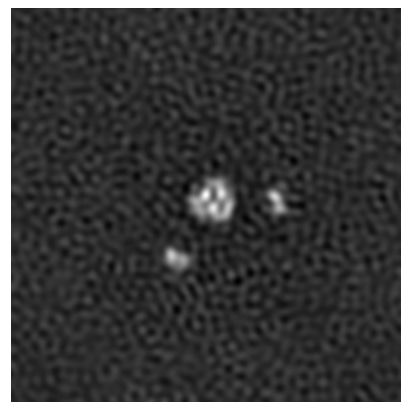
6.2.1 Primary map



X Index: 128



Y Index: 128

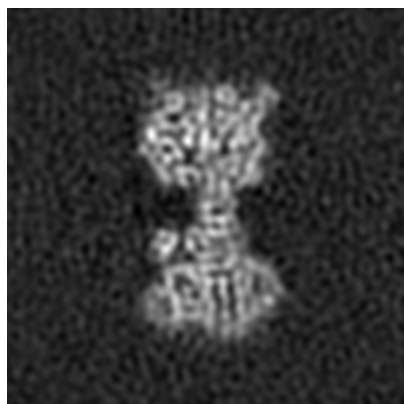


Z Index: 128

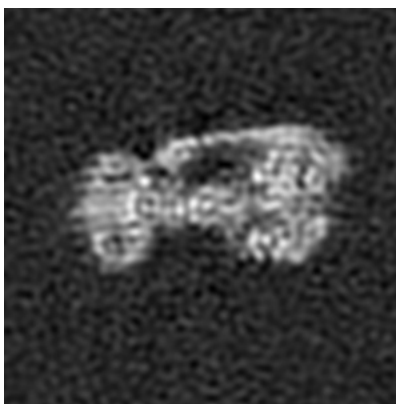
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

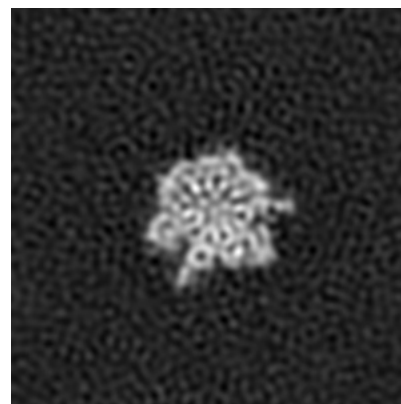
6.3.1 Primary map



X Index: 128



Y Index: 129

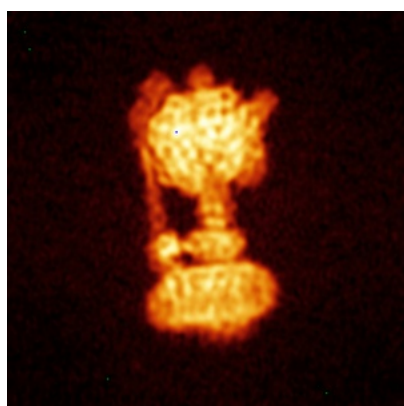


Z Index: 181

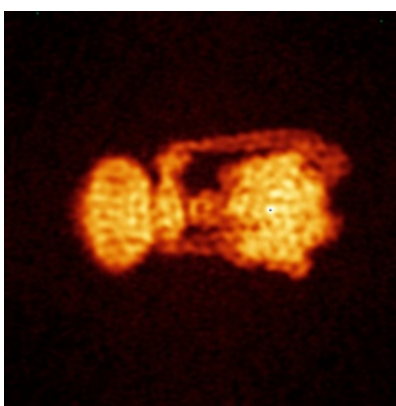
The images above show the largest variance slices of the map in three orthogonal directions.

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

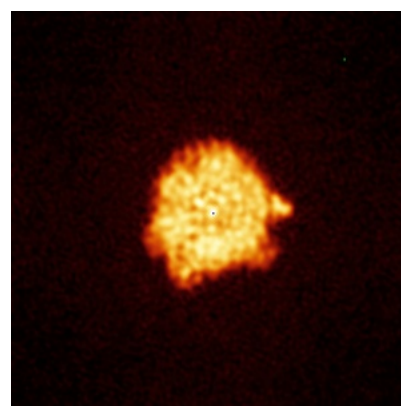
6.4.1 Primary map



X



Y



Z

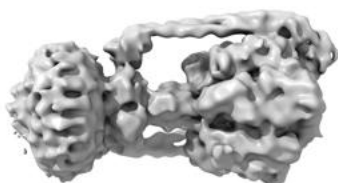
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

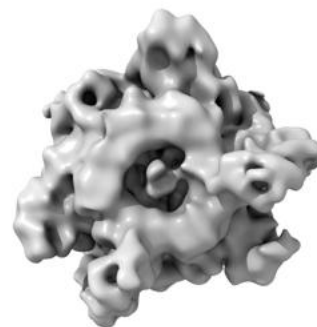
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.548. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

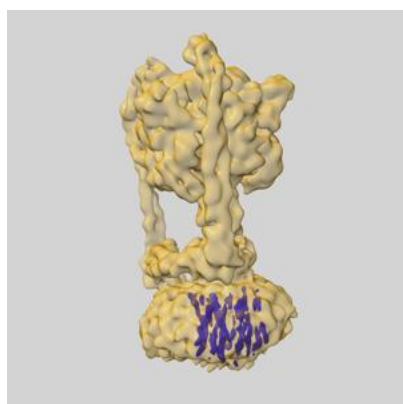
6.6 Mask visualisation [i](#)

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

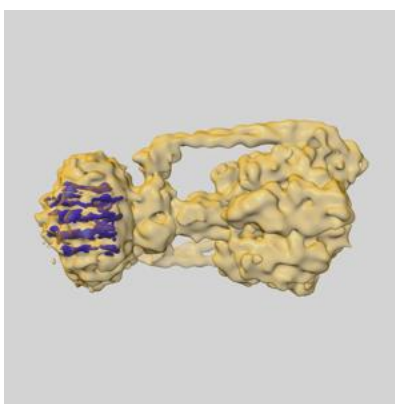
A mask typically either:

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

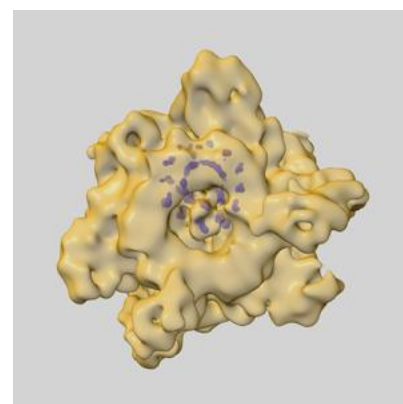
6.6.1 emd_5335_msk_2.map [i](#)



X

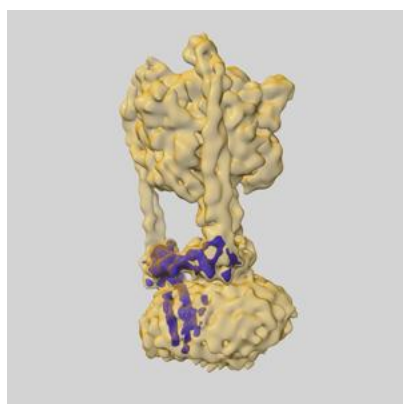


Y

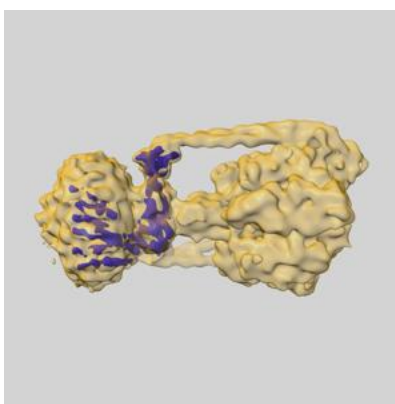


Z

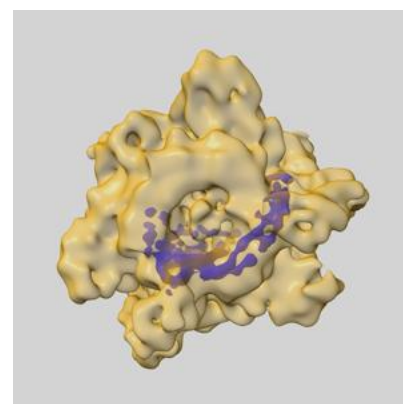
6.6.2 emd_5335_msk_1.map [i](#)



X

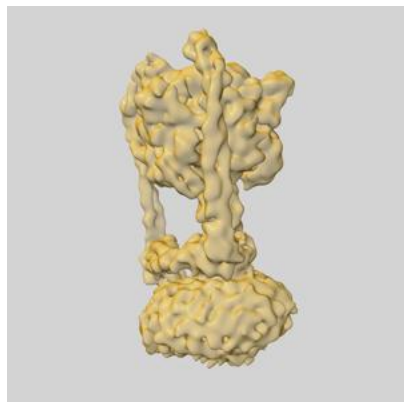


Y

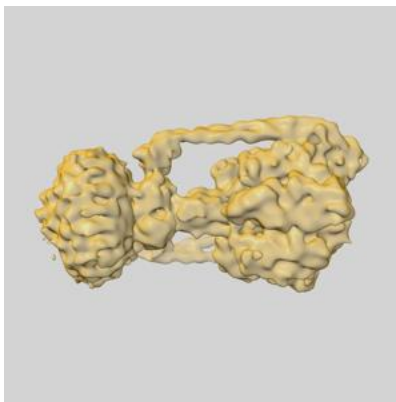


Z

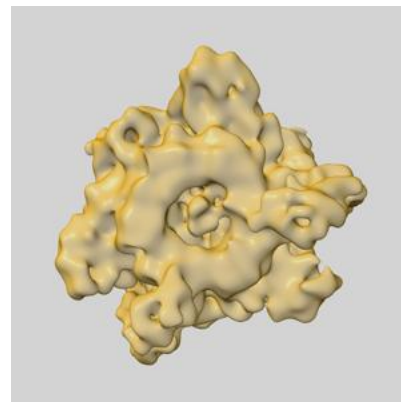
6.6.3 emd_5335_msk_3.map ⓘ



X



Y

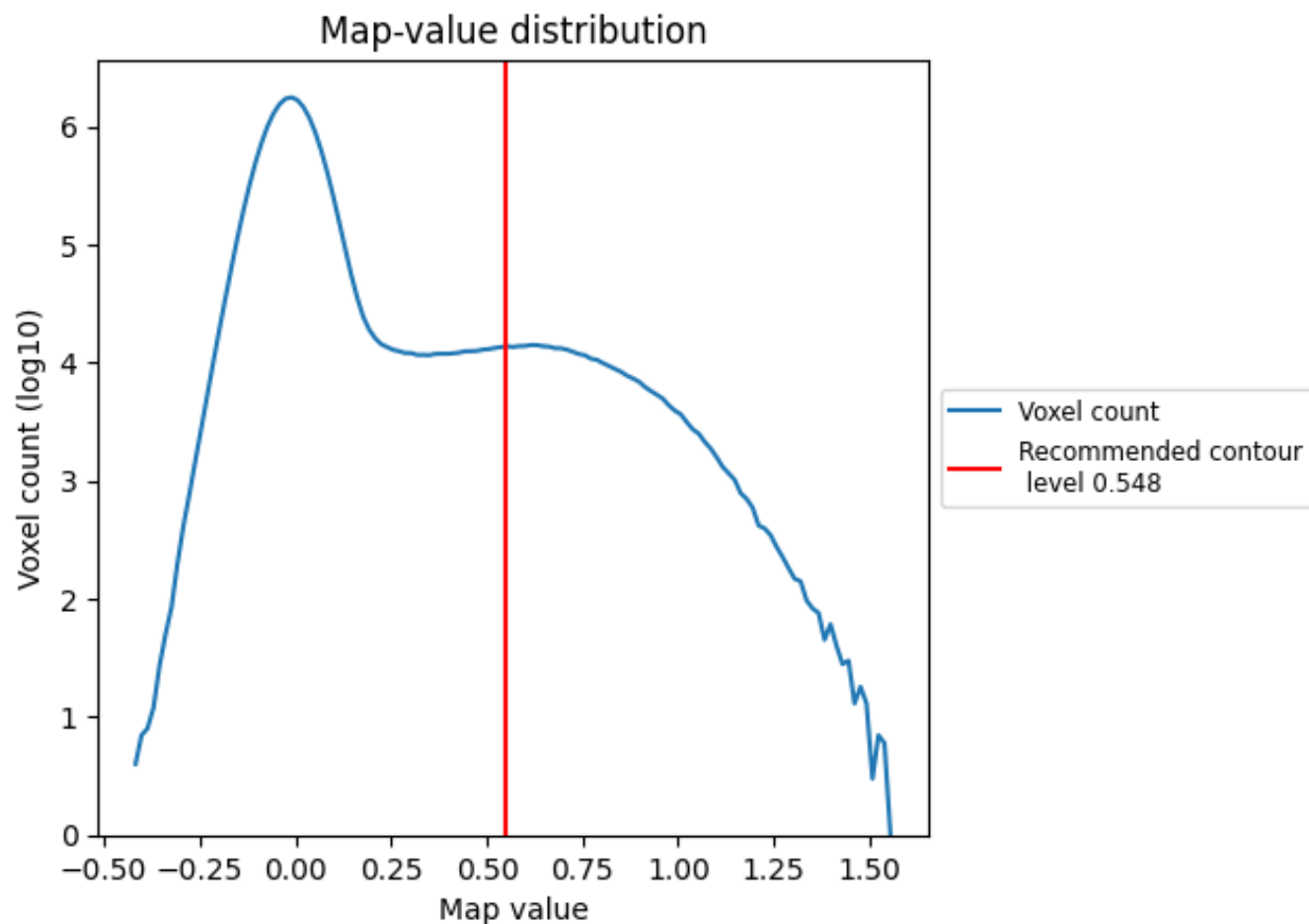


Z

7 Map analysis [i](#)

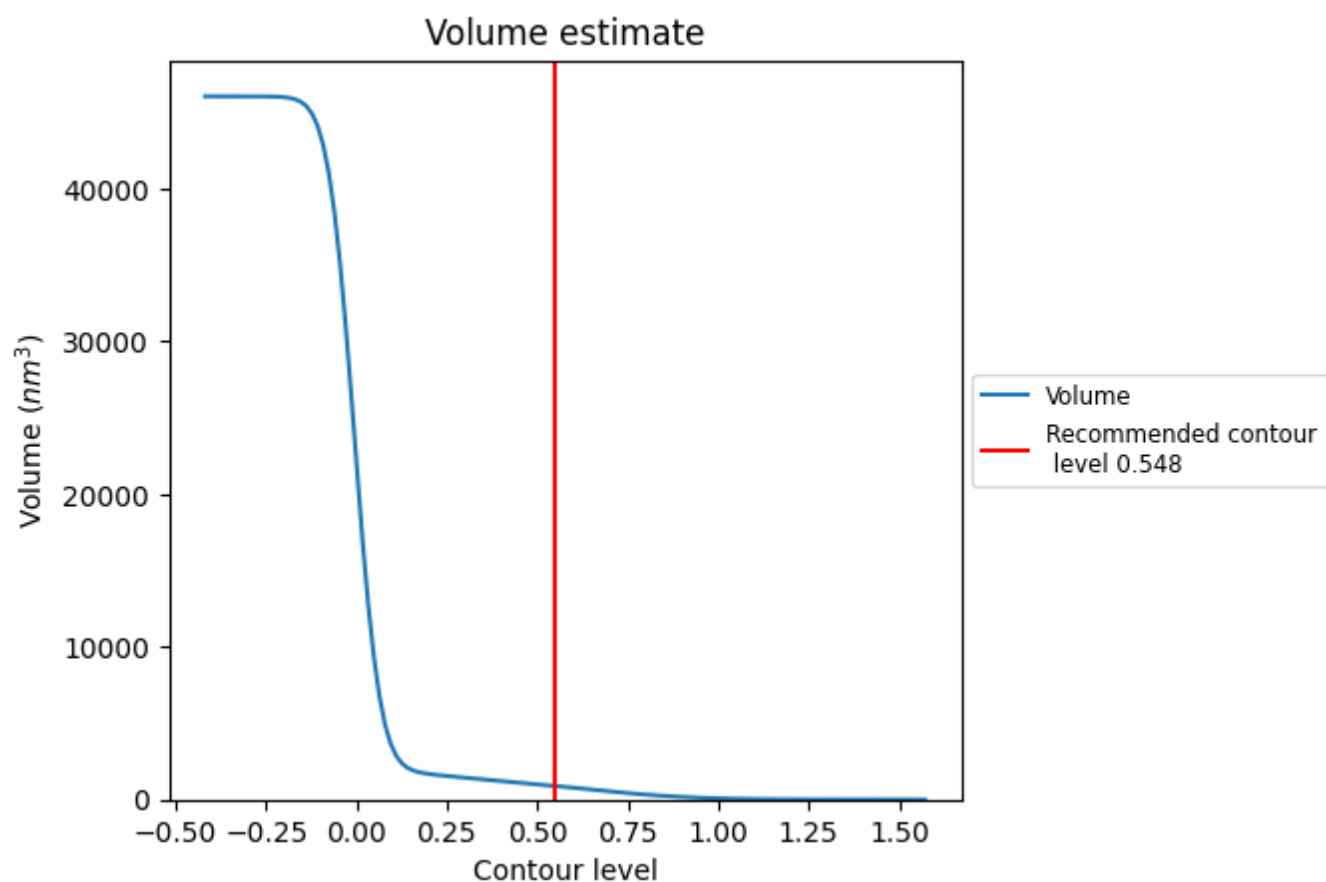
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

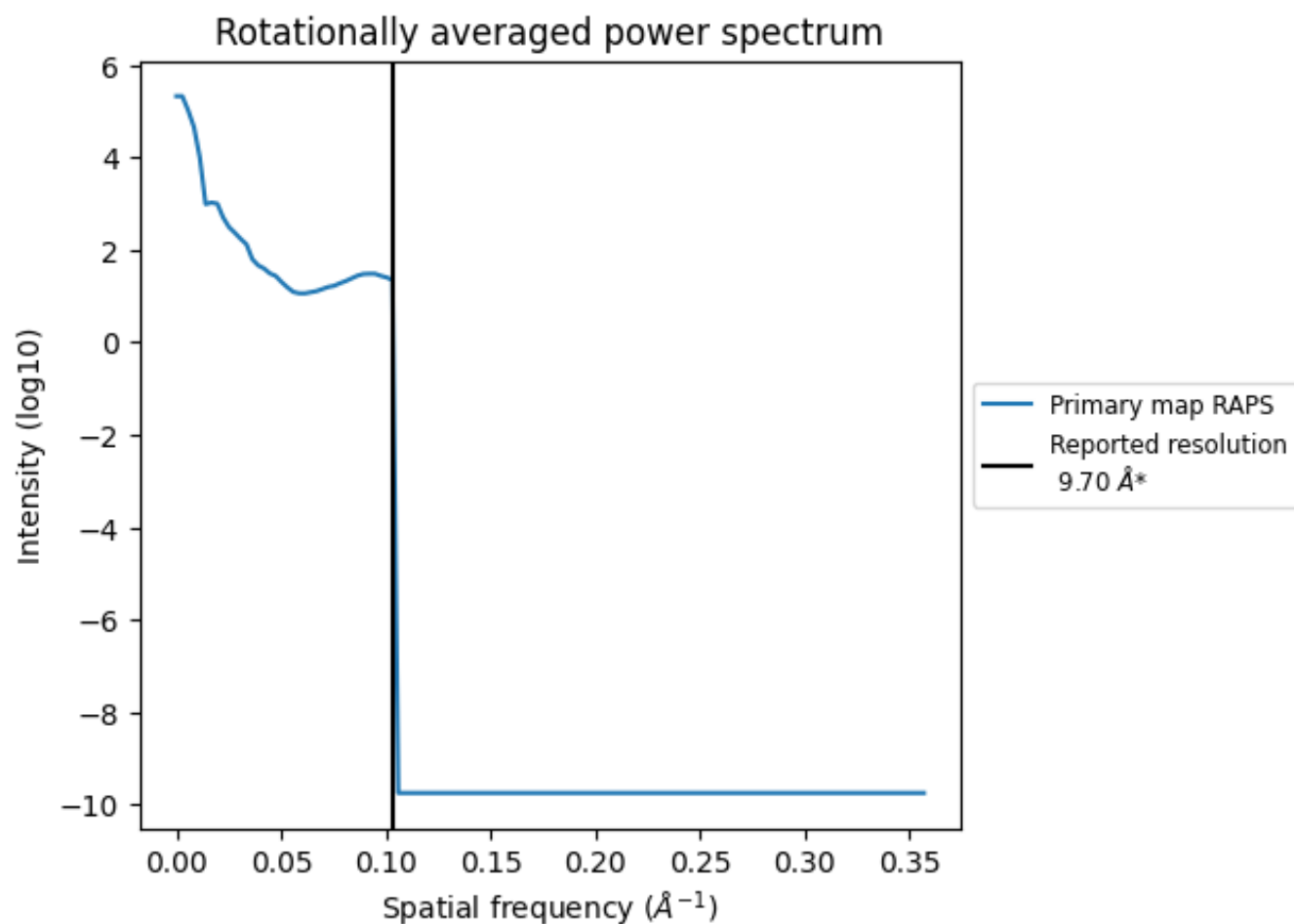
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 897 nm³; this corresponds to an approximate mass of 810 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 0.103 $\text{\AA}^{-1}$

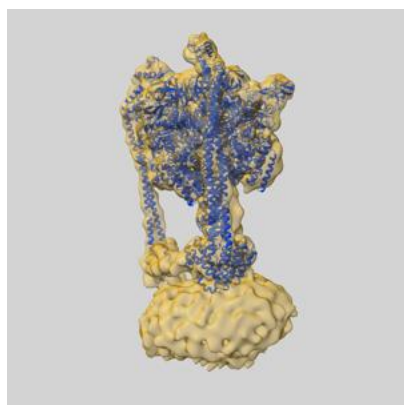
8 Fourier-Shell correlation

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

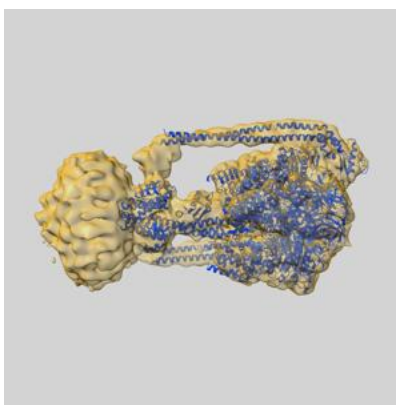
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5335 and PDB model 3J0J. Per-residue inclusion information can be found in section [3](#) on page [7](#).

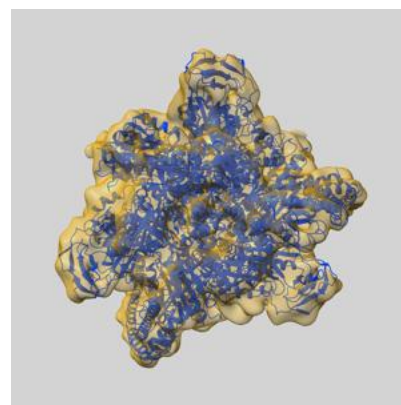
9.1 Map-model overlay [i](#)



X



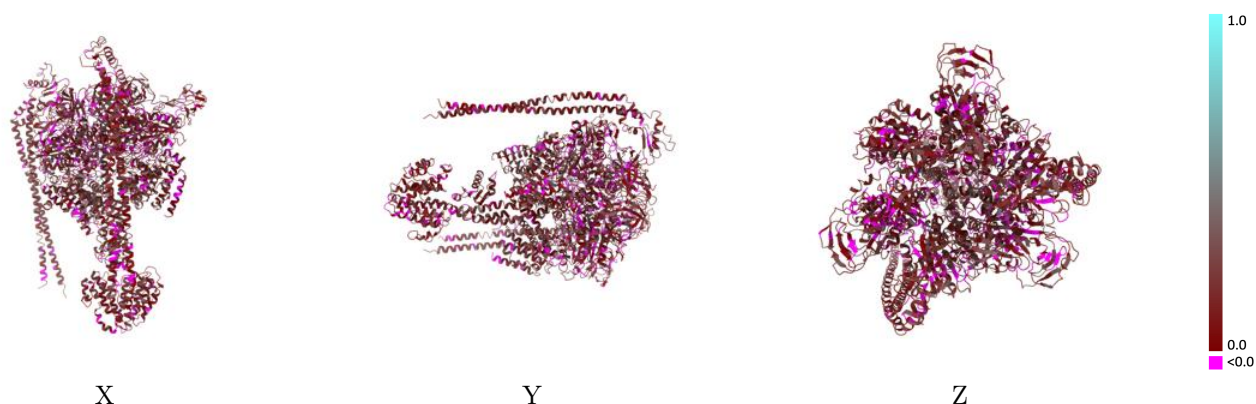
Y



Z

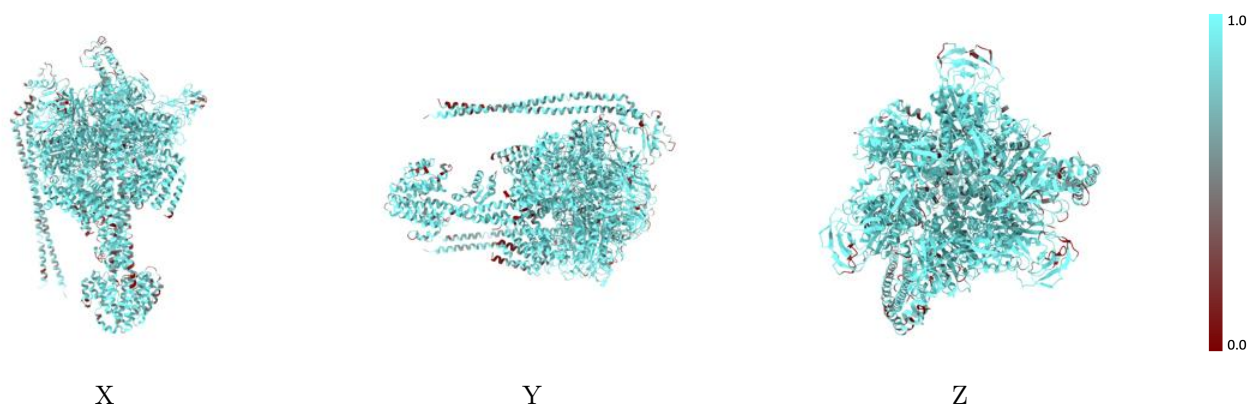
The images above show the 3D surface view of the map at the recommended contour level 0.548 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



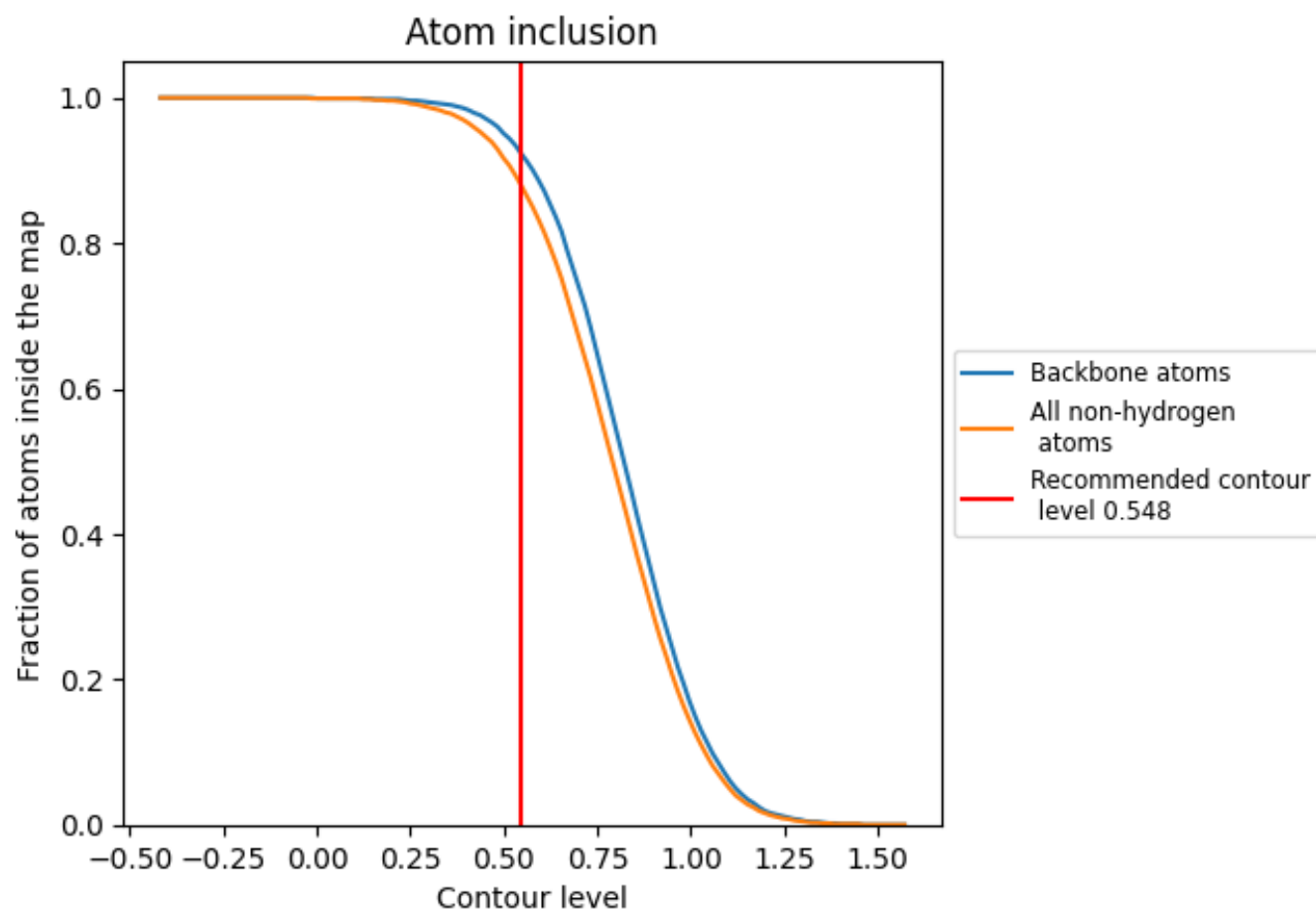
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.548).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.548) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.1440
A	 0.9290	 0.1400
B	 0.8820	 0.1230
C	 0.9210	 0.1560
D	 0.9210	 0.1460
E	 0.9320	 0.1560
F	 0.9220	 0.1460
G	 0.9530	 0.2040
H	 0.7860	 0.1280
I	 0.7140	 0.1430
J	 0.7770	 0.1530
K	 0.7610	 0.1440
L	 0.7340	 0.1470
M	 0.8460	 0.1260

