Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 10:59 AM EST

PDB ID	:	3J0J
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	:	1R5Z, 3K5B, 3A5C

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 (i) 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 (1)) were used in the production of this report:

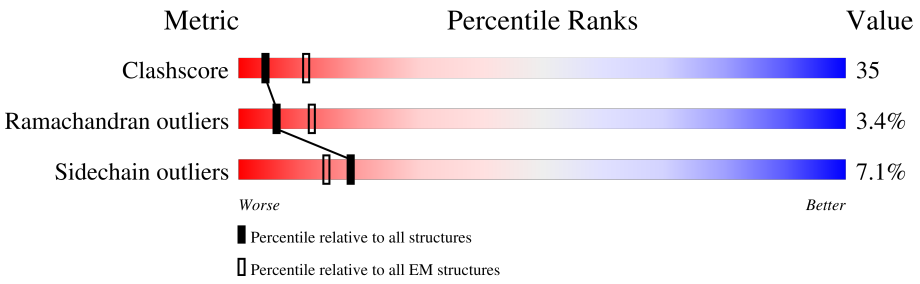
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	82% 13%
1	B	578	10% 85% 10%
1	C	578	6% 83% 12%
2	D	478	6% 83% 10% 6%
2	E	478	5% 82% 11% 6%
2	F	478	5% 82% 12% 6%
3	G	223	23% 24% 8% 42%
4	H	104	19% 79% 14% 7%

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Mol	Chain	Length	Quality of chain
5	I	104	12% 70% 24%
5	K	104	10% 73% 22%
6	J	188	11% 64% 25% 7%
6	L	188	17% 64% 26% 6%
7	M	323	7% 30% 63% 5%

2 Entry composition (i)

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
			Total	C	N	O		
1	A	561	2752	1630	561	561	0	0
1	B	561	2752	1630	561	561	0	0
1	C	561	2752	1630	561	561	0	0

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
6	J	184	1312	815	242	252	3	0	0
6	L	184	1312	815	242	252	3	0	0

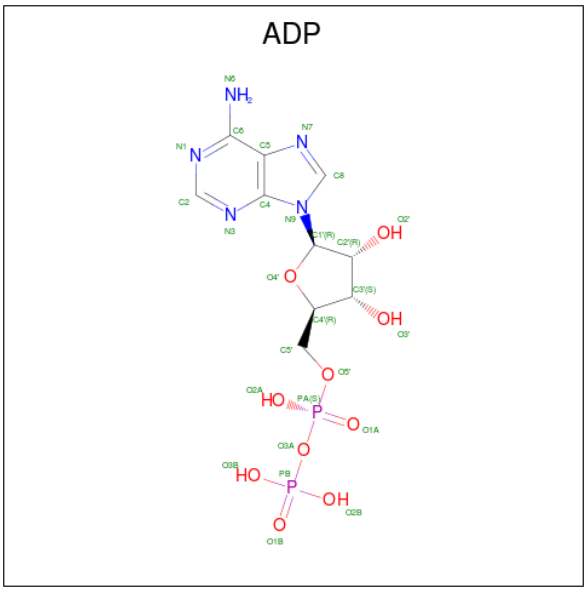
There are 6 discrepancies between the modelled and reference sequences:

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
			Total	C	N	O	S		
7	M	320	2514	1599	460	451	4	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



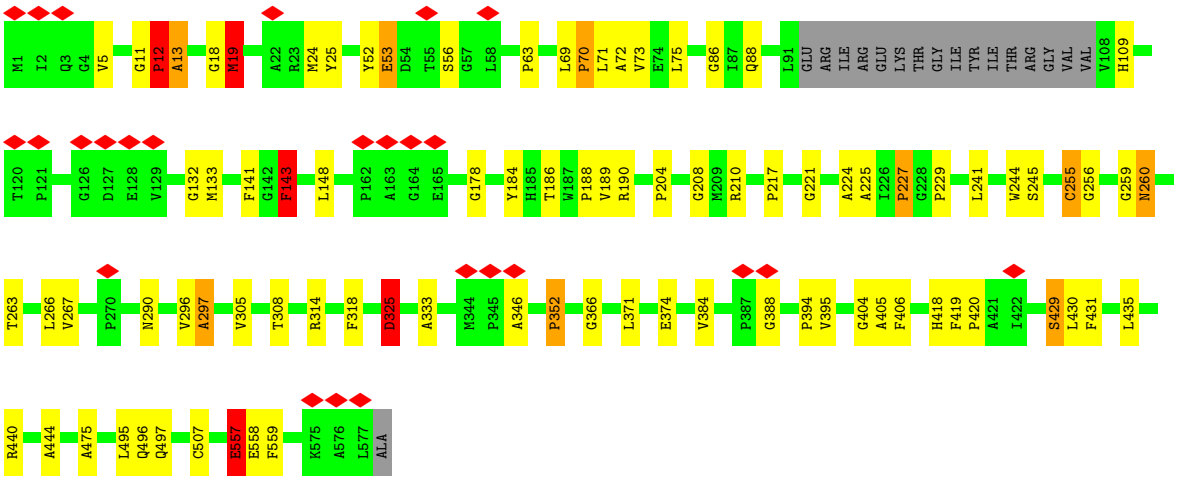
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

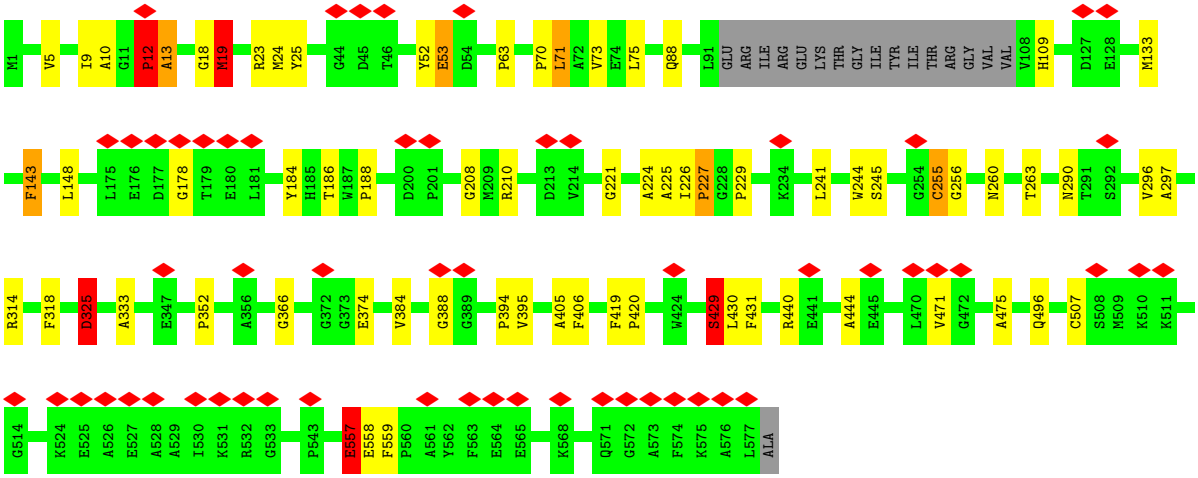
• Molecule 1: V-type ATP synthase alpha chain

Chain A:



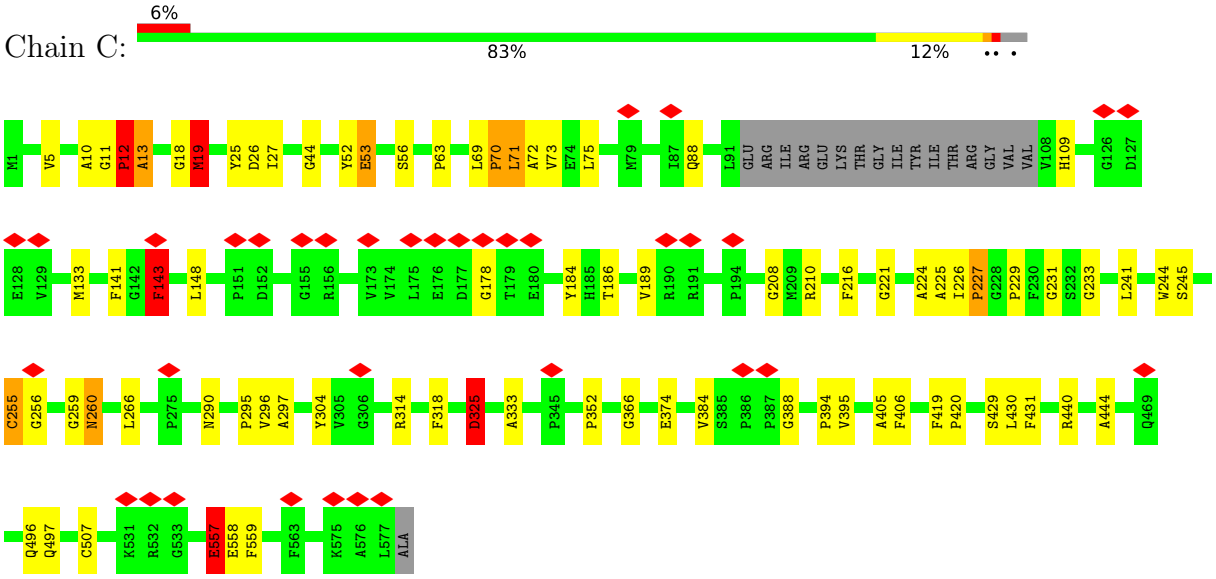
• Molecule 1: V-type ATP synthase alpha chain

Chain B:



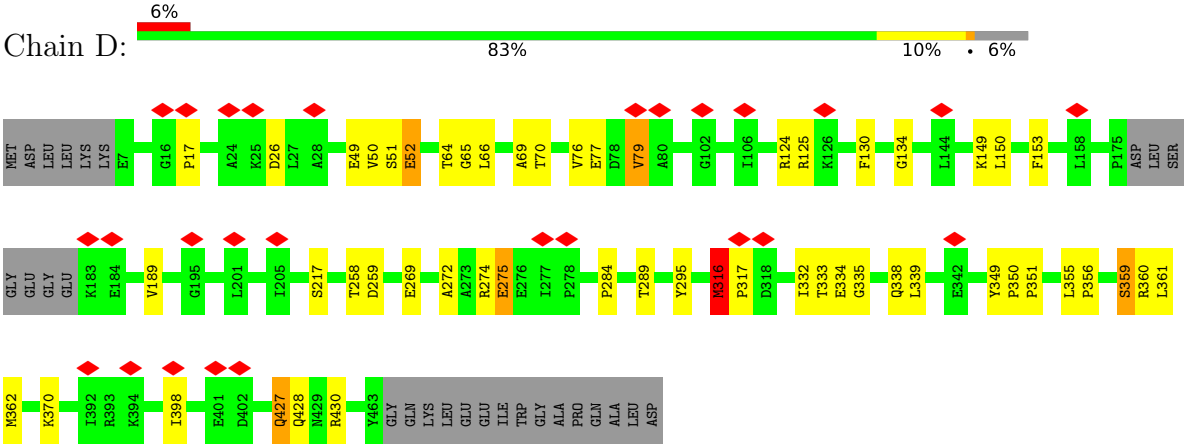
• Molecule 1: V-type ATP synthase alpha chain

Chain C:



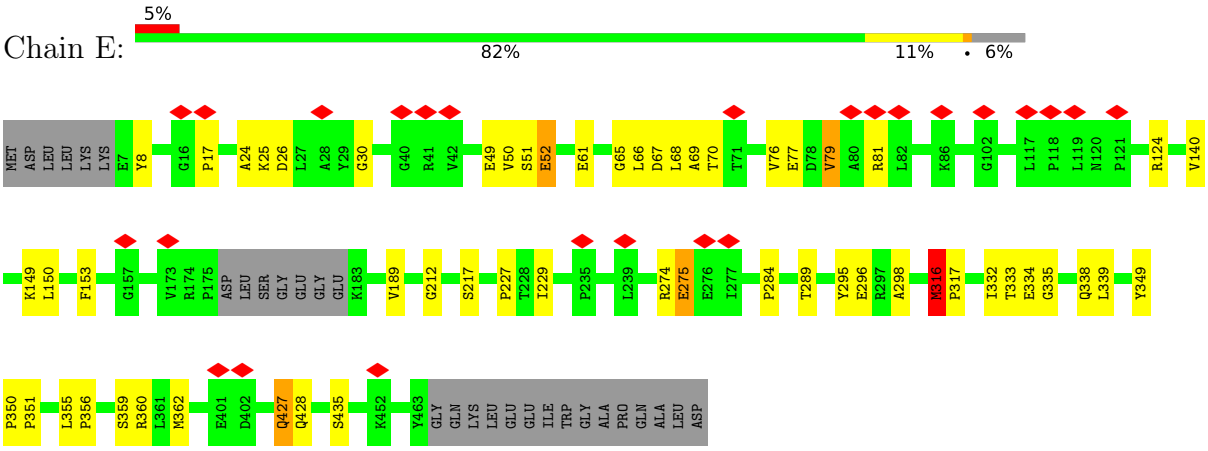
• Molecule 2: V-type ATP synthase beta chain

Chain D:



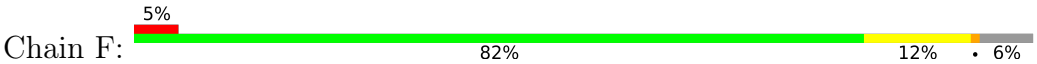
• Molecule 2: V-type ATP synthase beta chain

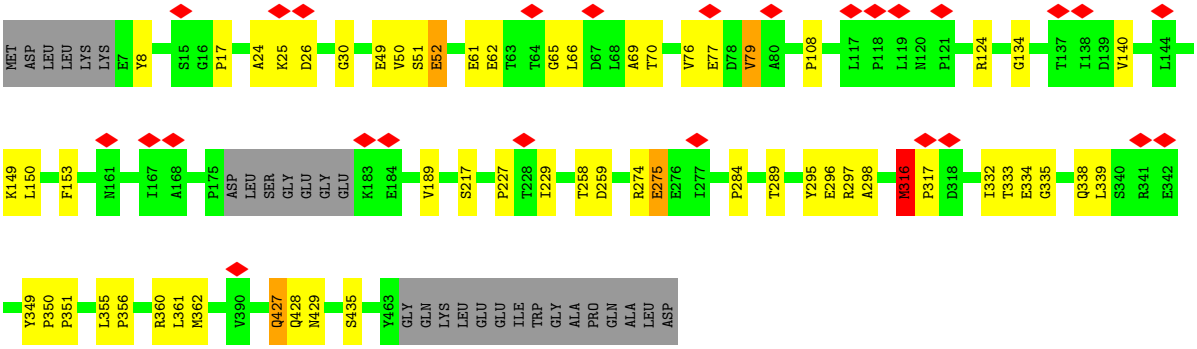
Chain E:



• Molecule 2: V-type ATP synthase beta chain

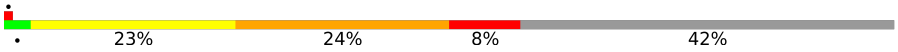
Chain F:

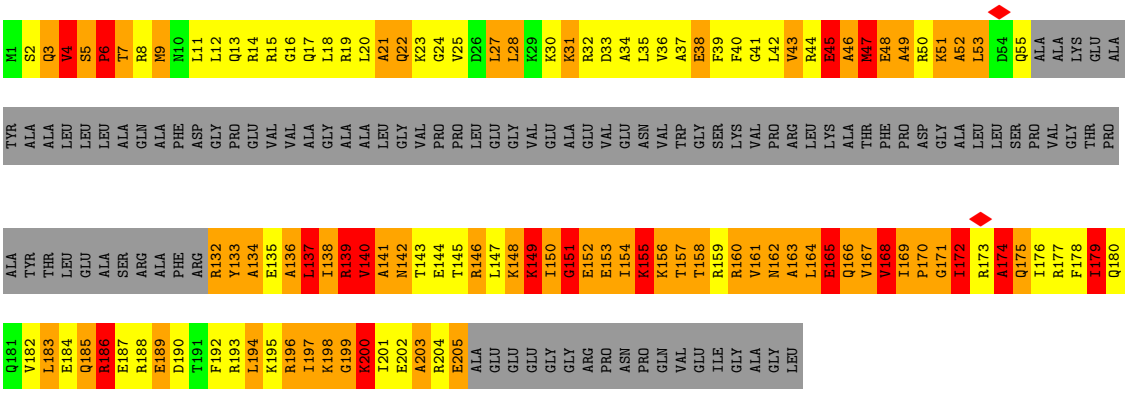




• Molecule 3: V-type ATP synthase subunit D

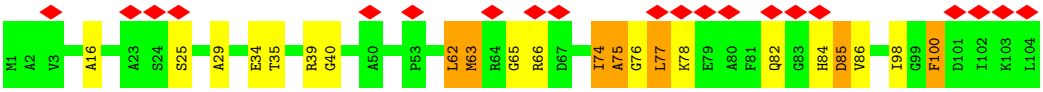
Chain G:





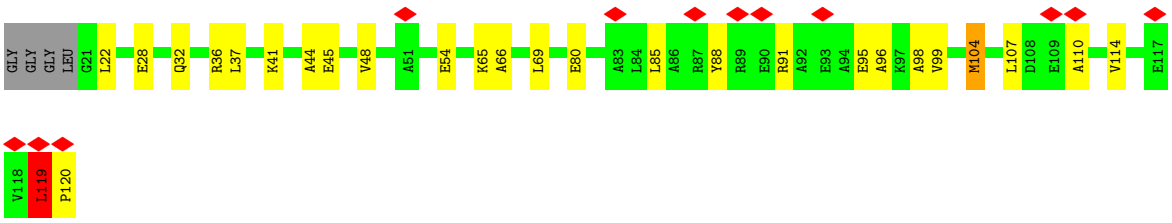
• Molecule 4: V-type ATP synthase subunit F

Chain H:



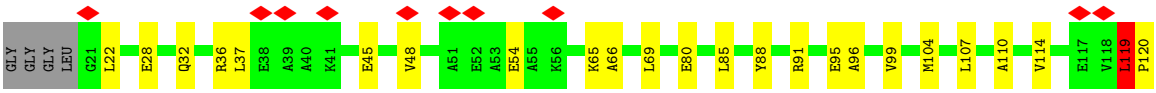
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain I:



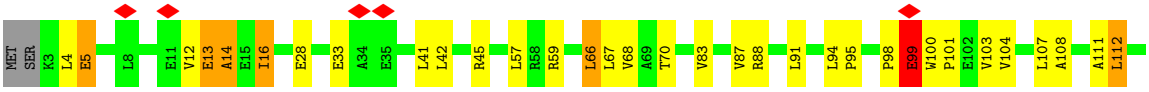
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

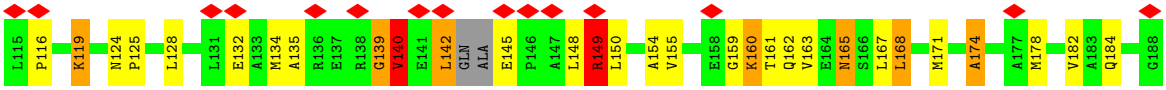
Chain K:



• Molecule 6: V-type ATP synthase subunit E

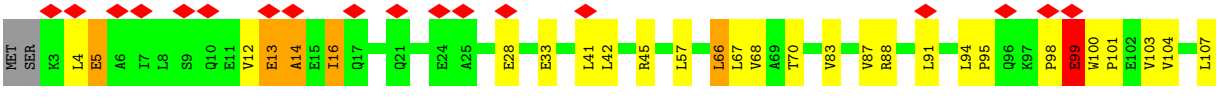
Chain J:

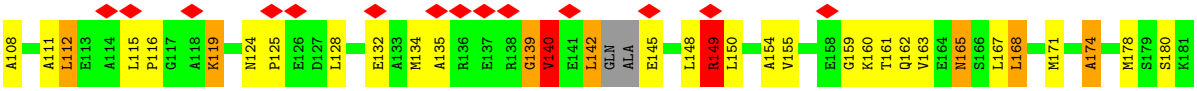




• Molecule 6: V-type ATP synthase subunit E

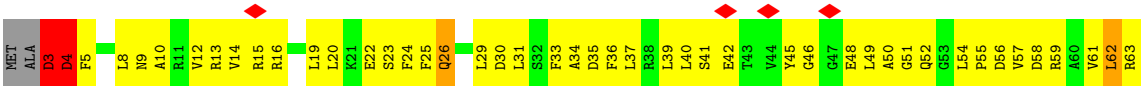
Chain L:

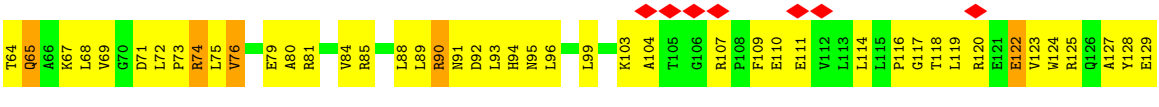


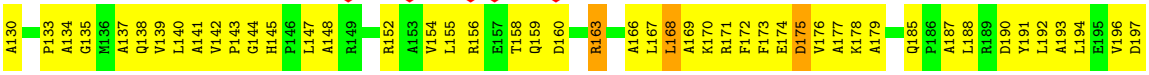


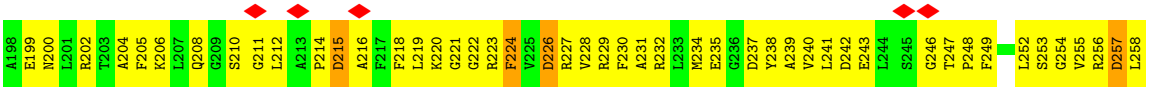
• Molecule 7: V-type ATP synthase subunit C

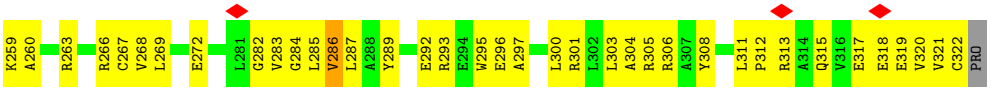
Chain M:











4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	B	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	C	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	E	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	125/637 (19.6%)	2.63	50/885 (5.6%)
4	H	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
5	I	0.42	1/749 (0.1%)	0.48	0/1004
5	K	0.42	1/749 (0.1%)	0.48	0/1004
6	J	0.45	2/1325 (0.2%)	0.53	0/1798
6	L	0.45	2/1325 (0.2%)	0.53	0/1798
7	M	1.22	5/2553 (0.2%)	1.11	12/3447 (0.3%)
All	All	1.02	164/22726 (0.7%)	1.19	138/31288 (0.4%)

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 (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	47	MET	CA-CB	-24.99	0.98	1.53
3	G	27	LEU	CA-CB	14.81	1.87	1.53
4	H	75	ALA	N-CA	13.46	1.73	1.46
3	G	7	THR	CA-CB	12.79	1.86	1.53
3	G	31	LYS	N-CA	12.37	1.71	1.46
3	G	138	ILE	CA-CB	-12.09	1.27	1.54
3	G	196	ARG	CA-C	12.06	1.84	1.52
4	H	76	GLY	CA-C	11.95	1.71	1.51
3	G	205	GLU	CA-CB	11.23	1.78	1.53
3	G	52	ALA	CA-CB	11.21	1.75	1.52
3	G	16	GLY	CA-C	11.03	1.69	1.51
4	H	75	ALA	CA-C	11.03	1.81	1.52
3	G	168	VAL	CA-CB	-10.99	1.31	1.54
3	G	167	VAL	CA-C	10.86	1.81	1.52
3	G	171	GLY	CA-C	10.62	1.68	1.51
4	H	34	GLU	C-O	10.58	1.43	1.23
3	G	16	GLY	C-O	10.31	1.40	1.23
3	G	189	GLU	CA-CB	10.16	1.76	1.53
3	G	4	VAL	CA-C	9.79	1.78	1.52
4	H	76	GLY	N-CA	9.78	1.60	1.46
3	G	19	ARG	N-CA	9.46	1.65	1.46
3	G	50	ARG	C-O	9.25	1.41	1.23
3	G	32	ARG	C-O	9.10	1.40	1.23
3	G	164	LEU	C-O	9.09	1.40	1.23
3	G	184	GLU	CA-CB	9.04	1.73	1.53
3	G	163	ALA	C-O	8.94	1.40	1.23
3	G	184	GLU	N-CA	8.91	1.64	1.46
3	G	169	ILE	C-O	8.78	1.40	1.23
3	G	142	ASN	CA-CB	8.67	1.75	1.53
3	G	6	PRO	C-O	8.66	1.40	1.23
3	G	183	LEU	C-O	8.57	1.39	1.23
3	G	194	LEU	CA-C	8.48	1.75	1.52
3	G	163	ALA	CA-C	8.37	1.74	1.52
3	G	38	GLU	N-CA	8.36	1.63	1.46
3	G	182	VAL	N-CA	8.30	1.62	1.46
4	H	40	GLY	C-O	8.28	1.36	1.23
3	G	155	LYS	N-CA	8.06	1.62	1.46
3	G	34	ALA	CA-CB	-8.01	1.35	1.52
3	G	185	GLN	C-O	7.88	1.38	1.23
3	G	195	LYS	N-CA	7.87	1.62	1.46
3	G	205	GLU	CA-C	7.86	1.73	1.52
3	G	170	PRO	CA-C	7.84	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	198	LYS	C-O	7.71	1.38	1.23
3	G	192	PHE	C-O	7.57	1.37	1.23
3	G	24	GLY	CA-C	7.57	1.64	1.51
3	G	46	ALA	C-O	7.52	1.37	1.23
3	G	51	LYS	C-O	7.48	1.37	1.23
3	G	4	VAL	CA-CB	7.45	1.70	1.54
3	G	134	ALA	N-CA	7.38	1.61	1.46
3	G	134	ALA	CA-CB	7.37	1.68	1.52
3	G	33	ASP	N-CA	7.36	1.61	1.46
3	G	146	ARG	CA-CB	7.29	1.70	1.53
3	G	22	GLN	C-O	7.24	1.37	1.23
3	G	53	LEU	N-CA	7.22	1.60	1.46
3	G	20	LEU	CA-C	7.20	1.71	1.52
3	G	172	ILE	N-CA	7.16	1.60	1.46
3	G	167	VAL	CA-CB	7.15	1.69	1.54
3	G	193	ARG	N-CA	7.12	1.60	1.46
3	G	6	PRO	CA-CB	7.12	1.67	1.53
3	G	27	LEU	N-CA	7.06	1.60	1.46
3	G	52	ALA	N-CA	7.05	1.60	1.46
3	G	188	ARG	N-CA	6.98	1.60	1.46
3	G	11	LEU	CA-CB	6.95	1.69	1.53
3	G	32	ARG	CA-C	6.86	1.70	1.52
3	G	156	LYS	CA-C	6.86	1.70	1.52
3	G	179	ILE	C-O	6.85	1.36	1.23
3	G	4	VAL	C-O	6.83	1.36	1.23
3	G	154	ILE	C-O	6.80	1.36	1.23
3	G	199	GLY	N-CA	6.75	1.56	1.46
4	H	75	ALA	C-N	6.70	1.45	1.33
3	G	169	ILE	N-CA	6.62	1.59	1.46
3	G	175	GLN	CA-CB	-6.58	1.39	1.53
3	G	32	ARG	C-N	6.57	1.49	1.34
3	G	204	ARG	N-CA	6.55	1.59	1.46
3	G	17	GLN	CA-CB	-6.46	1.39	1.53
3	G	148	LYS	CA-CB	6.43	1.68	1.53
3	G	189	GLU	CA-C	6.43	1.69	1.52
7	M	34	ALA	CA-CB	6.39	1.65	1.52
3	G	9	MET	CA-C	-6.38	1.36	1.52
3	G	5	SER	CA-CB	6.37	1.62	1.52
3	G	196	ARG	CA-CB	6.36	1.68	1.53
3	G	31	LYS	C-O	6.35	1.35	1.23
3	G	14	ARG	C-O	6.26	1.35	1.23
3	G	28	LEU	CA-C	6.20	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	14	ARG	N-CA	6.19	1.58	1.46
3	G	192	PHE	CA-C	6.19	1.69	1.52
3	G	24	GLY	C-O	6.16	1.33	1.23
4	H	40	GLY	C-N	6.14	1.44	1.33
3	G	45	GLU	C-O	6.11	1.34	1.23
1	B	13	ALA	CA-CB	-6.07	1.39	1.52
3	G	203	ALA	N-CA	-6.04	1.34	1.46
1	C	13	ALA	CA-CB	-6.04	1.39	1.52
3	G	201	ILE	CA-CB	-6.02	1.41	1.54
3	G	194	LEU	C-O	6.02	1.34	1.23
3	G	164	LEU	N-CA	6.02	1.58	1.46
3	G	205	GLU	C-O	5.98	1.34	1.23
1	A	13	ALA	CA-CB	-5.97	1.40	1.52
3	G	7	THR	CA-C	5.95	1.68	1.52
3	G	166	GLN	CA-CB	-5.92	1.41	1.53
5	I	104	MET	CG-SD	5.92	1.96	1.81
5	K	104	MET	CG-SD	5.89	1.96	1.81
7	M	224	PHE	CE2-CZ	5.82	1.48	1.37
3	G	14	ARG	CA-CB	5.78	1.66	1.53
3	G	141	ALA	CA-CB	5.75	1.64	1.52
7	M	293	ARG	CG-CD	5.74	1.66	1.51
3	G	21	ALA	C-O	5.74	1.34	1.23
3	G	23	LYS	N-CA	5.69	1.57	1.46
2	D	275	GLU	CA-CB	-5.67	1.41	1.53
3	G	52	ALA	C-O	5.66	1.34	1.23
7	M	297	ALA	CA-CB	5.66	1.64	1.52
2	F	275	GLU	CA-CB	-5.66	1.41	1.53
3	G	37	ALA	CA-CB	-5.61	1.40	1.52
3	G	170	PRO	N-CA	5.61	1.56	1.47
6	J	134	MET	CG-SD	5.59	1.95	1.81
6	L	134	MET	CG-SD	5.59	1.95	1.81
2	E	275	GLU	CA-CB	-5.58	1.41	1.53
3	G	25	VAL	N-CA	5.56	1.57	1.46
3	G	47	MET	C-O	5.56	1.33	1.23
3	G	158	THR	CA-CB	-5.55	1.39	1.53
3	G	49	ALA	N-CA	5.52	1.57	1.46
2	D	289	THR	C-N	5.51	1.46	1.34
3	G	15	ARG	CA-CB	5.51	1.66	1.53
4	H	25	SER	CA-CB	5.50	1.61	1.52
3	G	49	ALA	CA-CB	-5.50	1.41	1.52
3	G	148	LYS	N-CA	5.48	1.57	1.46
3	G	187	GLU	CA-C	5.48	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	171	GLY	C-O	5.48	1.32	1.23
6	L	178	MET	CG-SD	5.42	1.95	1.81
3	G	163	ALA	C-N	5.42	1.46	1.34
2	D	316	MET	C-N	-5.40	1.24	1.34
3	G	36	VAL	CA-C	5.40	1.67	1.52
6	J	178	MET	CG-SD	5.40	1.95	1.81
2	F	316	MET	C-N	-5.39	1.24	1.34
3	G	7	THR	C-O	5.38	1.33	1.23
1	B	19	MET	CA-CB	-5.38	1.42	1.53
1	A	19	MET	CA-CB	-5.37	1.42	1.53
2	F	289	THR	C-N	5.36	1.46	1.34
3	G	28	LEU	C-O	5.35	1.33	1.23
2	E	289	THR	C-N	5.34	1.46	1.34
1	C	19	MET	CA-CB	-5.33	1.42	1.53
2	E	316	MET	C-N	-5.33	1.24	1.34
1	A	352	PRO	CA-CB	-5.32	1.43	1.53
1	B	352	PRO	CA-CB	-5.31	1.43	1.53
1	C	352	PRO	CA-CB	-5.29	1.43	1.53
3	G	7	THR	N-CA	5.28	1.56	1.46
4	H	29	ALA	CA-CB	-5.25	1.41	1.52
3	G	196	ARG	C-O	5.24	1.33	1.23
3	G	49	ALA	CA-C	-5.22	1.39	1.52
3	G	138	ILE	CA-C	-5.20	1.39	1.52
3	G	153	GLU	N-CA	5.18	1.56	1.46
3	G	15	ARG	C-O	5.16	1.33	1.23
3	G	143	THR	N-CA	5.12	1.56	1.46
3	G	201	ILE	C-O	5.12	1.33	1.23
3	G	165	GLU	C-O	5.11	1.33	1.23
3	G	162	ASN	C-O	5.11	1.33	1.23
3	G	36	VAL	CA-CB	5.10	1.65	1.54
3	G	200	LYS	CA-C	5.09	1.66	1.52
3	G	132	ARG	C-O	5.05	1.32	1.23
3	G	165	GLU	N-CA	5.05	1.56	1.46
3	G	36	VAL	C-O	5.04	1.32	1.23
3	G	22	GLN	C-N	5.04	1.45	1.34
3	G	37	ALA	C-O	5.03	1.32	1.23
3	G	160	ARG	C-O	5.02	1.32	1.23
7	M	122	GLU	CD-OE1	5.00	1.31	1.25

All (138) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	ASP	O-C-N	-39.91	58.85	122.70
1	B	325	ASP	O-C-N	-39.91	58.85	122.70
1	C	325	ASP	O-C-N	-39.84	58.95	122.70
1	C	70	PRO	C-N-CA	-27.46	53.06	121.70
4	H	76	GLY	N-CA-C	26.73	179.94	113.10
1	A	429	SER	O-C-N	25.73	163.87	122.70
1	A	429	SER	CA-C-N	-25.54	61.01	117.20
1	A	429	SER	C-N-CA	-21.28	68.49	121.70
1	C	70	PRO	CA-C-N	-19.69	73.89	117.20
4	H	74	ILE	O-C-N	-18.88	92.50	122.70
1	C	325	ASP	C-N-CA	-18.24	76.09	121.70
1	B	325	ASP	C-N-CA	-18.23	76.13	121.70
1	A	325	ASP	C-N-CA	-18.17	76.28	121.70
2	D	316	MET	O-C-N	-15.64	91.39	121.10
2	E	316	MET	O-C-N	-15.58	91.50	121.10
2	F	316	MET	O-C-N	-15.54	91.57	121.10
1	A	325	ASP	CA-C-N	15.11	150.44	117.20
1	B	325	ASP	CA-C-N	15.05	150.31	117.20
1	C	325	ASP	CA-C-N	15.00	150.21	117.20
4	H	76	GLY	CA-C-N	14.65	149.44	117.20
1	C	70	PRO	O-C-N	13.41	144.16	122.70
4	H	74	ILE	CA-C-N	12.93	145.65	117.20
4	H	75	ALA	N-CA-C	12.21	143.97	111.00
4	H	77	LEU	C-N-CA	-11.86	92.05	121.70
4	H	76	GLY	CA-C-O	-11.46	99.97	120.60
3	G	47	MET	N-CA-C	10.65	139.76	111.00
3	G	139	ARG	N-CA-C	-10.47	82.73	111.00
4	H	76	GLY	C-N-CA	10.12	146.99	121.70
3	G	6	PRO	C-N-CA	-9.83	97.13	121.70
3	G	6	PRO	N-CA-CB	9.48	114.67	103.30
2	E	316	MET	CA-C-N	9.46	143.59	117.10
2	D	316	MET	CA-C-N	9.45	143.55	117.10
2	F	316	MET	CA-C-N	9.43	143.52	117.10
3	G	9	MET	C-N-CA	-9.37	98.27	121.70
1	B	429	SER	O-C-N	-9.33	107.77	122.70
3	G	49	ALA	C-N-CA	-9.14	98.84	121.70
4	H	75	ALA	C-N-CA	9.11	141.44	122.30
1	A	63	PRO	N-CA-CB	8.73	113.78	103.30
4	H	77	LEU	CA-C-N	8.73	136.42	117.20
1	C	63	PRO	N-CA-CB	8.61	113.63	103.30
3	G	47	MET	C-N-CA	-8.59	100.23	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	PRO	N-CA-CB	8.54	113.55	103.30
7	M	3	ASP	CB-CG-OD2	8.50	125.95	118.30
3	G	187	GLU	N-CA-C	8.37	133.59	111.00
3	G	31	LYS	CA-C-N	-8.27	99.00	117.20
4	H	76	GLY	O-C-N	-8.05	109.82	122.70
3	G	186	ARG	C-N-CA	-7.86	102.06	121.70
3	G	203	ALA	N-CA-C	-7.82	89.89	111.00
7	M	160	ASP	CB-CG-OD2	7.60	125.14	118.30
3	G	167	VAL	O-C-N	-7.44	110.80	122.70
4	H	63	MET	N-CA-C	7.36	130.88	111.00
3	G	31	LYS	O-C-N	7.29	134.37	122.70
3	G	167	VAL	C-N-CA	-7.29	103.48	121.70
2	D	289	THR	O-C-N	-7.28	111.05	122.70
2	F	289	THR	O-C-N	-7.16	111.25	122.70
3	G	7	THR	C-N-CA	-7.15	103.82	121.70
2	E	289	THR	O-C-N	-7.13	111.29	122.70
3	G	133	TYR	N-CA-C	-7.10	91.82	111.00
3	G	30	LYS	C-N-CA	7.10	139.44	121.70
3	G	170	PRO	N-CA-CB	7.07	111.78	103.30
3	G	157	THR	N-CA-C	-7.02	92.03	111.00
3	G	182	VAL	O-C-N	7.00	133.90	122.70
3	G	153	GLU	N-CA-C	6.99	129.88	111.00
4	H	77	LEU	O-C-N	-6.95	111.59	122.70
3	G	156	LYS	N-CA-C	6.90	129.63	111.00
3	G	202	GLU	CA-C-N	-6.88	102.06	117.20
3	G	151	GLY	N-CA-C	-6.83	96.02	113.10
3	G	167	VAL	CA-C-N	6.67	131.87	117.20
1	C	12	PRO	N-CA-CB	6.66	111.29	103.30
3	G	12	LEU	N-CA-C	-6.66	93.03	111.00
1	B	12	PRO	N-CA-CB	6.61	111.23	103.30
1	A	12	PRO	N-CA-CB	6.58	111.19	103.30
3	G	49	ALA	CA-C-N	-6.50	102.90	117.20
3	G	154	ILE	N-CA-C	-6.44	93.61	111.00
3	G	156	LYS	C-N-CA	-6.44	105.60	121.70
1	A	143	PHE	N-CA-C	6.43	128.37	111.00
2	D	289	THR	CA-C-N	6.43	131.35	117.20
2	F	289	THR	CA-C-N	6.41	131.31	117.20
3	G	196	ARG	N-CA-CB	-6.41	99.06	110.60
1	C	143	PHE	N-CA-C	6.40	128.27	111.00
3	G	196	ARG	CB-CA-C	6.38	123.16	110.40
1	B	143	PHE	N-CA-C	6.37	128.20	111.00
2	E	289	THR	CA-C-N	6.35	131.17	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	PRO	N-CA-CB	6.33	110.90	103.30
1	B	229	PRO	N-CA-CB	6.26	110.81	103.30
3	G	199	GLY	N-CA-C	-6.25	97.49	113.10
7	M	286	VAL	CG1-CB-CG2	-6.24	100.92	110.90
1	C	229	PRO	N-CA-CB	6.19	110.72	103.30
2	D	360	ARG	N-CA-C	-6.16	94.36	111.00
3	G	21	ALA	O-C-N	6.14	132.52	122.70
7	M	4	ASP	CB-CA-C	6.11	122.62	110.40
7	M	293	ARG	NE-CZ-NH1	6.04	123.32	120.30
7	M	163	ARG	NE-CZ-NH2	-5.96	117.32	120.30
3	G	194	LEU	N-CA-C	5.94	127.03	111.00
3	G	149	LYS	N-CA-C	-5.92	95.00	111.00
2	D	17	PRO	N-CA-CB	5.91	110.39	103.30
2	D	284	PRO	N-CA-CB	5.91	110.39	103.30
2	F	284	PRO	N-CA-CB	5.91	110.39	103.30
2	F	351	PRO	N-CA-CB	5.89	110.37	103.30
2	E	351	PRO	N-CA-CB	5.88	110.36	103.30
2	F	17	PRO	N-CA-CB	5.88	110.35	103.30
2	E	17	PRO	N-CA-CB	5.86	110.33	103.30
2	E	284	PRO	N-CA-CB	5.83	110.30	103.30
7	M	293	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	D	351	PRO	N-CA-CB	5.79	110.25	103.30
3	G	21	ALA	CB-CA-C	-5.78	101.43	110.10
1	B	557	GLU	O-C-N	-5.77	113.46	122.70
3	G	136	ALA	N-CA-C	-5.76	95.45	111.00
3	G	188	ARG	N-CA-CB	5.74	120.94	110.60
1	C	557	GLU	O-C-N	-5.71	113.57	122.70
1	A	557	GLU	O-C-N	-5.70	113.59	122.70
3	G	47	MET	N-CA-CB	-5.66	100.41	110.60
1	A	244	TRP	N-CA-C	5.63	126.19	111.00
1	C	244	TRP	N-CA-C	5.62	126.18	111.00
1	B	244	TRP	N-CA-C	5.62	126.17	111.00
3	G	142	ASN	N-CA-C	-5.58	95.94	111.00
7	M	168	LEU	CA-CB-CG	5.57	128.11	115.30
7	M	175	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	429	SER	CA-C-N	5.44	129.17	117.20
2	D	359	SER	N-CA-C	-5.40	96.41	111.00
4	H	35	THR	CB-CA-C	-5.40	97.01	111.60
3	G	174	ALA	C-N-CA	-5.38	108.24	121.70
3	G	155	LYS	C-N-CA	-5.38	108.25	121.70
3	G	47	MET	CA-C-O	5.37	131.38	120.10
3	G	140	VAL	N-CA-C	5.37	125.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	PRO	N-CA-C	-5.27	98.39	112.10
3	G	171	GLY	N-CA-C	-5.22	100.05	113.10
7	M	237	ASP	CB-CG-OD2	5.20	122.98	118.30
7	M	30	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	430	LEU	N-CA-C	-5.18	97.01	111.00
3	G	31	LYS	CB-CA-C	-5.17	100.06	110.40
3	G	137	LEU	O-C-N	-5.14	114.47	122.70
3	G	156	LYS	CA-C-N	5.10	128.42	117.20
7	M	226	ASP	CB-CG-OD2	5.08	122.88	118.30
2	E	81	ARG	N-CA-C	5.06	124.67	111.00
3	G	21	ALA	CA-C-N	-5.06	106.07	117.20
4	H	62	LEU	C-N-CA	-5.03	109.12	121.70
3	G	47	MET	CB-CA-C	-5.01	100.38	110.40

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	Peptide,Mainchain
2	E	316	MET	Mainchain
2	E	427	GLN	Peptide
2	E	79	VAL	Mainchain

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Mol	Chain	Res	Type	Group
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 (i)

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	122	0
1	B	2752	0	1303	59	0
1	C	2752	0	1302	86	0
2	D	2212	0	1009	80	0
2	E	2212	0	1009	84	0
2	F	2212	0	1009	83	0
3	G	639	0	299	136	0
4	H	509	0	255	23	0
5	I	747	0	726	21	0
5	K	747	0	726	18	0
6	J	1312	0	1240	74	0
6	L	1312	0	1240	56	0
7	M	2514	0	2583	624	0
8	A	27	0	12	0	0
8	C	27	0	12	4	0
All	All	22726	0	14025	1287	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 35.

All (1287) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:194:LEU:C	3:G:194:LEU:CA	1.75	1.56
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
3:G:163:ALA:C	3:G:163:ALA:CA	1.74	1.53
3:G:4:VAL:C	3:G:4:VAL:CA	1.78	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: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
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
4:H:75:ALA:C	4:H:75:ALA:CA	1.81	1.48
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
3:G:196:ARG:C	3:G:196:ARG:CA	1.84	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
3:G:167:VAL:C	3:G:167:VAL:CA	1.81	1.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:266:LEU:C	2:F:124:ARG:CB	1.93	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
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
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
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
7:M:88:LEU:HB3	7:M:117:GLY:C	1.48	1.30
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
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:A:259:GLY:O	2:F:296:GLU:C	1.73	1.27
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
2:E:24:ALA:C	6:J:161:THR:HA	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:11:GLY:HA3	2:F:50:VAL:C	1.58	1.23
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
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
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
7:M:51:GLY:HA3	7:M:56:ASP:HB3	1.26	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
7:M:170:LYS:CG	7:M:174:GLU:OE2	1.92	1.15
1:B:263:THR:CB	2:D:125:ARG:C	2.15	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
2:E:24:ALA:HB1	6:J:159:GLY:C	1.69	1.13
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:24:MET:C	2:D:66:LEU:H	1.53	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
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
1:A:259:GLY:C	2:F:296:GLU:C	2.06	1.09
2:D:334:GLU:O	2:D:361:LEU:N	1.86	1.09
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
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:232:ARG:HH12	7:M:243:GLU:CD	1.60	1.04
7:M:263:ARG:HG3	7:M:321:VAL:O	1.56	1.04
1:C:259:GLY:O	2:E:296:GLU:C	1.97	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:M:259:LYS:HZ3	7:M:318:GLU:CB	1.72	1.03
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
1:A:267:VAL:N	2:F:124:ARG:CA	2.22	1.00
3:G:7:THR:O	3:G:8:ARG:C	1.98	1.00
7:M:29:LEU:HD13	7:M:313:ARG:NE	1.76	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
2:F:360:ARG:C	2:F:362:MET:H	1.67	0.98
7:M:20:LEU:HD21	7:M:24:PHE:CD1	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:M:204:ALA:HA	7:M:234:MET:HE2	1.42	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
2:E:24:ALA:C	6:J:161:THR:CA	2.33	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
7:M:259:LYS:HZ3	7:M:318:GLU:HB3	1.15	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
3:G:199:GLY:C	3:G:203:ALA:HB2	1.86	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:M:3:ASP:HB3	7:M:79:GLU:CB	1.89	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: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: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
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: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
1:A:419:PHE:CB	1:A:497:GLN:O	2.20	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
3:G:135:GLU:C	3:G:137:LEU:N	2.17	0.90
7:M:214:PRO:CG	7:M:231:ALA:HB1	1.91	0.90
7:M:312:PRO:HG3	7:M:315:GLN:CD	1.92	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
1:B:263:THR:CB	2:D:125:ARG:CA	2.51	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
7:M:119:LEU:CD1	7:M:140:LEU:HD23	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:178:LYS:CE	7:M:221:GLY:HA2	1.71	0.88
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
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:C:259:GLY:C	2:E:296:GLU:C	2.33	0.87
1:A:419:PHE:N	1:A:496:GLN:HA	1.89	0.87
7:M:33:PHE:CE1	7:M:308:TYR:CD1	2.63	0.87
3:G:47:MET:O	3:G:48:GLU:C	2.09	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:226:ASP:CG	7:M:229:ARG:HB2	1.95	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:204:ALA:CA	7:M:234:MET:HE2	2.05	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
3:G:174:ALA:O	3:G:175:GLN:C	2.09	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
7:M:266:ARG:C	7:M:322:CYS:SG	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:266:ARG:HD3	7:M:295:TRP:CD2	2.11	0.84
7:M:88:LEU:CB	7:M:117:GLY:C	2.42	0.84
7:M:61:VAL:CG1	7:M:65:GLN:HG3	2.08	0.84
2:E:140:VAL:CB	2:E:435:SER:CB	2.56	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
4:H:75:ALA:C	4:H:75:ALA:HA	1.95	0.83
1:A:25:TYR:C	2:D:65:GLY:HA2	1.98	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: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
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
3:G:167:VAL:O	3:G:168:VAL:C	2.19	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:51:GLY:C	7:M:56:ASP:HB3	2.02	0.80
7:M:73:PRO:HG2	7:M:88:LEU:HD12	1.62	0.80
1:C:259:GLY:C	2:E:296:GLU:CA	2.38	0.80
7:M:93:LEU:CD1	7:M:168:LEU:HD23	2.12	0.80
2:F:134:GLY:O	2:F:429:ASN:HA	1.82	0.79
6:J:87:VAL:HG12	6:J:171:MET:CE	2.12	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
2:E:24:ALA:CB	6:J:159:GLY:C	2.44	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
2:F:108:PRO:O	6:L:180:SER:CB	2.30	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
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
6:L:87:VAL:HG12	6:L:171:MET:CE	2.12	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
7:M:170:LYS:CG	7:M:174:GLU:CD	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:223:ARG:NE	7:M:224:PHE:HE2	1.82	0.77
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:204:ALA:HA	7:M:234:MET:HE1	1.66	0.76
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
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
1:C:259:GLY:C	2:E:296:GLU:HA	1.81	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:204:ALA:CB	7:M:234:MET:HE2	2.16	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
7:M:170:LYS:HG2	7:M:174:GLU:CD	2.07	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
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
1:C:52:TYR:C	1:C:295:PRO:CB	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:132:ARG:C	3:G:134:ALA:N	2.37	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
3:G:199:GLY:C	3:G:203:ALA:CB	2.56	0.74
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
6:J:87:VAL:HG12	6:J:171:MET:HE1	1.70	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
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: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
3:G:45:GLU:O	3:G:46:ALA:C	2.27	0.72
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
3:G:163:ALA:C	3:G:163:ALA:HA	2.04	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: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:259:LYS:HZ1	7:M:318:GLU:HB3	1.55	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:10:ALA:HA	7:M:13:ARG:NH1	2.05	0.71
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
7:M:56:ASP:OD1	7:M:59:ARG:NH2	2.22	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: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
4:H:75:ALA:C	4:H:75:ALA:CB	2.60	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
2:D:359:SER:C	2:D:361:LEU:N	2.39	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:232:ARG:NH1	7:M:243:GLU:OE2	2.23	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
3:G:135:GLU:O	3:G:136:ALA:C	2.28	0.69
1:A:24:MET:HA	2:D:66:LEU:N	1.97	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:185:GLN:HE22	7:M:282:GLY:CA	2.06	0.68
7:M:51:GLY:HA3	7:M:56:ASP:CG	2.13	0.68
1:A:5:VAL:CB	1:A:18:GLY:O	2.42	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
7:M:69:VAL:HA	7:M:72:LEU:HD12	1.72	0.68
7:M:267:CYS:SG	7:M:322:CYS:O	2.51	0.68
1:B:5:VAL:CB	1:B:18:GLY:O	2.42	0.68
2:E:25:LYS:CB	6:J:161:THR:C	2.62	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:194:LEU:C	3:G:194:LEU:HA	2.04	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
6:L:87:VAL:HG12	6:L:171:MET:HE2	1.76	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
3:G:48:GLU:C	3:G:51:LYS:H	1.97	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
7:M:170:LYS:HG3	7:M:174:GLU:CD	2.12	0.67
7:M:259:LYS:HZ3	7:M:318:GLU:CG	2.06	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
6:L:87:VAL:HG12	6:L:171:MET:HE1	1.75	0.66
7:M:40:LEU:CD2	7:M:49:LEU:HD22	2.21	0.66
3:G:196:ARG:C	3:G:196:ARG:HA	2.05	0.66
6:J:150:LEU:HD23	6:J:168:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:256:ARG:O	7:M:257:ASP:CB	2.44	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
6:L:150:LEU:HD23	6:L:168:LEU:HD21	1.78	0.65
1:C:259:GLY:C	2:E:296:GLU:O	2.35	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
1:C:27:ILE:HA	1:C:71:LEU:H	1.61	0.65
1:A:25:TYR:H	2:D:65:GLY:C	1.96	0.65
3:G:141:ALA:HA	3:G:144:GLU:CB	2.26	0.65
2:F:149:LYS:O	2:F:333:THR:C	2.35	0.65
7:M:88:LEU:CB	7:M:117:GLY:HA2	2.27	0.65
7:M:51:GLY:C	7:M:56:ASP:CB	2.64	0.64
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
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:54:LEU:HB3	7:M:55:PRO:HD3	1.80	0.64
2:D:149:LYS:O	2:D:333:THR:C	2.35	0.64
7:M:166:ALA:C	7:M:170:LYS:HB3	2.16	0.64
7:M:64:THR:O	7:M:67:LYS:HG2	1.97	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
2:E:149:LYS:O	2:E:333:THR:C	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:419:PHE:C	1:B:496:GLN:HA	2.13	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: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
3:G:141:ALA:HA	3:G:145:THR:H	1.62	0.63
3:G:151:GLY:O	3:G:152:GLU:C	2.37	0.63
6:J:67:LEU:O	6:J:67:LEU:HD23	1.98	0.63
4:H:74:ILE:C	4:H:75:ALA:HA	2.16	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
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
2:E:76:VAL:O	2:E:77:GLU:CB	2.47	0.62
6:J:87:VAL:HG12	6:J:171:MET:HE2	1.81	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
4:H:62:LEU:O	4:H:63:MET:CB	2.46	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
7:M:103:LYS:NZ	7:M:128:TYR:O	2.27	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
1:C:429:SER:C	1:C:431:PHE:H	2.03	0.61
7:M:8:LEU:CD1	7:M:12:VAL:HG23	2.30	0.61
7:M:31:LEU:HD22	7:M:35:ASP:HB3	1.82	0.61
1:A:208:GLY:O	1:A:507:CYS:O	2.18	0.61
7:M:68:LEU:O	7:M:72:LEU:CD1	2.44	0.61
3:G:156:LYS:C	3:G:158:THR:N	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:8:LEU:HG	7:M:12:VAL:HG21	1.83	0.61
3:G:4:VAL:C	3:G:4:VAL:HA	2.07	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
3:G:135:GLU:O	3:G:137:LEU:N	2.33	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
3:G:170:PRO:O	3:G:174:ALA:HB2	2.00	0.60
7:M:266:ARG:HD2	7:M:322:CYS:SG	2.41	0.60
3:G:41:GLY:O	3:G:42:LEU:C	2.38	0.60
7:M:29:LEU:CD1	7:M:313:ARG:HE	2.12	0.60
4:H:74:ILE:C	4:H:75:ALA:CA	2.62	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
3:G:156:LYS:O	3:G:157:THR:C	2.33	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
1:B:12:PRO:O	1:B:13:ALA:HB3	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
3:G:132:ARG:O	3:G:133:TYR:C	2.37	0.59
7:M:39:LEU:O	7:M:42:GLU:HG2	2.02	0.59
7:M:312:PRO:CG	7:M:315:GLN:CD	2.62	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:150:ILE:C	3:G:151:GLY:O	2.39	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
3:G:158:THR:C	3:G:161:VAL:CB	2.70	0.59
7:M:166:ALA:O	7:M:170:LYS:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:SER:CB	1:A:431:PHE:H	2.16	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:HG2	7:M:322:CYS:C	2.23	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
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:193:ALA:HB1	7:M:222:GLY:C	2.24	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
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
7:M:8:LEU:HG	7:M:12:VAL:HG23	1.85	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
7:M:266:ARG:HG2	7:M:322:CYS:HG	1.67	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
7:M:204:ALA:CA	7:M:234:MET:CE	2.69	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
1:A:419:PHE:HA	1:A:420:PRO:C	2.25	0.57
1:B:419:PHE:HA	1:B:420:PRO:C	2.25	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
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
7:M:15:ARG:HH12	7:M:68:LEU:HD23	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:226:ASP:OD1	7:M:229:ARG:CB	2.51	0.57
1:C:419:PHE:HA	1:C:420:PRO:C	2.25	0.57
1:A:259:GLY:C	2:F:296:GLU:O	2.31	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
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
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
3:G:47:MET:C	3:G:49:ALA:N	2.57	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: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
3:G:47:MET:C	3:G:49:ALA:H	2.09	0.56
7:M:89:LEU:H	7:M:118:THR:HG23	1.68	0.56
7:M:169:ALA:O	7:M:170:LYS:C	2.44	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
7:M:69:VAL:HA	7:M:72:LEU:HD11	1.86	0.55
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:137:LEU:O	3:G:140:VAL:N	2.40	0.54
7:M:71:ASP:C	7:M:73:PRO:HD2	2.28	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
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: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
7:M:170:LYS:O	7:M:174:GLU:N	2.30	0.54
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
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
7:M:51:GLY:CA	7:M:56:ASP:CG	2.75	0.53
1:C:11:GLY:HA2	2:E:49:GLU:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:12:VAL:O	7:M:13:ARG:C	2.45	0.53
7:M:242:ASP:OD1	7:M:254:GLY:HA2	2.09	0.53
3:G:165:GLU:O	3:G:166:GLN:C	2.47	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
3:G:45:GLU:C	3:G:47:MET:N	2.58	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
5:K:65:LYS:HG3	6:L:42:LEU:HD11	1.91	0.52
7:M:152:ARG:HB3	7:M:156:ARG:CZ	2.40	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:145:THR:O	3:G:149:LYS:CB	2.57	0.52
7:M:107:ARG:NH1	7:M:111:GLU:OE1	2.40	0.52
3:G:42:LEU:O	3:G:45:GLU:CB	2.57	0.52
3:G:167:VAL:C	3:G:169:ILE:N	2.61	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
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
1:A:132:GLY:HA3	1:A:371:LEU:C	2.30	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
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:57:VAL:C	7:M:301:ARG:HH12	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:G:132:ARG:C	3:G:134:ALA:H	2.13	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:B:263:THR:CB	2:D:124:ARG:C	2.78	0.52
1:C:11:GLY:CA	2:E:50:VAL:H	2.14	0.52
3:G:44:ARG:C	3:G:47:MET:CB	2.72	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
7:M:61:VAL:HG21	7:M:301:ARG:HD2	1.92	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
3:G:7:THR:O	3:G:9:MET:N	2.42	0.51
7:M:52:GLN:H	7:M:56:ASP:CG	2.13	0.51
7:M:33:PHE:CG	7:M:308:TYR:CG	2.77	0.51
7:M:312:PRO:HG2	7:M:315:GLN:CB	2.41	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:D:359:SER:C	2:D:361:LEU:H	2.07	0.50
2:E:25:LYS:CB	6:J:161:THR:HG23	1.19	0.50
1:C:259:GLY:CA	2:E:296:GLU:C	2.60	0.50
6:L:12:VAL:O	6:L:14:ALA:N	2.44	0.50
7:M:211:GLY:C	7:M:235:GLU:OE1	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:MET:CB	2:D:66:LEU:HA	2.29	0.50
3:G:52:ALA:CB	3:G:52:ALA:C	2.74	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
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
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
7:M:71:ASP:C	7:M:73:PRO:CD	2.80	0.50
3:G:146:ARG:O	3:G:147:LEU:C	2.50	0.49
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
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
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
1:A:557:GLU:C	1:A:559:PHE:N	2.66	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:HA	1:C:429:SER:CB	2.43	0.49
1:C:557:GLU:C	1:C:559:PHE:N	2.66	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
1:B:557:GLU:C	1:B:559:PHE:N	2.66	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: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
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
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
3:G:198:LYS:O	3:G:199:GLY:O	2.31	0.48
7:M:92:ASP:CB	7:M:124:TRP:CH2	2.96	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:200:LYS:HA	3:G:203:ALA:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:429:SER:C	1:C:431:PHE:N	2.60	0.48
3:G:43:VAL:O	3:G:44:ARG:C	2.51	0.48
7:M:88:LEU:C	7:M:118:THR:HG23	2.31	0.48
3:G:138:ILE:C	3:G:139:ARG:O	2.45	0.48
3:G:167:VAL:C	3:G:169:ILE:H	2.18	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
1:B:429:SER:C	1:B:431:PHE:H	2.17	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
3:G:135:GLU:C	3:G:137:LEU:H	2.03	0.47
3:G:198:LYS:O	3:G:199:GLY:C	2.52	0.47
6:J:107:LEU:HD23	6:J:165:ASN:OD1	2.15	0.47
7:M:3:ASP:OD1	7:M:79:GLU:C	2.44	0.47
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
1:B:24:MET:CB	2:E:66:LEU:C	2.83	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
3:G:4:VAL:CA	3:G:5:SER:N	2.68	0.47
7:M:154:VAL:CG1	7:M:167:LEU:HD13	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:150:LEU:C	2:E:335:GLY:O	2.53	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
2:D:150:LEU:C	2:D:335:GLY:O	2.52	0.47
3:G:189:GLU:CB	3:G:189:GLU:N	2.69	0.47
7:M:204:ALA:CB	7:M:234:MET:CE	2.90	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
2:F:150:LEU:C	2:F:335:GLY:O	2.53	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
2:D:134:GLY:C	2:D:430:ARG:O	2.54	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
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
1:C:419:PHE:N	1:C:496:GLN:HA	2.31	0.46
6:L:98:PRO:C	6:L:100:TRP:H	2.20	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
4:H:77:LEU:O	4:H:78:LYS:C	2.37	0.45
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
1:B:70:PRO:O	1:B:71:LEU:C	2.55	0.45
6:J:124:ASN:OD1	6:J:148:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
1:A:11:GLY:C	2:F:50:VAL:O	2.54	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
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
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
7:M:286:VAL:O	7:M:287:LEU:C	2.54	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
7:M:259:LYS:HZ3	7:M:318:GLU:HG2	1.80	0.45
1:A:217:PRO:C	1:A:431:PHE:CB	2.84	0.45
1:B:208:GLY:O	1:B:507:CYS:CB	2.65	0.45
7:M:74:ARG:HG3	7:M:74:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:J:98:PRO:C	6:J:100:TRP:H	2.20	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:141:ALA:C	7:M:143:PRO:HD2	2.38	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
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: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:79:GLU:CD	7:M:185:GLN:HE21	2.21	0.44
7:M:147:LEU:HD13	7:M:172:PHE:HD1	1.67	0.44
1:A:296:VAL:CA	1:A:333:ALA:HB1	2.47	0.44
4:H:84:HIS:O	4:H:85:ASP:C	2.48	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
2:E:153:PHE:O	2:E:338:GLN:HA	2.18	0.44
3:G:179:ILE:O	3:G:180:GLN:C	2.55	0.44
6:J:171:MET:O	6:J:174:ALA:HB3	2.17	0.44
7:M:12:VAL:C	7:M:14:VAL:N	2.72	0.44
1:A:56:SER:CB	2:F:30:GLY:H	2.29	0.43
2:E:349:TYR:HA	2:E:350:PRO:C	2.39	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
7:M:141:ALA:O	7:M:142:VAL:C	2.55	0.43
7:M:252:LEU:O	7:M:253:SER:C	2.55	0.43
7:M:283:VAL:HG22	7:M:286:VAL:CG1	2.46	0.43
7:M:138:GLN:O	7:M:142:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:O	1:A:184:TYR:HA	2.19	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: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
3:G:194:LEU:C	3:G:194:LEU:CB	2.73	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
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
2:D:349:TYR:HA	2:D:350:PRO:C	2.38	0.43
2:F:360:ARG:C	2:F:362:MET:N	2.38	0.43
3:G:175:GLN:O	3:G:177:ARG:N	2.51	0.43
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
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
2:F:349:TYR:HA	2:F:350:PRO:C	2.38	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
1:C:259:GLY:HA2	2:E:296:GLU:C	2.22	0.42
6:J:101:PRO:HA	6:J:104:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:12:PRO:N	2:E:49:GLU:CB	2.83	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
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:88:LEU:HD13	7:M:117:GLY:C	2.39	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
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: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
3:G:177:ARG:C	3:G:179:ILE:N	2.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:LYS:C	3:G:149:LYS:O	2.59	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
7:M:283:VAL:O	7:M:284:GLY:C	2.59	0.41
3:G:146:ARG:O	3:G:149:LYS:CB	2.69	0.41
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
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:4:VAL:C	3:G:6:PRO:N	2.71	0.41
3:G:43:VAL:O	3:G:45:GLU:N	2.54	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
7:M:57:VAL:HG11	7:M:301:ARG:HG2	2.03	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
2:D:334:GLU:C	2:D:361:LEU:CB	2.88	0.41
7:M:170:LYS:O	7:M:174:GLU:HB2	2.21	0.41
7:M:263:ARG:HG3	7:M:321:VAL:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	4	29
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	4	26
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	4	27
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	7	38
2	E	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	7	38
2	F	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	6	35
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	7	38
5	I	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	98/104 (94%)	90 (92%)	6 (6%)	2 (2%)	7	38
6	J	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	2	19
6	L	180/188 (96%)	156 (87%)	14 (8%)	10 (6%)	2	19
7	M	318/323 (98%)	281 (88%)	32 (10%)	5 (2%)	9	44
All	All	4110/4402 (93%)	3678 (90%)	293 (7%)	139 (3%)	6	26

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

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Mol	Chain	Res	Type
1	C	395	VAL
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

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Mol	Chain	Res	Type
1	C	255	CYS
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

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Mol	Chain	Res	Type
6	J	13	GLU
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	62/76 (82%)	59 (95%)	3 (5%)	25	51
5	K	62/76 (82%)	59 (95%)	3 (5%)	25	51
6	J	108/141 (77%)	94 (87%)	14 (13%)	4	18
6	L	108/141 (77%)	94 (87%)	14 (13%)	4	18
7	M	254/256 (99%)	246 (97%)	8 (3%)	40	62
All	All	594/690 (86%)	552 (93%)	42 (7%)	18	39

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	54	GLU
5	I	69	LEU
5	I	119	LEU
6	J	16	ILE
6	J	28	GLU
6	J	33	GLU
6	J	66	LEU
6	J	88	ARG
6	J	99	GLU
6	J	112	LEU
6	J	132	GLU
6	J	140	VAL
6	J	142	LEU
6	J	149	ARG
6	J	165	ASN
6	J	168	LEU
6	J	184	GLN
5	K	54	GLU
5	K	69	LEU
5	K	119	LEU
6	L	16	ILE
6	L	28	GLU
6	L	33	GLU
6	L	66	LEU
6	L	88	ARG
6	L	99	GLU
6	L	112	LEU
6	L	132	GLU
6	L	140	VAL
6	L	142	LEU
6	L	149	ARG
6	L	165	ASN
6	L	168	LEU
6	L	184	GLN
7	M	3	ASP
7	M	4	ASP
7	M	26	GLN
7	M	62	LEU
7	M	65	GLN
7	M	74	ARG
7	M	76	VAL
7	M	90	ARG

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 monosaccharides 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	A	600	-	24,29,29	1.09	2 (8%)	29,45,45	0.88	0
8	ADP	C	600	-	24,29,29	1.00	2 (8%)	29,45,45	1.07	4 (13%)

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	A	600	-	-	2/12/32/32	0/3/3/3
8	ADP	C	600	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ADP	O4'-C1'	2.60	1.44	1.41
8	C	600	ADP	PB-O2B	-2.44	1.45	1.54
8	A	600	ADP	PB-O2B	-2.35	1.45	1.54
8	C	600	ADP	PA-O1A	-2.32	1.42	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	600	ADP	O3B-PB-O2B	2.38	116.74	107.64
8	C	600	ADP	C5-C6-N6	2.37	123.95	120.35
8	C	600	ADP	O5'-PA-O1A	2.05	117.09	109.07
8	C	600	ADP	O4'-C4'-C3'	-2.05	101.06	105.11

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.

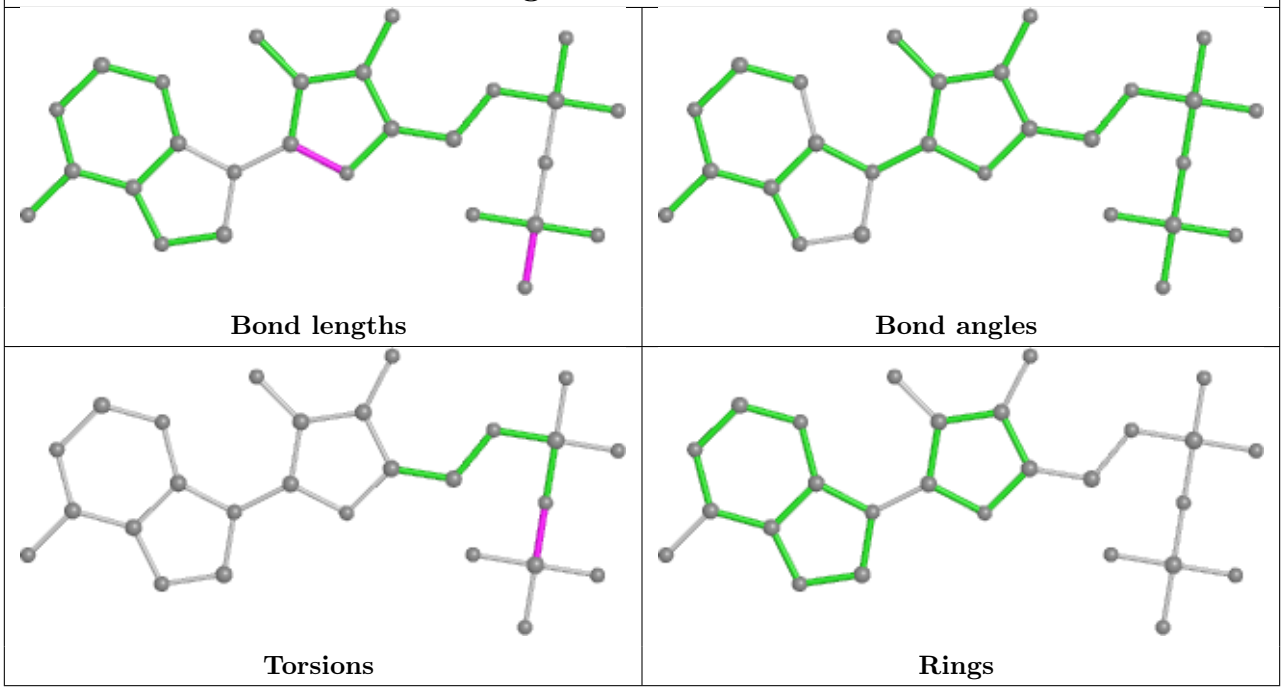
1 monomer is involved in 4 short contacts:

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

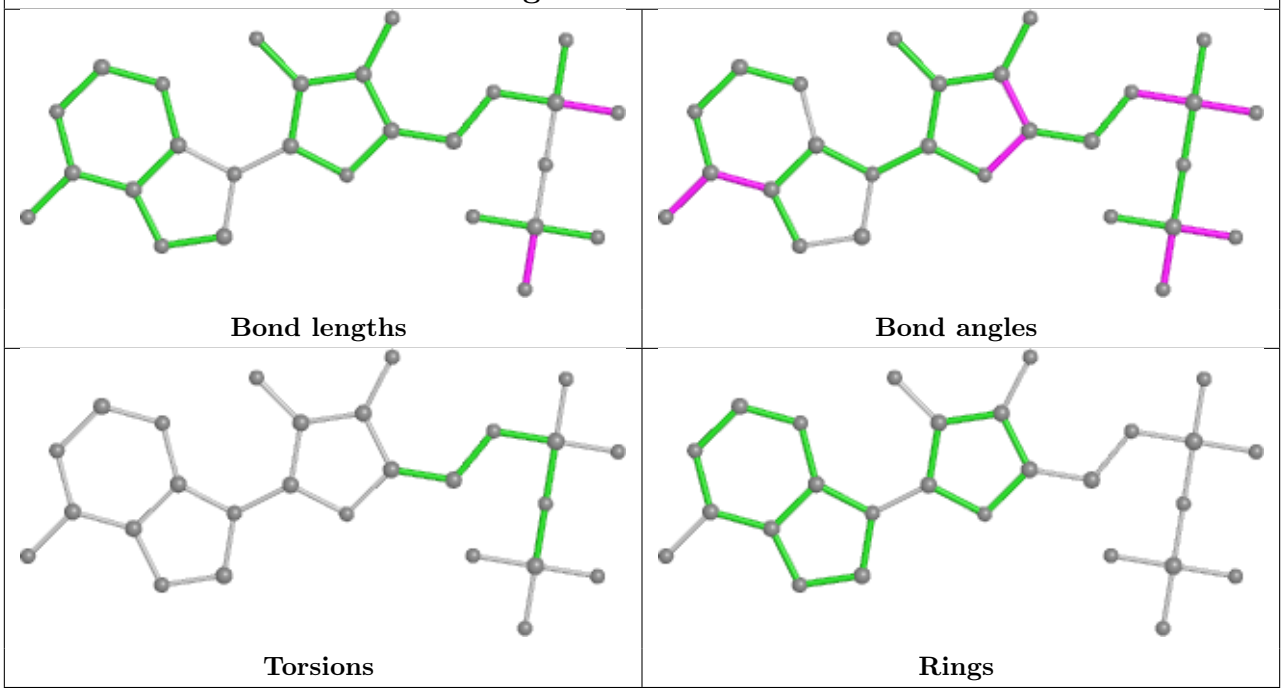
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ADP A 600



Ligand ADP C 600



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.

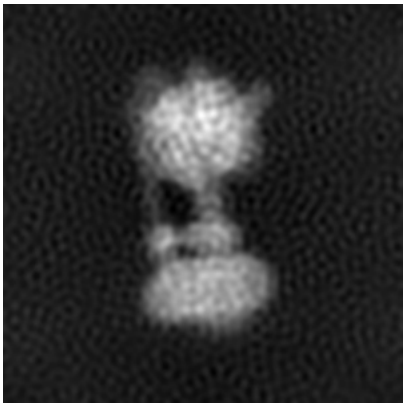
6 Map visualisation (i)

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.

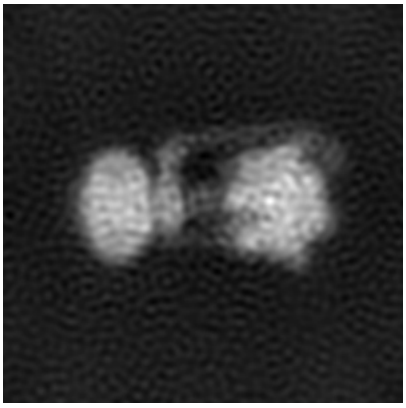
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

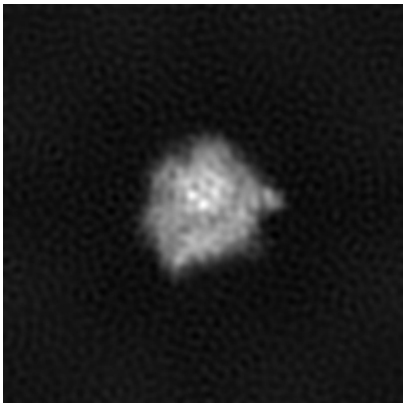
6.1.1 Primary map



X



Y

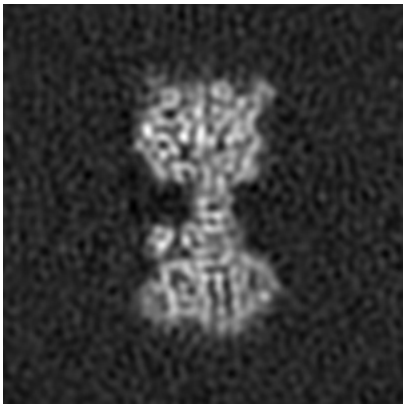


Z

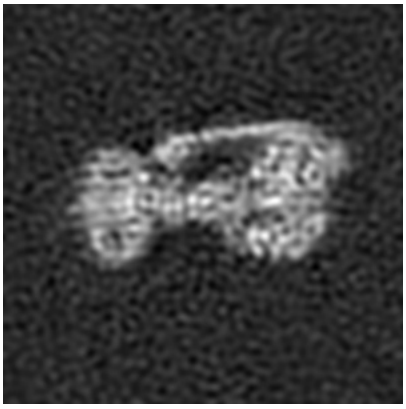
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

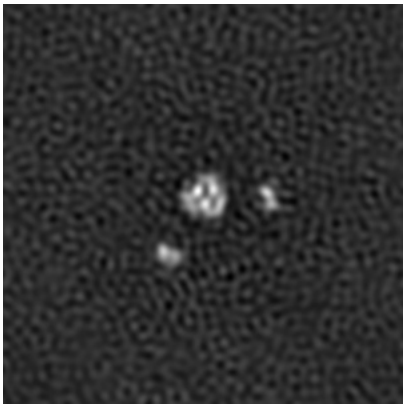
6.2.1 Primary map



X Index: 128



Y Index: 128

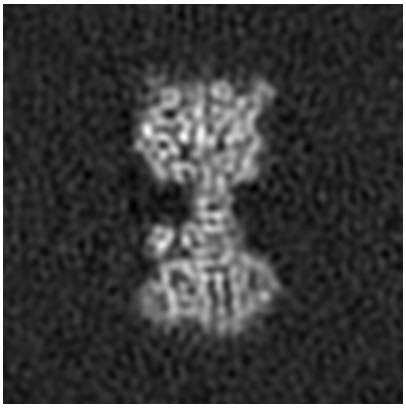


Z Index: 128

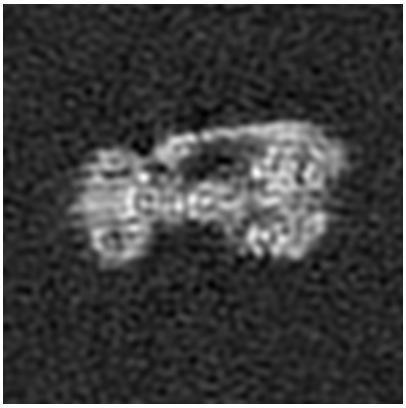
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

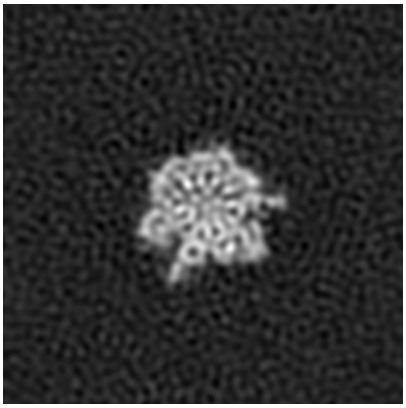
6.3.1 Primary map



X Index: 128



Y Index: 129



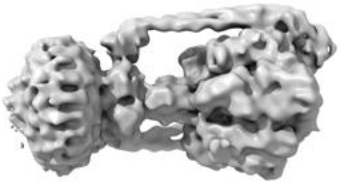
Z Index: 181

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

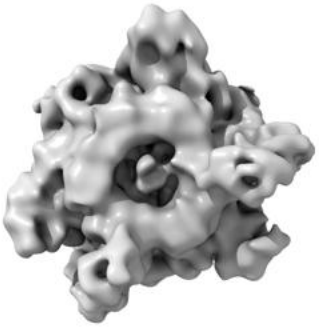
6.4 Orthogonal surface views (i)

6.4.1 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.

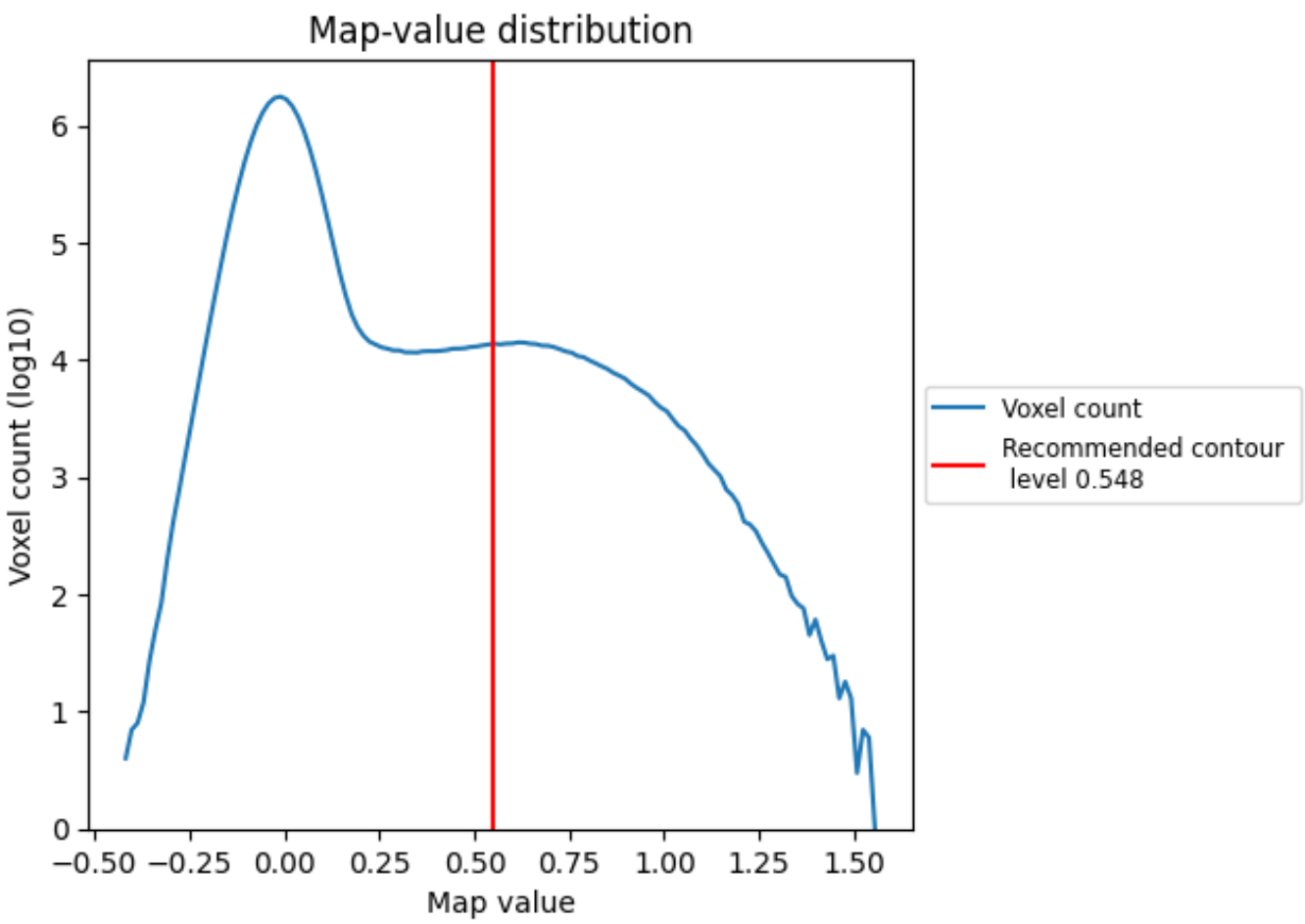
6.5 Mask visualisation (i)

This section was not generated.

7 Map analysis (i)

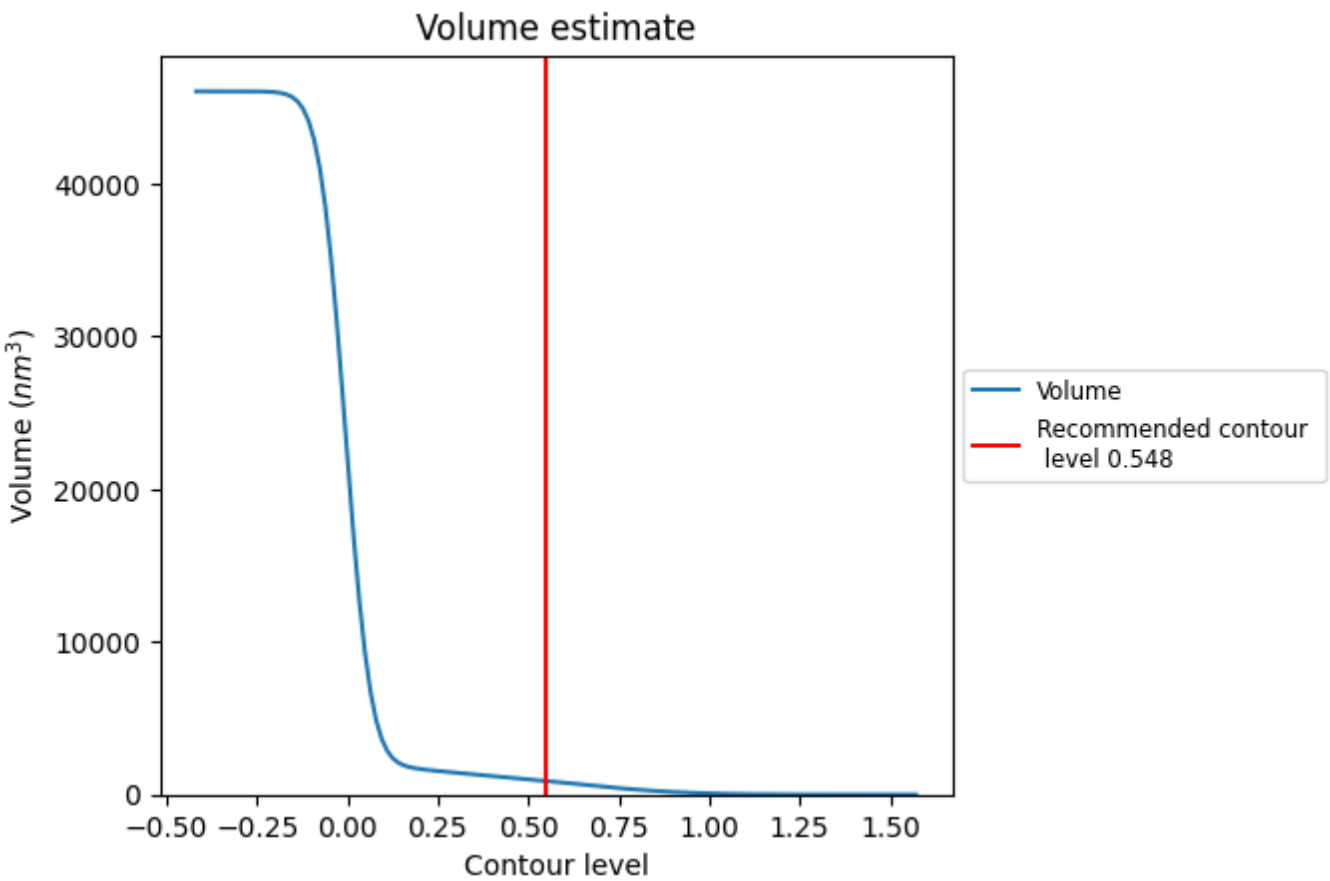
This section contains the results of statistical analysis of the map.

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.

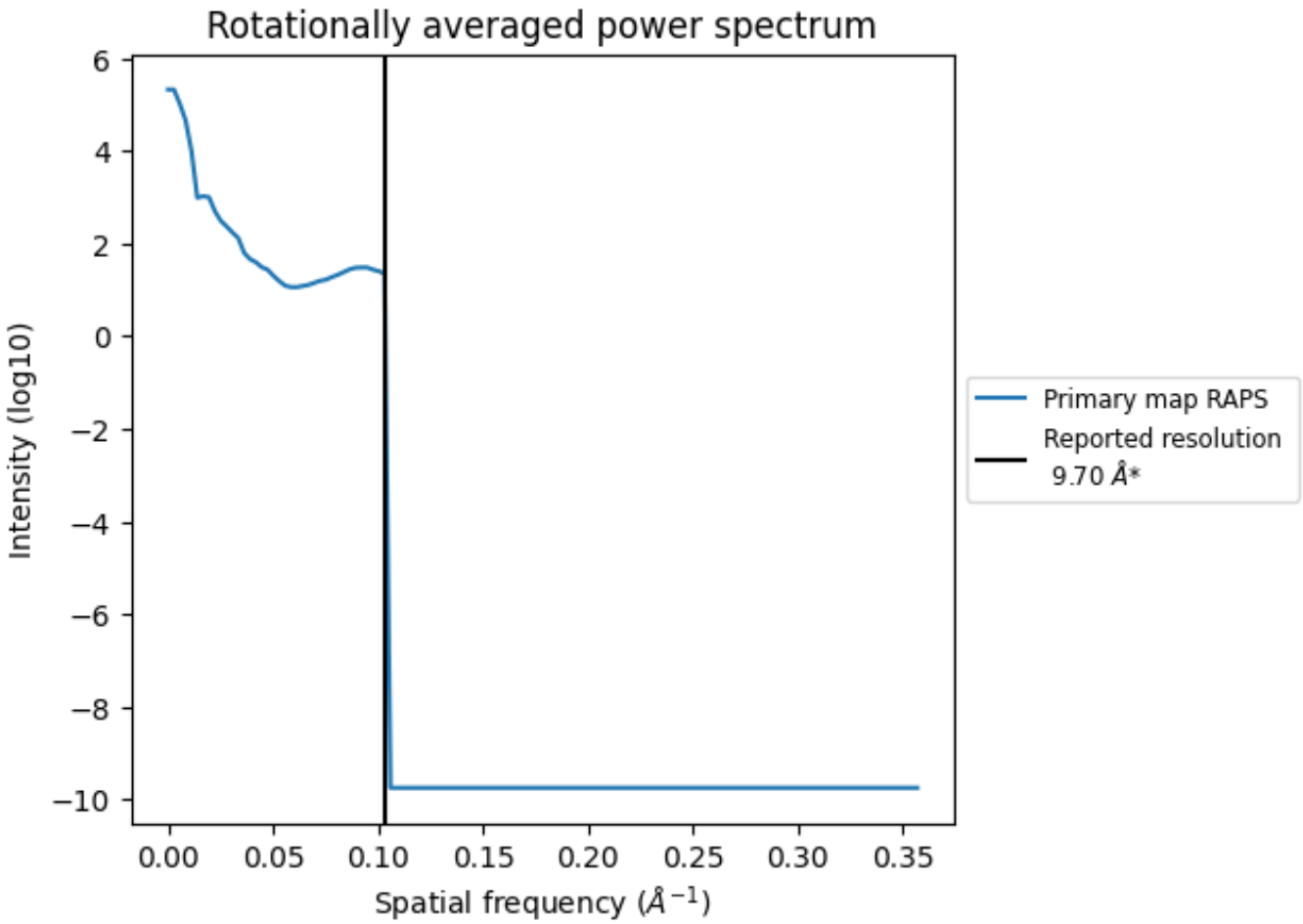
7.2 Volume estimate (i)



The volume at the recommended contour level is 897 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.103 Å^{-1}

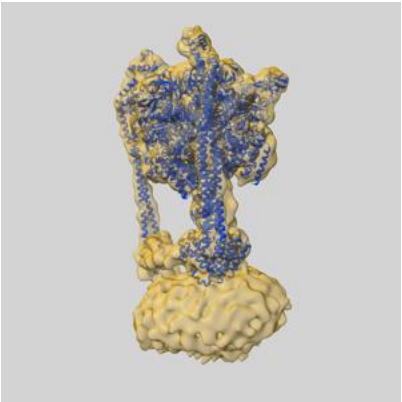
8 Fourier-Shell correlation (i)

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

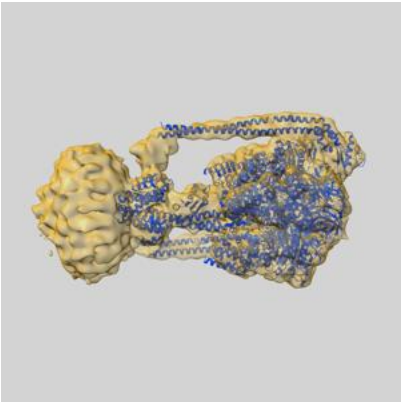
9 Map-model fit (i)

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.

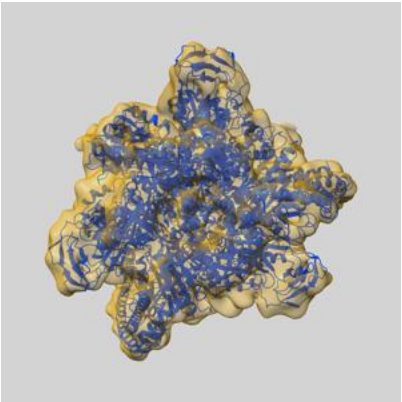
9.1 Map-model overlay (i)



X



Y



Z

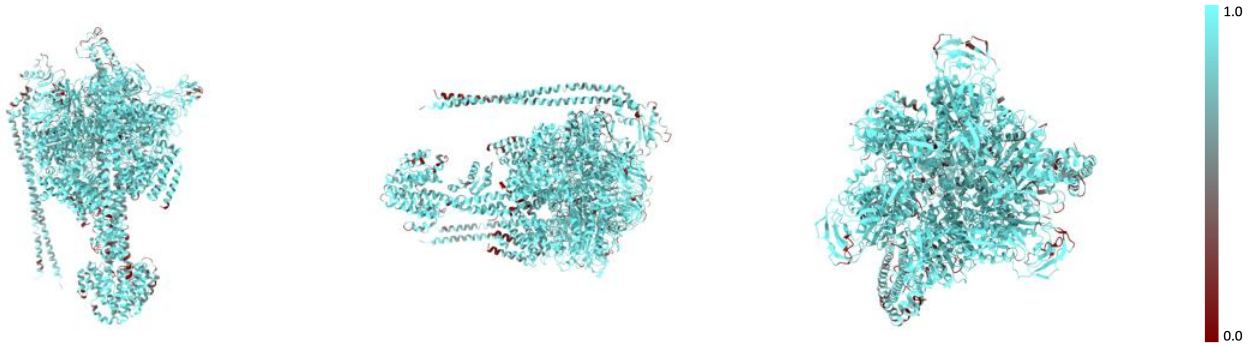
The images above show the 3D surface view of the map at the recommended contour level 0.548 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

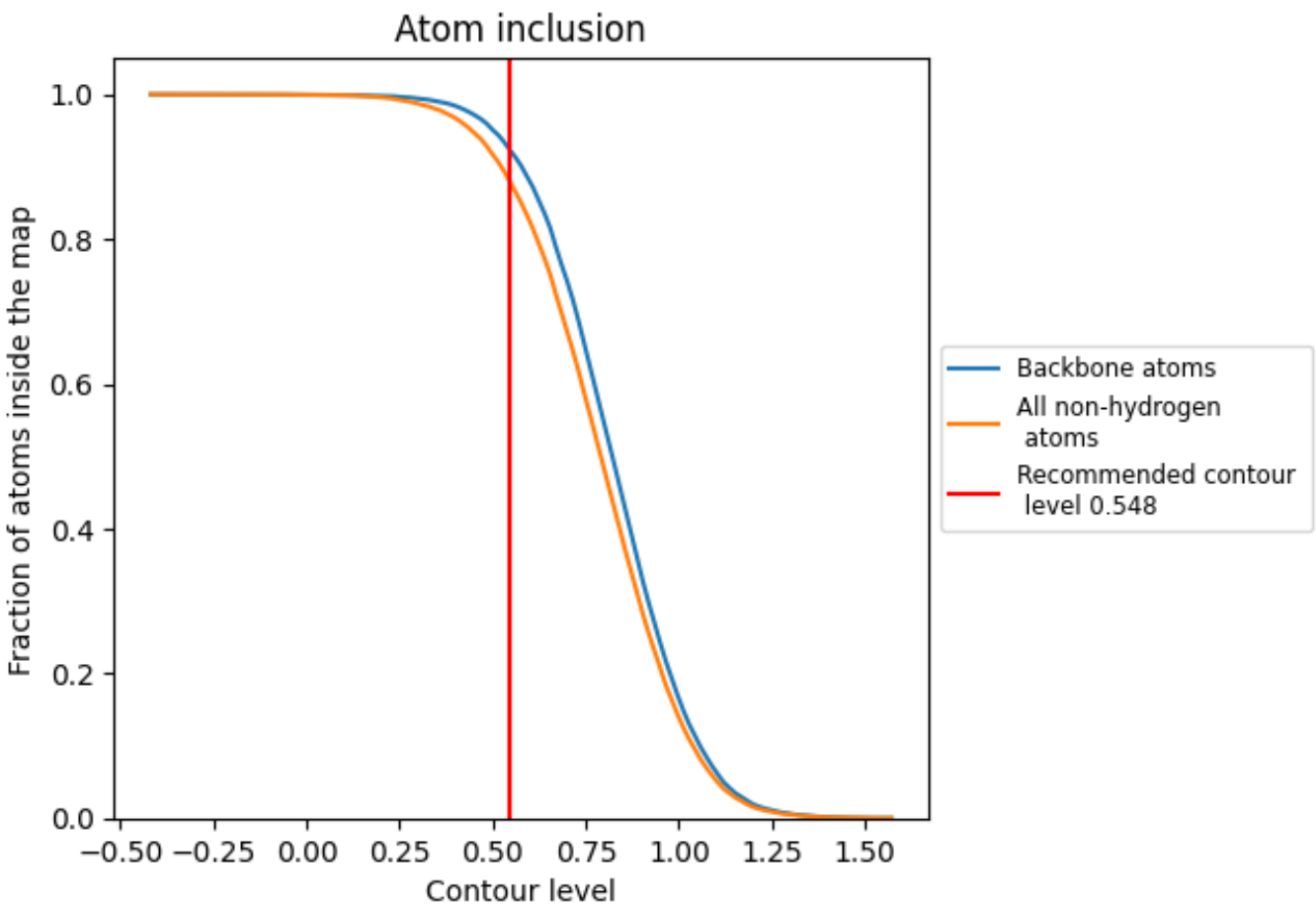
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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	0.8776	0.1440
A	0.9291	0.1400
B	0.8823	0.1230
C	0.9208	0.1560
D	0.9213	0.1460
E	0.9322	0.1560
F	0.9222	0.1460
G	0.9531	0.2040
H	0.7859	0.1280
I	0.7139	0.1430
J	0.7766	0.1530
K	0.7607	0.1440
L	0.7344	0.1470
M	0.8456	0.1260