



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 8JXM / pdb_00008jxm
EMDB ID : EMD-36705
Title : Human 3-methylcrotonyl-CoA carboxylase in BCCP-H2 state with MCoA
Authors : Liu, D.S.; Su, J.Y.; Tian, X.Y.
Deposited on : 2023-06-30
Resolution : 3.49 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

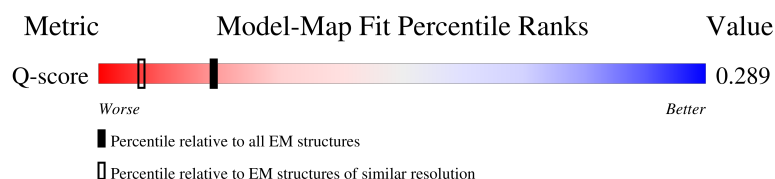
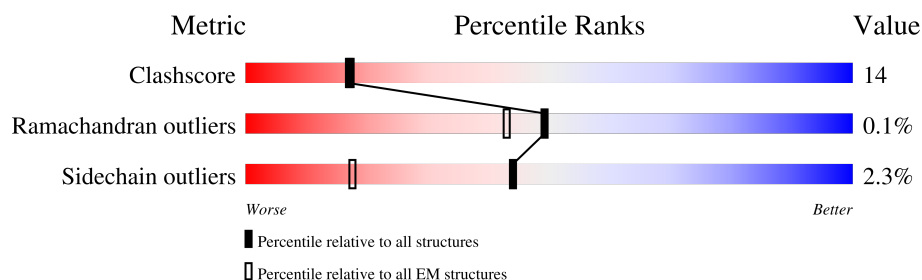
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 (2.99 - 3.99)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	563	
1	C	563	
1	E	563	
1	H	563	

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Mol	Chain	Length	Quality of chain
1	J	563	
1	K	563	
2	B	725	
2	F	725	
2	G	725	
2	I	725	
2	L	725	
2	M	725	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTI	C	601	-	-	X	-
4	BTI	H	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51993 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.

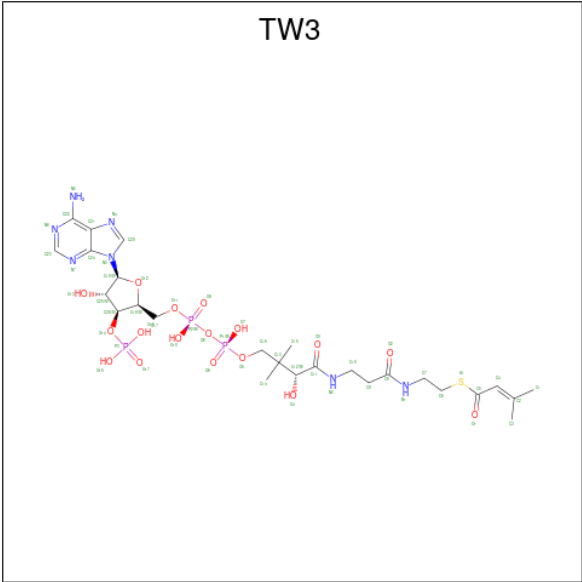
- Molecule 1 is a protein called Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		
1	A	541	Total	C	N	O	S	0	0
			4154	2633	726	776	19		
1	C	520	Total	C	N	O	S	0	0
			4006	2538	704	745	19		
1	H	520	Total	C	N	O	S	0	0
			4006	2538	704	745	19		
1	E	524	Total	C	N	O	S	0	0
			4038	2562	708	749	19		
1	J	522	Total	C	N	O	S	0	0
			4025	2553	706	747	19		

- Molecule 2 is a protein called Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial.

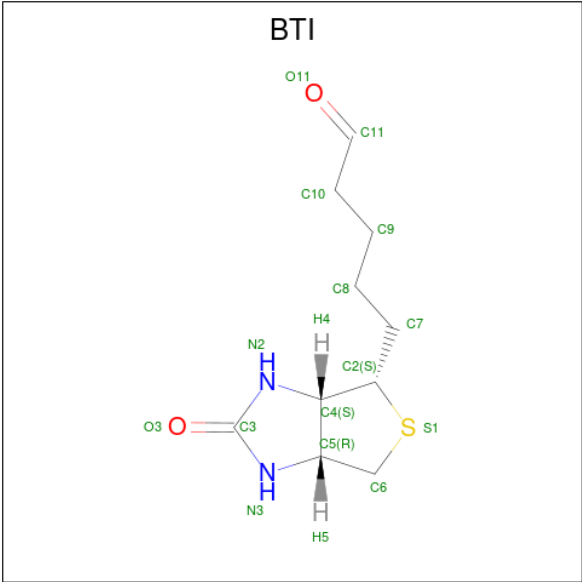
Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	541	Total	C	N	O	S	0	0
			4192	2646	730	790	26		
2	B	541	Total	C	N	O	S	0	0
			4192	2646	730	790	26		
2	F	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		
2	G	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		
2	I	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		
2	M	607	Total	C	N	O	S	0	0
			4703	2961	821	892	29		

- Molecule 3 is {S}-[2-[3-[[[2 {R}]-4-[[[2 {S},3 {S},4 {S},5 {S}]-5-(6-aminopurin-9-yl)-4-oxidan-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] 3-methylbut-2-enethioate (CCD ID: TW3) (formula: C₂₆H₄₂N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	K	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	A	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	C	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	H	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	E	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	
3	J	1	Total	C	N	O	P	S	0
			54	26	7	17	3	1	

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).

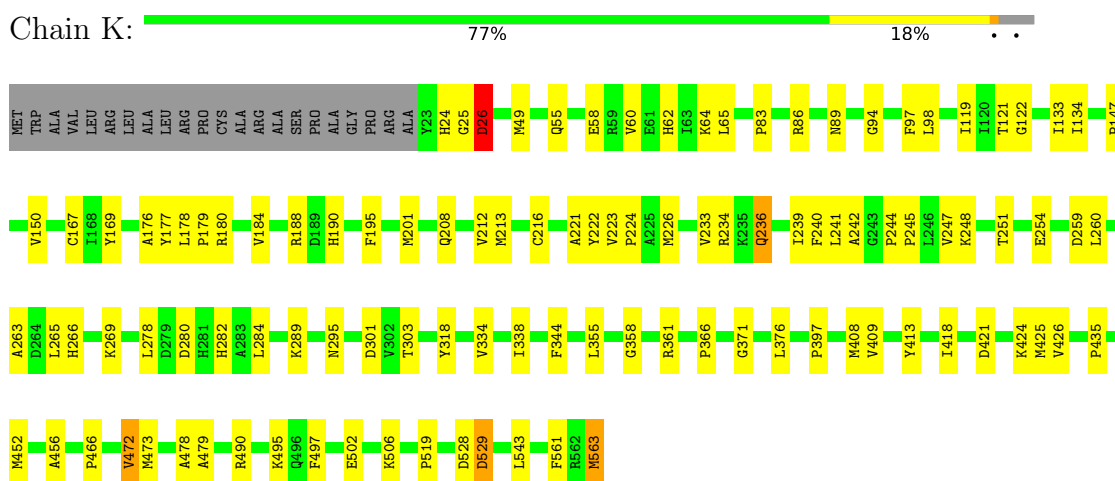


Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	F	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	G	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	H	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	I	1	Total	C	N	O	S	0
			15	10	2	2	1	
4	M	1	Total	C	N	O	S	0
			15	10	2	2	1	

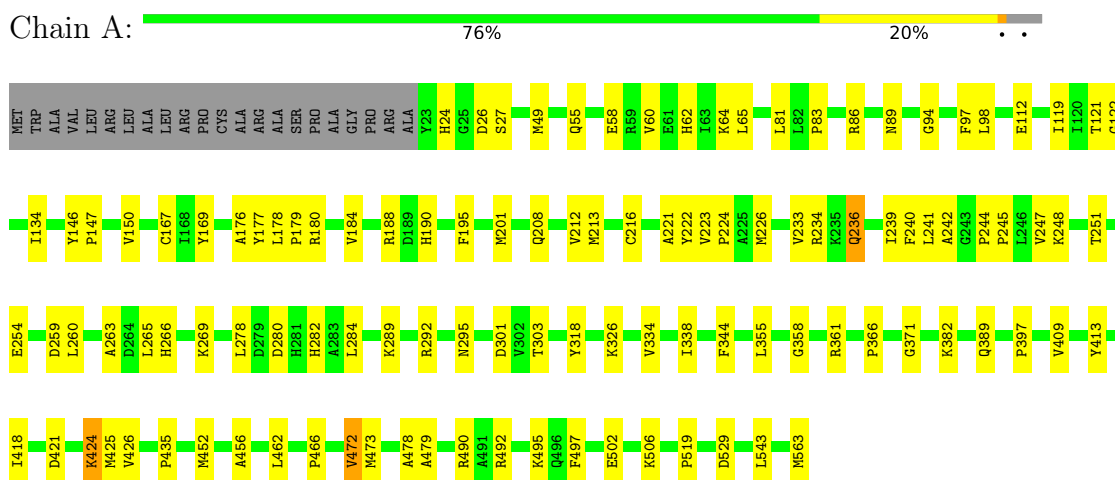
3 Residue-property plots

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

- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial



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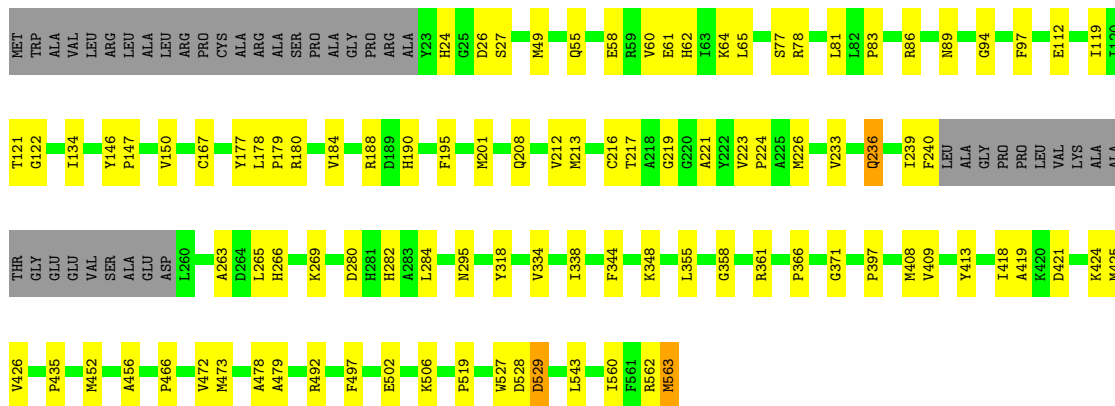
- Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial





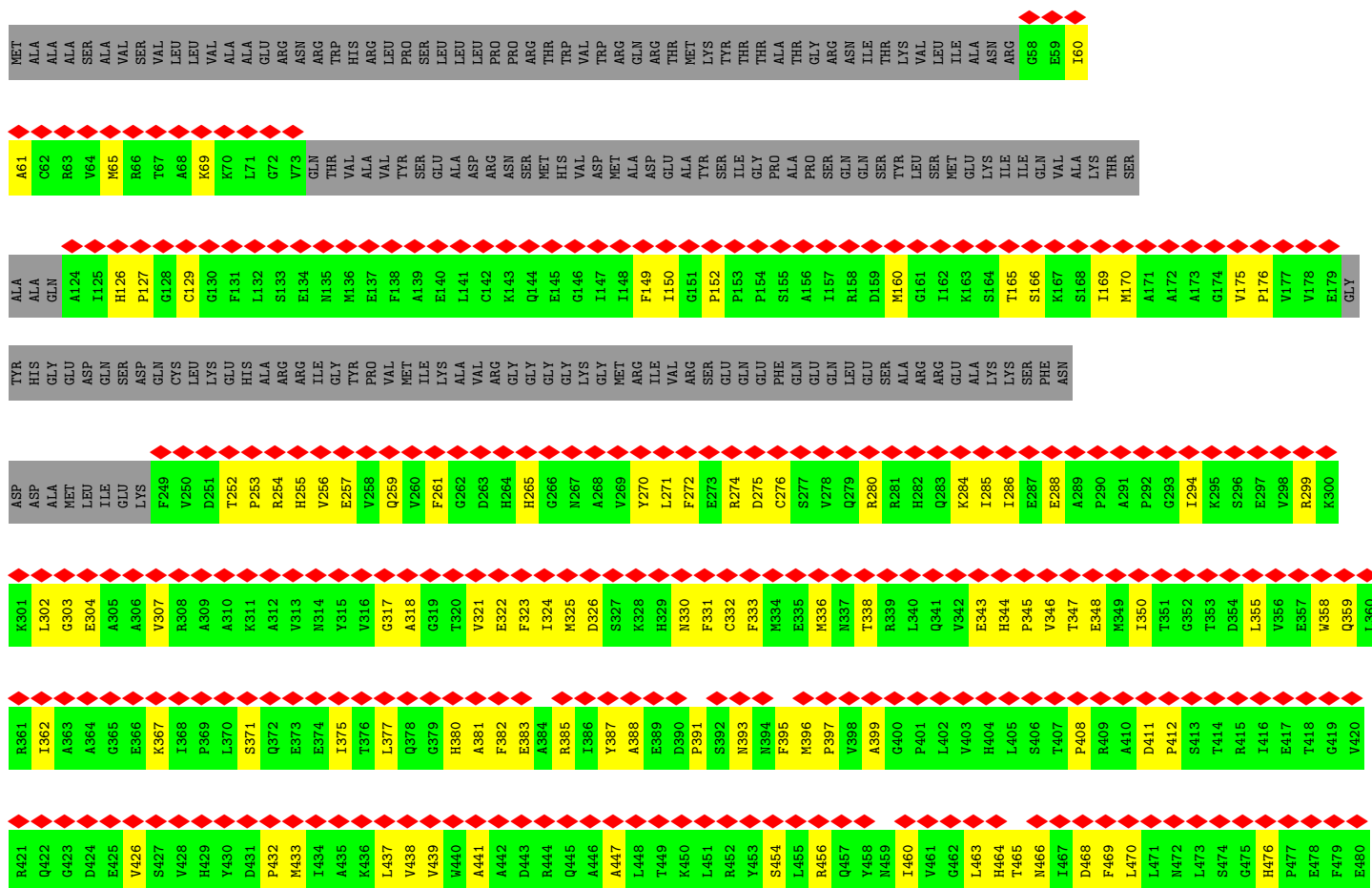
• Molecule 1: Methylcrotonoyl-CoA carboxylase beta chain, mitochondrial

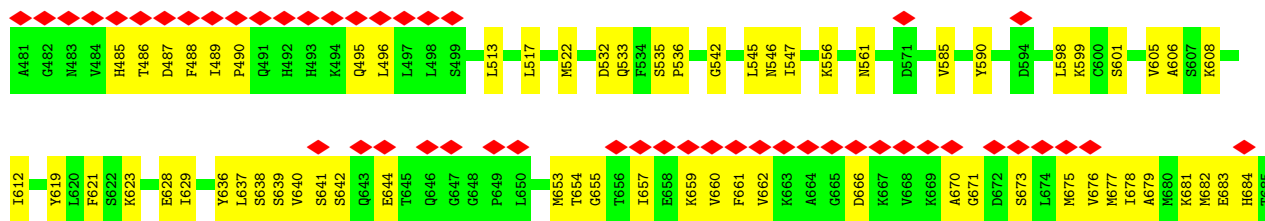
Chain J: 75% 17% 7%



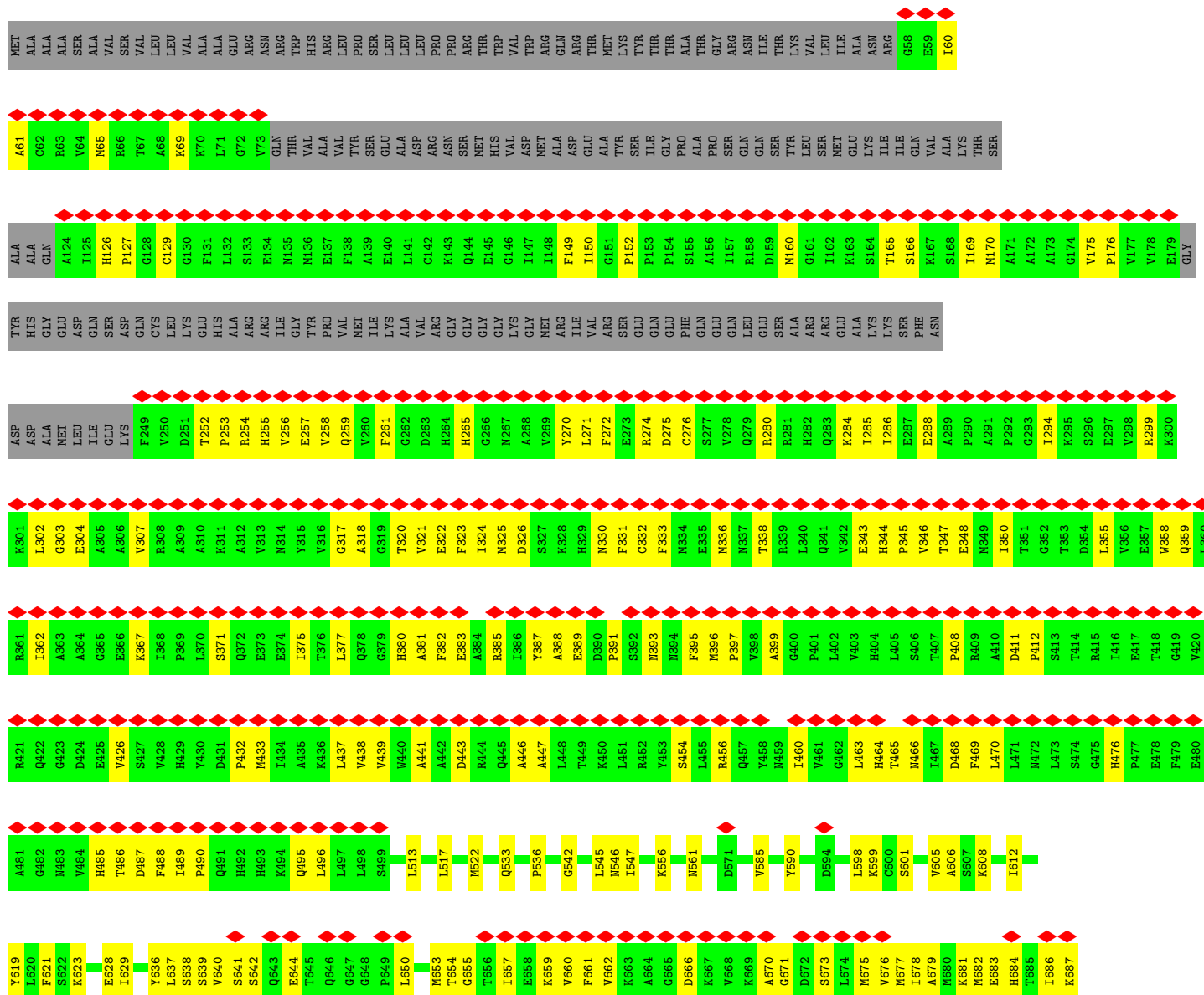
• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

Chain L: 52% 49% 26% 25%



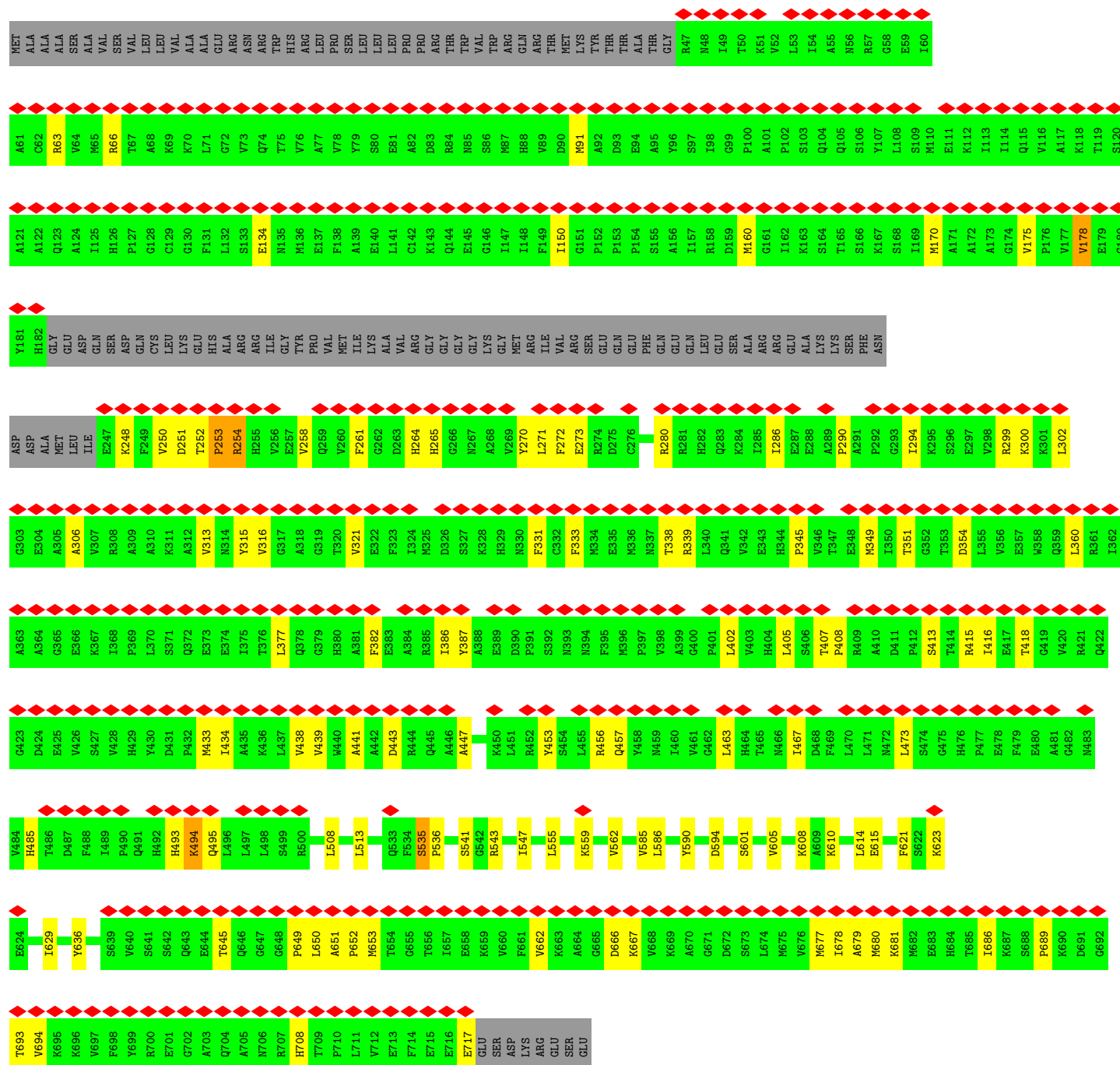


• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial



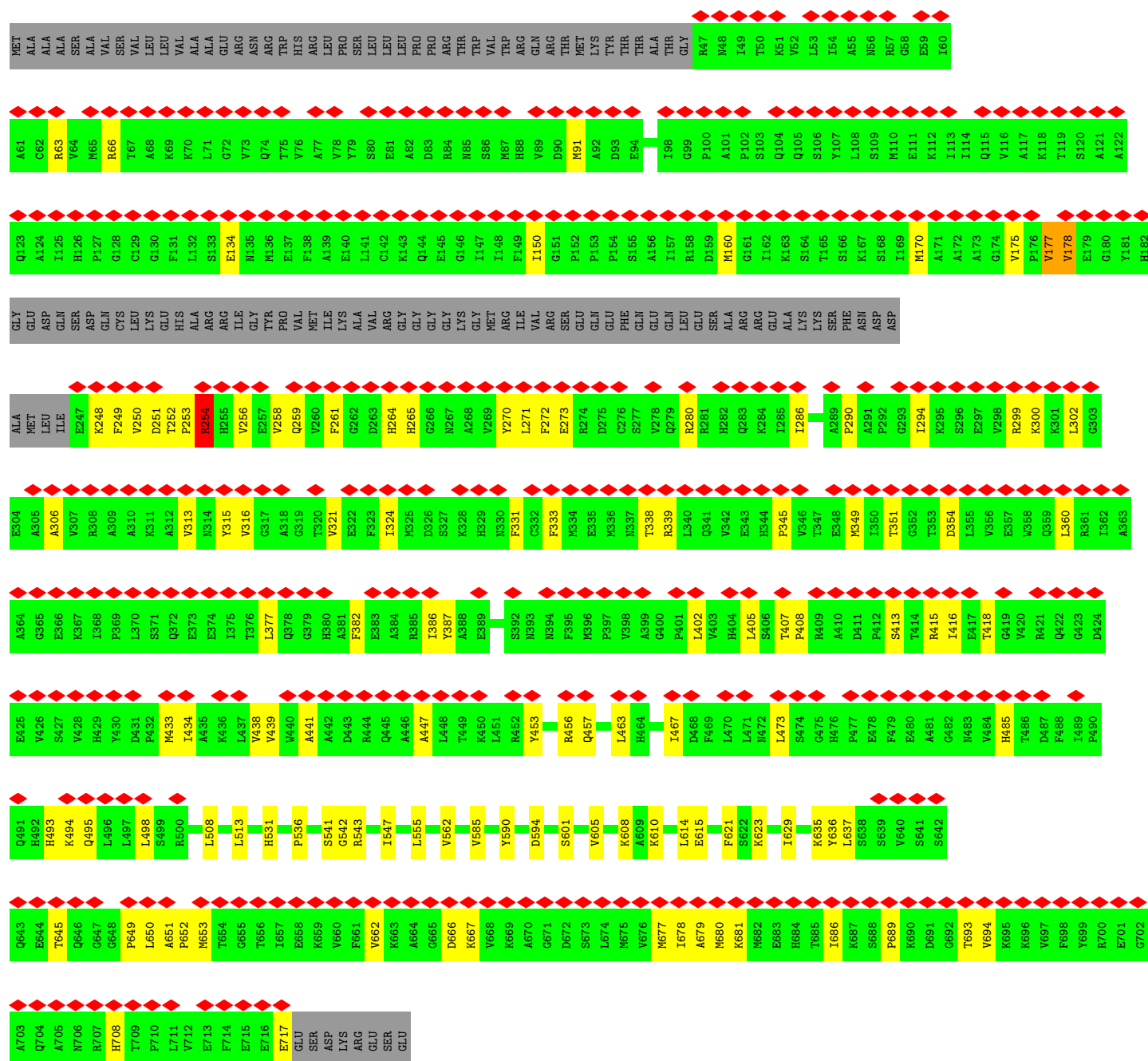


• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial

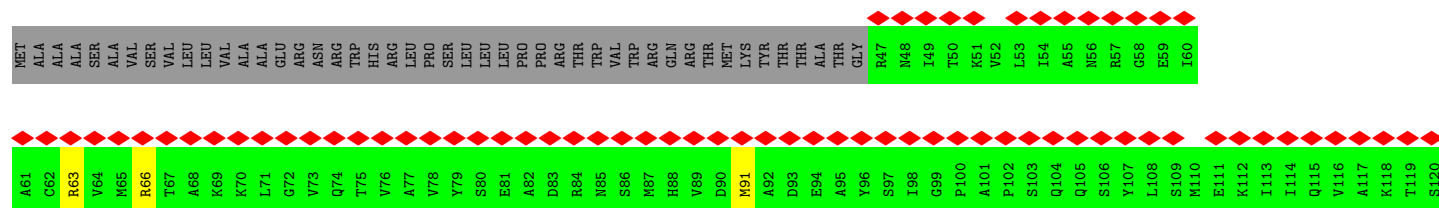


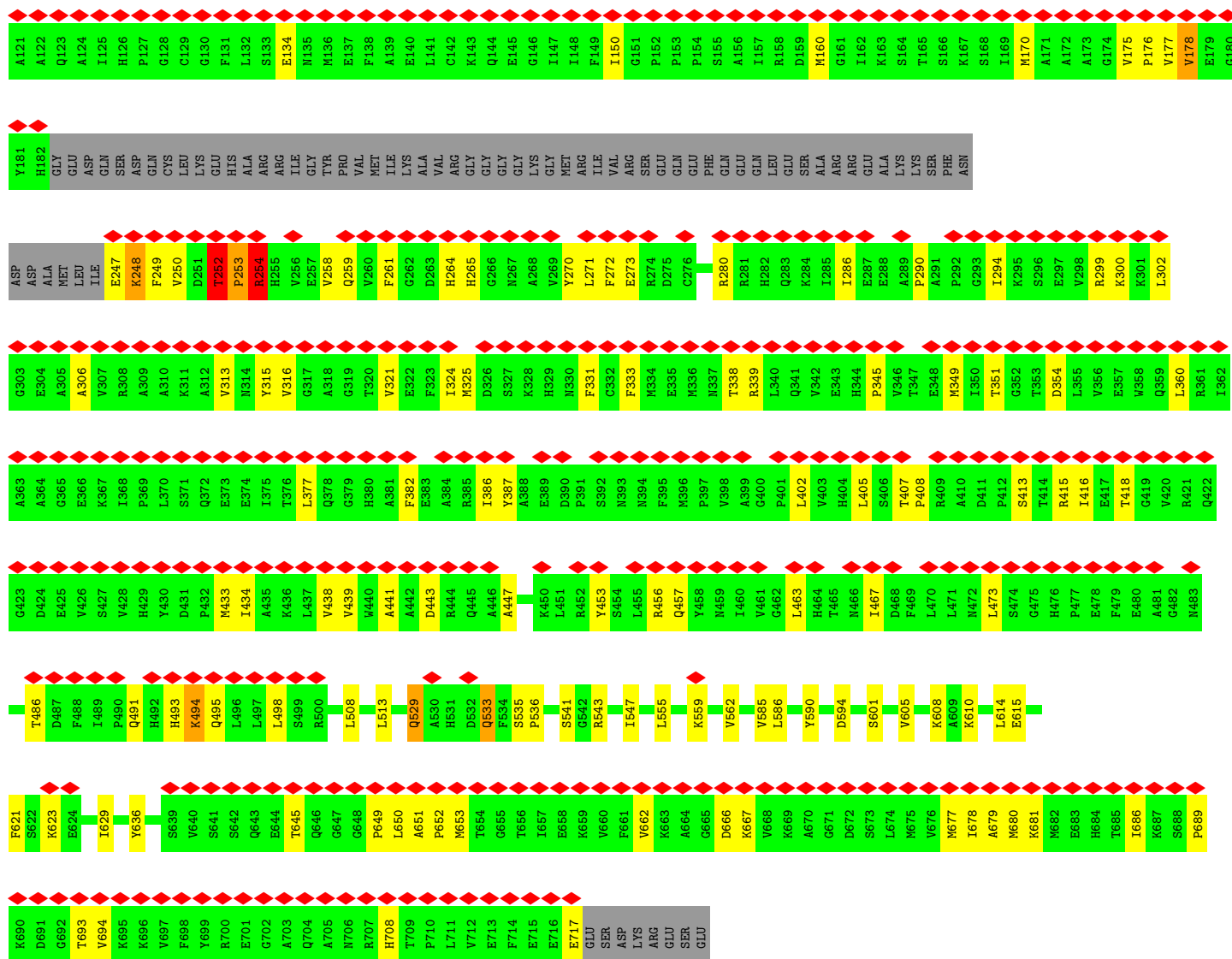
• Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial



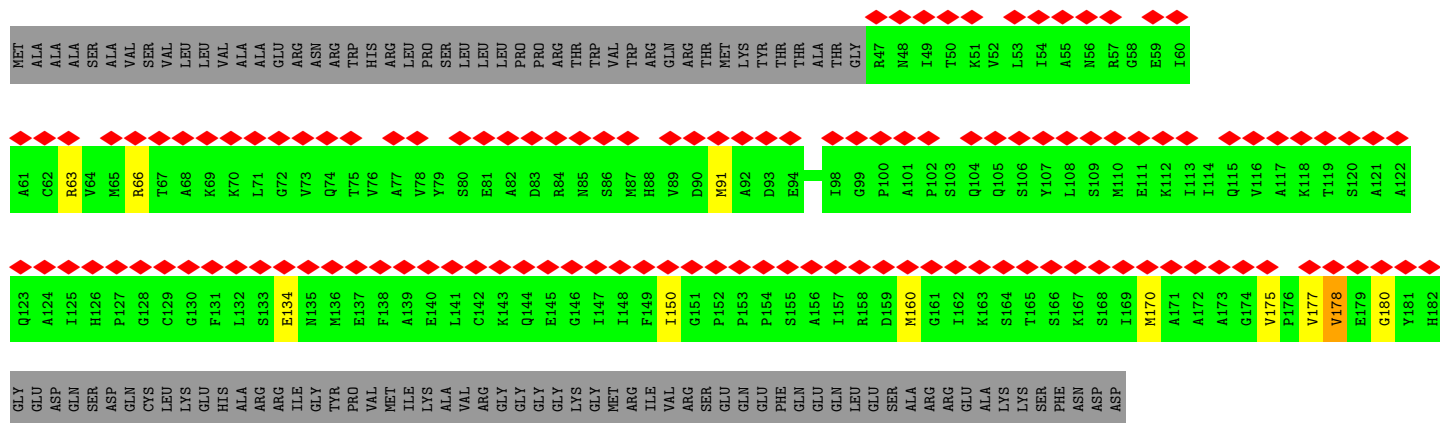


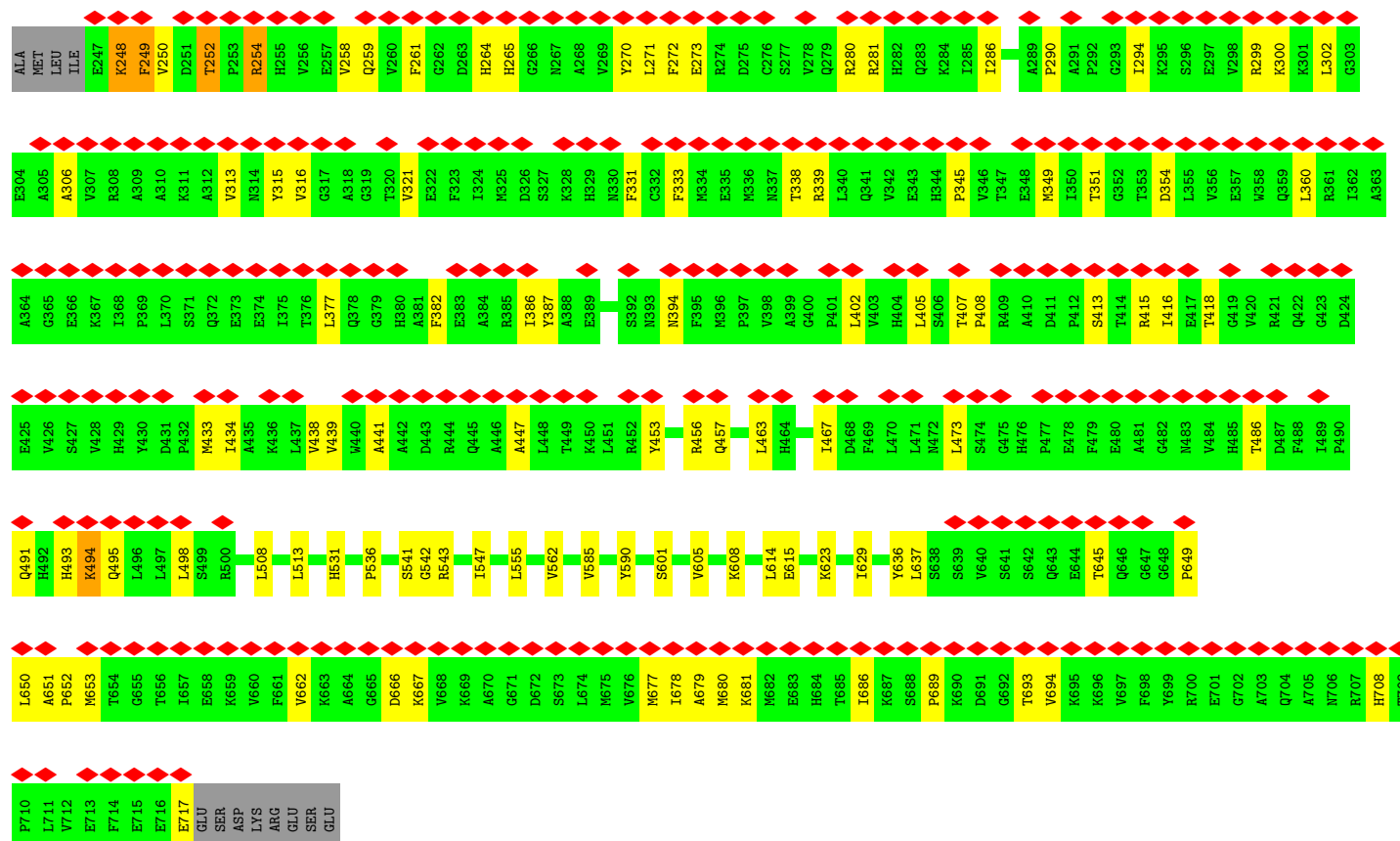
● Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial





● Molecule 2: Methylcrotonoyl-CoA carboxylase subunit alpha, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.782	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.09	Depositor
Map size ($\text{\AA}$)	349.2, 349.2, 349.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.97, 0.97, 0.97	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TW3, BTI

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	0.39	1/4239 (0.0%)	0.54	0/5731
1	C	0.51	1/4087 (0.0%)	0.74	7/5521 (0.1%)
1	E	0.40	1/4120 (0.0%)	0.55	0/5566
1	H	0.51	1/4087 (0.0%)	0.74	8/5521 (0.1%)
1	J	0.38	1/4107 (0.0%)	0.55	0/5548
1	K	0.38	1/4239 (0.0%)	0.54	0/5731
2	B	0.15	1/4273 (0.0%)	0.22	0/5771
2	F	0.75	0/4793	1.08	6/6476 (0.1%)
2	G	0.74	0/4793	1.08	5/6476 (0.1%)
2	I	0.75	0/4793	1.08	8/6476 (0.1%)
2	L	0.15	1/4273 (0.0%)	0.22	0/5771
2	M	0.75	0/4793	1.07	4/6476 (0.1%)
All	All	0.54	8/52597 (0.0%)	0.78	38/71064 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	PRO	N-CD	5.33	1.55	1.47
1	K	435	PRO	N-CD	5.32	1.55	1.47
1	H	435	PRO	N-CD	5.29	1.55	1.47
1	C	435	PRO	N-CD	5.28	1.55	1.47
1	E	435	PRO	N-CD	5.28	1.55	1.47
1	J	435	PRO	N-CD	5.28	1.55	1.47
2	L	689	PRO	N-CD	5.11	1.54	1.47
2	B	689	PRO	N-CD	5.05	1.54	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	254	ARG	N-CA-C	7.48	120.54	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	250	VAL	N-CA-C	6.83	117.58	110.62
2	I	535	SER	CA-C-N	-6.10	113.33	119.56
2	I	535	SER	C-N-CA	-6.10	113.33	119.56
2	G	652	PRO	N-CA-C	-6.03	105.14	113.53
2	F	652	PRO	N-CA-C	-6.02	105.16	113.53
1	H	186	PRO	N-CA-C	6.00	121.44	113.40
2	I	652	PRO	N-CA-C	-5.99	105.20	113.53
2	M	652	PRO	N-CA-C	-5.99	105.21	113.53
1	C	186	PRO	N-CA-C	5.97	121.40	113.40
2	F	254	ARG	N-CA-C	5.81	119.52	110.17
2	G	177	VAL	N-CA-C	5.78	118.75	113.20
2	F	253	PRO	N-CA-C	5.77	123.40	114.98
2	M	177	VAL	N-CA-C	5.67	118.44	112.83
2	I	253	PRO	N-CA-C	5.65	120.46	111.26
2	I	177	VAL	N-CA-C	5.61	118.38	112.83
2	I	252	THR	N-CA-C	5.60	121.12	113.16
1	C	220	GLY	N-CA-C	-5.58	106.37	115.46
1	H	220	GLY	N-CA-C	-5.56	106.39	115.46
1	C	366	PRO	CA-C-O	-5.52	115.16	121.56
1	C	525	ARG	N-CA-C	-5.51	103.42	110.53
1	H	525	ARG	N-CA-C	-5.51	103.42	110.53
2	F	535	SER	CA-C-N	-5.50	113.95	119.56
2	F	535	SER	C-N-CA	-5.50	113.95	119.56
1	H	425	MET	N-CA-C	-5.43	105.28	111.14
1	H	366	PRO	CA-C-O	-5.39	115.19	121.34
2	I	178	VAL	N-CA-C	5.33	117.30	109.63
2	M	178	VAL	N-CA-C	5.28	117.23	109.63
1	C	212	VAL	CA-C-O	-5.28	118.04	122.63
2	M	531	HIS	N-CA-C	-5.27	106.11	112.54
1	H	212	VAL	CA-C-O	-5.23	118.08	122.63
1	H	189	ASP	N-CA-C	-5.20	107.46	112.97
1	C	189	ASP	N-CA-C	-5.20	107.46	112.97
2	G	531	HIS	N-CA-C	-5.17	105.82	111.82
1	H	524	ALA	N-CA-C	-5.11	105.71	111.28
1	C	524	ALA	N-CA-C	-5.10	105.72	111.28
2	F	178	VAL	N-CA-C	5.05	116.91	109.63
2	G	178	VAL	N-CA-C	5.05	116.74	109.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4154	0	4130	147	0
1	C	4006	0	3982	136	0
1	E	4038	0	4018	123	0
1	H	4006	0	3982	143	0
1	J	4025	0	4002	129	0
1	K	4154	0	4130	140	0
2	B	4192	0	4199	225	0
2	F	4703	0	4703	93	0
2	G	4703	0	4703	95	0
2	I	4703	0	4703	101	0
2	L	4192	0	4199	227	0
2	M	4703	0	4703	97	0
3	A	54	0	0	2	0
3	C	54	0	0	7	0
3	E	54	0	0	3	0
3	H	54	0	0	6	0
3	J	54	0	0	4	0
3	K	54	0	0	2	0
4	C	15	0	16	7	0
4	F	15	0	15	3	0
4	G	15	0	15	3	0
4	H	15	0	16	9	0
4	I	15	0	15	3	0
4	M	15	0	15	3	0
All	All	51993	0	51546	1431	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 14.

All (1431) 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)
1:A:278:LEU:HD11	2:B:641:SER:CB	1.30	1.61
1:K:278:LEU:HD11	2:L:641:SER:CB	1.30	1.56
2:F:681:LYS:NZ	4:F:801:BTI:C11	1.71	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:681:LYS:NZ	4:M:801:BTI:C11	1.71	1.53
2:G:681:LYS:NZ	4:G:801:BTI:C11	1.71	1.52
1:A:278:LEU:CD1	2:B:641:SER:HB3	1.38	1.52
1:K:278:LEU:CD1	2:L:641:SER:HB3	1.38	1.49
2:I:681:LYS:NZ	4:I:801:BTI:C11	1.71	1.47
2:B:681:LYS:NZ	4:C:601:BTI:C11	1.81	1.44
2:L:681:LYS:NZ	4:H:601:BTI:C11	1.81	1.42
2:L:681:LYS:NZ	4:H:601:BTI:H11	1.28	1.41
1:A:426:VAL:CG1	1:H:226:MET:HE1	1.52	1.38
1:K:426:VAL:CG1	1:C:226:MET:HE1	1.51	1.38
1:E:241:LEU:HD13	1:J:419:ALA:CB	1.53	1.38
2:B:681:LYS:HZ2	4:C:601:BTI:C11	1.41	1.26
2:B:681:LYS:NZ	4:C:601:BTI:H11	0.95	1.26
1:E:241:LEU:HD22	1:J:419:ALA:N	1.50	1.24
1:K:426:VAL:HG11	1:C:226:MET:HE1	1.18	1.17
1:C:217:THR:HG21	3:C:602:TW3:C14	1.74	1.16
1:H:217:THR:HG21	3:H:602:TW3:C14	1.74	1.16
1:E:226:MET:HE1	1:J:426:VAL:HG11	1.28	1.16
2:B:662:VAL:HG21	2:B:694:VAL:HG11	1.26	1.15
2:B:348:GLU:HG2	2:B:355:LEU:HD13	1.15	1.14
2:L:662:VAL:HG21	2:L:694:VAL:HG11	1.26	1.12
1:E:426:VAL:HG11	1:J:226:MET:HE1	1.27	1.11
2:L:348:GLU:HG2	2:L:355:LEU:HD13	1.15	1.11
1:E:241:LEU:HD13	1:J:419:ALA:HB2	1.16	1.08
1:A:426:VAL:HG11	1:H:226:MET:HE1	1.18	1.08
1:H:217:THR:CG2	3:H:602:TW3:C14	2.32	1.07
1:A:247:VAL:HG22	1:H:409:VAL:CG1	1.84	1.07
1:K:247:VAL:HG22	1:C:409:VAL:CG1	1.84	1.07
1:C:217:THR:CG2	3:C:602:TW3:C14	2.32	1.07
1:K:426:VAL:HG12	1:C:226:MET:HE1	1.34	1.06
1:A:226:MET:HE1	1:H:426:VAL:HG11	1.36	1.06
2:L:272:PHE:CE1	2:L:377:LEU:HD23	1.89	1.06
1:A:426:VAL:HG12	1:H:226:MET:HE1	1.35	1.06
2:B:272:PHE:CE1	2:B:377:LEU:HD23	1.89	1.06
1:E:426:VAL:HG11	1:J:226:MET:CE	1.87	1.05
1:K:241:LEU:HD13	1:C:419:ALA:HB2	1.39	1.05
1:A:241:LEU:HD13	1:H:419:ALA:HB2	1.39	1.04
1:K:247:VAL:HG22	1:C:409:VAL:HG12	1.38	1.02
1:A:241:LEU:HD13	1:H:419:ALA:CB	1.89	1.02
1:E:226:MET:CE	1:J:426:VAL:HG11	1.87	1.02
1:E:241:LEU:CD1	1:J:419:ALA:HB2	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:681:LYS:HZ2	4:H:601:BTI:C11	1.48	1.02
1:H:167:CYS:SG	1:H:201:MET:HE1	2.00	1.01
1:C:167:CYS:SG	1:C:201:MET:HE1	2.00	1.00
1:A:247:VAL:HG22	1:H:409:VAL:HG12	1.38	1.00
1:K:241:LEU:HD13	1:C:419:ALA:CB	1.90	1.00
2:L:276:CYS:SG	2:L:284:LYS:HG2	2.02	1.00
2:B:411:ASP:CG	2:B:412:PRO:HD2	1.87	1.00
2:B:276:CYS:SG	2:B:284:LYS:HG2	2.02	1.00
1:K:426:VAL:CG1	1:C:226:MET:CE	2.40	0.99
2:L:411:ASP:CG	2:L:412:PRO:HD2	1.87	0.99
1:A:226:MET:CE	1:H:426:VAL:HG11	1.92	0.99
1:E:241:LEU:HD22	1:J:419:ALA:CA	1.93	0.99
2:G:636:TYR:CB	1:J:282:HIS:CD2	2.47	0.98
1:A:426:VAL:CG1	1:H:226:MET:CE	2.41	0.97
2:M:636:TYR:CB	1:E:282:HIS:CD2	2.47	0.97
1:E:241:LEU:HD13	1:J:419:ALA:HB1	1.46	0.97
2:B:304:GLU:O	2:B:307:VAL:HG12	1.68	0.93
2:L:304:GLU:O	2:L:307:VAL:HG12	1.68	0.93
1:E:241:LEU:CD1	1:J:419:ALA:CB	2.45	0.92
1:E:426:VAL:CG1	1:J:226:MET:CE	2.49	0.91
1:H:282:HIS:CD2	2:I:636:TYR:CB	2.54	0.91
2:G:636:TYR:HB2	1:J:282:HIS:CD2	2.06	0.91
2:M:170:MET:HG3	2:M:333:PHE:CZ	2.07	0.91
2:F:681:LYS:HZ2	4:F:801:BTI:C11	1.63	0.90
2:G:170:MET:HG3	2:G:333:PHE:CZ	2.06	0.90
2:F:170:MET:HG3	2:F:333:PHE:CZ	2.06	0.90
1:C:282:HIS:CD2	2:F:636:TYR:CB	2.54	0.90
2:M:636:TYR:HB2	1:E:282:HIS:CD2	2.06	0.89
1:E:226:MET:CE	1:J:426:VAL:CG1	2.49	0.89
2:L:411:ASP:OD1	2:L:412:PRO:HD2	1.73	0.89
2:I:170:MET:HG3	2:I:333:PHE:CZ	2.06	0.89
1:A:239:ILE:HB	1:A:266:HIS:CE1	2.08	0.89
2:I:681:LYS:HZ2	4:I:801:BTI:C11	1.56	0.88
1:J:265:LEU:CD2	1:J:266:HIS:CD2	2.56	0.88
1:K:426:VAL:HG11	1:C:226:MET:CE	2.02	0.88
1:K:147:PRO:O	1:K:150:VAL:HG12	1.73	0.88
1:A:147:PRO:O	1:A:150:VAL:HG12	1.73	0.88
1:K:265:LEU:CD2	1:K:266:HIS:CD2	2.56	0.88
1:A:265:LEU:CD2	1:A:266:HIS:CD2	2.56	0.88
1:J:147:PRO:O	1:J:150:VAL:HG12	1.73	0.88
2:B:411:ASP:OD1	2:B:412:PRO:HD2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:LEU:CD2	1:E:266:HIS:CD2	2.56	0.88
2:I:387:TYR:CE1	2:I:433:MET:HG2	2.09	0.88
1:H:282:HIS:CD2	2:I:636:TYR:HB2	2.09	0.88
1:E:239:ILE:HB	1:E:266:HIS:CE1	2.08	0.88
2:M:387:TYR:CE1	2:M:433:MET:HG2	2.09	0.87
2:G:681:LYS:HZ2	4:G:801:BTI:C11	1.56	0.87
2:M:681:LYS:HZ2	4:M:801:BTI:C11	1.86	0.87
1:J:239:ILE:HB	1:J:266:HIS:CE1	2.08	0.87
1:K:239:ILE:HB	1:K:266:HIS:CE1	2.08	0.87
1:H:147:PRO:O	1:H:150:VAL:HG12	1.73	0.87
1:E:147:PRO:O	1:E:150:VAL:HG12	1.73	0.87
2:G:387:TYR:CE1	2:G:433:MET:HG2	2.09	0.87
2:G:636:TYR:CG	1:J:282:HIS:CD2	2.63	0.87
2:M:636:TYR:CG	1:E:282:HIS:CD2	2.63	0.87
1:J:265:LEU:CD2	1:J:266:HIS:HD2	1.88	0.87
1:K:265:LEU:CD2	1:K:266:HIS:HD2	1.88	0.87
2:F:387:TYR:CE1	2:F:433:MET:HG2	2.09	0.87
2:B:675:MET:CE	2:B:711:LEU:HB3	2.04	0.86
1:C:147:PRO:O	1:C:150:VAL:HG12	1.73	0.86
1:E:265:LEU:CD2	1:E:266:HIS:HD2	1.88	0.86
2:L:160:MET:HE1	2:L:338:THR:CG2	2.06	0.86
1:C:282:HIS:CD2	2:F:636:TYR:HB2	2.09	0.86
2:B:675:MET:HE1	2:B:711:LEU:HB3	1.57	0.86
2:I:306:ALA:HB1	2:I:321:VAL:HG21	1.57	0.86
2:L:675:MET:HE1	2:L:711:LEU:HB3	1.57	0.86
1:C:404:ILE:CD1	1:C:448:GLY:C	2.49	0.86
2:F:253:PRO:HB2	2:F:485:HIS:HB2	1.57	0.86
1:H:404:ILE:CD1	1:H:448:GLY:C	2.48	0.86
2:G:306:ALA:HB1	2:G:321:VAL:HG21	1.57	0.86
2:L:675:MET:CE	2:L:711:LEU:HB3	2.04	0.86
2:B:160:MET:HE1	2:B:338:THR:CG2	2.06	0.86
2:F:306:ALA:HB1	2:F:321:VAL:HG21	1.57	0.86
1:A:265:LEU:CD2	1:A:266:HIS:HD2	1.88	0.85
2:B:681:LYS:HZ1	4:C:601:BTI:H11	1.05	0.85
2:B:377:LEU:O	2:B:377:LEU:HD12	1.77	0.85
1:E:426:VAL:CG1	1:J:226:MET:HE1	2.07	0.85
1:A:426:VAL:HG11	1:H:226:MET:CE	2.02	0.85
2:B:662:VAL:CG2	2:B:694:VAL:HG21	2.06	0.85
2:B:653:MET:O	2:B:677:MET:HE1	1.77	0.85
2:B:252:THR:HB	2:B:326:ASP:HB3	1.58	0.85
2:L:662:VAL:CG2	2:L:694:VAL:HG21	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:HB3	1:H:409:VAL:HG11	1.59	0.84
1:K:242:ALA:HB3	1:C:409:VAL:CG1	2.08	0.84
1:E:226:MET:HE1	1:J:426:VAL:CG1	2.07	0.84
1:J:265:LEU:HD23	1:J:266:HIS:HD2	1.43	0.84
1:A:226:MET:CE	1:H:426:VAL:CG1	2.55	0.83
2:M:306:ALA:HB1	2:M:321:VAL:HG21	1.57	0.83
2:L:377:LEU:O	2:L:377:LEU:HD12	1.77	0.83
2:L:681:LYS:HZ1	4:H:601:BTI:H11	1.12	0.83
2:L:653:MET:O	2:L:677:MET:HE1	1.77	0.83
2:L:252:THR:HB	2:L:326:ASP:HB3	1.58	0.83
2:L:662:VAL:HG22	2:L:694:VAL:HG21	1.60	0.83
1:A:242:ALA:HB3	1:H:409:VAL:CG1	2.08	0.83
1:A:265:LEU:HD23	1:A:266:HIS:HD2	1.43	0.83
2:B:160:MET:HE1	2:B:338:THR:HG23	1.61	0.83
1:K:242:ALA:HB3	1:C:409:VAL:HG11	1.59	0.83
1:K:265:LEU:HD23	1:K:266:HIS:HD2	1.43	0.82
1:A:178:LEU:HD12	1:H:482:LEU:CD2	2.09	0.82
2:L:681:LYS:HZ1	4:H:601:BTI:C11	1.63	0.82
2:M:636:TYR:CG	1:E:282:HIS:HD2	1.97	0.82
1:K:178:LEU:HD12	1:C:482:LEU:CD2	2.08	0.82
2:B:662:VAL:HG22	2:B:694:VAL:HG21	1.60	0.82
2:L:160:MET:HE1	2:L:338:THR:HG23	1.61	0.81
2:G:636:TYR:CG	1:J:282:HIS:HD2	1.97	0.81
1:E:265:LEU:HD23	1:E:266:HIS:HD2	1.43	0.80
1:A:382:LYS:HG2	1:A:424:LYS:NZ	1.95	0.80
2:B:411:ASP:CG	2:B:412:PRO:CD	2.54	0.80
1:H:372:ASN:OD1	1:H:404:ILE:CG2	2.30	0.80
1:C:372:ASN:OD1	1:C:404:ILE:CG2	2.30	0.80
2:L:411:ASP:CG	2:L:412:PRO:CD	2.54	0.80
1:K:278:LEU:CG	2:L:641:SER:HB3	2.12	0.80
1:E:241:LEU:CD2	1:J:419:ALA:N	2.41	0.80
2:I:681:LYS:NZ	4:I:801:BTI:C10	2.45	0.79
1:A:282:HIS:CD2	2:B:636:TYR:CB	2.66	0.79
1:C:404:ILE:HD12	1:C:448:GLY:C	2.08	0.79
1:E:226:MET:HE2	1:J:426:VAL:CG1	2.13	0.79
1:J:265:LEU:HD23	1:J:266:HIS:CD2	2.18	0.79
2:G:681:LYS:NZ	4:G:801:BTI:C10	2.45	0.79
2:F:681:LYS:NZ	4:F:801:BTI:C10	2.45	0.79
1:E:426:VAL:CG1	1:J:226:MET:HE2	2.12	0.79
2:M:175:VAL:HG12	2:M:333:PHE:HB2	1.65	0.79
2:M:681:LYS:NZ	4:M:801:BTI:C10	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:CG	2:B:641:SER:HB3	2.12	0.78
1:K:278:LEU:HD11	2:L:641:SER:OG	1.83	0.78
1:K:282:HIS:CD2	2:L:636:TYR:CB	2.66	0.78
1:A:278:LEU:HD11	2:B:641:SER:OG	1.83	0.78
1:C:282:HIS:CD2	2:F:636:TYR:CG	2.72	0.78
1:E:265:LEU:HD23	1:E:266:HIS:CD2	2.18	0.78
2:M:175:VAL:CG1	2:M:333:PHE:HB2	2.13	0.78
2:B:276:CYS:SG	2:B:284:LYS:CG	2.71	0.78
2:L:662:VAL:CG2	2:L:694:VAL:HG11	2.11	0.77
1:H:404:ILE:HD12	1:H:448:GLY:C	2.08	0.77
2:I:175:VAL:CG1	2:I:333:PHE:HB2	2.13	0.77
1:K:265:LEU:HD23	1:K:266:HIS:CD2	2.18	0.77
1:H:282:HIS:CD2	2:I:636:TYR:CG	2.72	0.77
2:L:276:CYS:SG	2:L:284:LYS:CG	2.71	0.77
1:A:178:LEU:HD12	1:H:482:LEU:HD21	1.66	0.77
2:M:650:LEU:HB3	2:M:708:HIS:HA	1.68	0.76
1:A:563:MET:OXT	1:E:382:LYS:HB3	1.85	0.76
2:I:650:LEU:HB3	2:I:708:HIS:HA	1.67	0.76
1:K:178:LEU:HD12	1:C:482:LEU:HD21	1.65	0.76
2:L:659:LYS:HA	2:L:701:GLU:HG2	1.67	0.76
1:A:265:LEU:HD23	1:A:266:HIS:CD2	2.18	0.76
2:I:175:VAL:HG12	2:I:333:PHE:HB2	1.65	0.76
2:F:650:LEU:HB3	2:F:708:HIS:HA	1.68	0.76
2:B:662:VAL:CG2	2:B:694:VAL:HG11	2.11	0.76
1:A:278:LEU:CD1	2:B:641:SER:CB	2.22	0.76
1:A:282:HIS:CD2	2:B:636:TYR:HB2	2.21	0.75
2:G:650:LEU:HB3	2:G:708:HIS:HA	1.68	0.75
2:L:681:LYS:HZ2	4:H:601:BTI:H11	1.00	0.75
1:J:239:ILE:O	1:J:266:HIS:CE1	2.40	0.75
1:A:382:LYS:HG2	1:A:424:LYS:HZ1	1.50	0.75
1:H:217:THR:HG23	3:H:602:TW3:C14	2.15	0.75
1:K:239:ILE:O	1:K:266:HIS:CE1	2.40	0.74
1:A:226:MET:HE2	1:H:426:VAL:CG1	2.16	0.74
2:B:681:LYS:HZ1	4:C:601:BTI:C11	1.72	0.74
2:F:457:GLN:HE22	2:F:623:LYS:HG2	1.53	0.74
2:B:259:GLN:HB3	2:B:271:LEU:HB2	1.69	0.74
1:A:226:MET:HE1	1:H:426:VAL:CG1	2.15	0.74
2:B:411:ASP:OD1	2:B:412:PRO:CD	2.36	0.74
1:E:239:ILE:O	1:E:266:HIS:CE1	2.40	0.74
1:K:282:HIS:CD2	2:L:636:TYR:HB2	2.21	0.74
2:L:411:ASP:OD1	2:L:412:PRO:CD	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:O	1:A:266:HIS:CE1	2.40	0.74
2:B:275:ASP:HB3	2:B:288:GLU:HG3	1.69	0.74
2:I:457:GLN:HE22	2:I:623:LYS:HG2	1.53	0.74
2:B:659:LYS:HA	2:B:701:GLU:HG2	1.67	0.73
2:M:457:GLN:HE22	2:M:623:LYS:HG2	1.53	0.73
2:G:457:GLN:HE22	2:G:623:LYS:HG2	1.53	0.73
1:C:282:HIS:HD2	2:F:636:TYR:CG	2.07	0.73
2:L:275:ASP:HB3	2:L:288:GLU:HG3	1.69	0.72
2:B:397:PRO:HB3	2:B:432:PRO:HG3	1.71	0.72
1:C:217:THR:HG23	3:C:602:TW3:C14	2.16	0.72
2:L:259:GLN:HB3	2:L:271:LEU:HB2	1.70	0.72
1:E:241:LEU:CG	1:J:419:ALA:HB2	2.19	0.72
2:B:695:LYS:N	2:B:713:GLU:O	2.22	0.72
1:E:241:LEU:CD2	1:J:419:ALA:CA	2.68	0.72
1:H:282:HIS:HD2	2:I:636:TYR:CG	2.07	0.72
2:L:695:LYS:N	2:L:713:GLU:O	2.22	0.71
2:L:397:PRO:HB3	2:L:432:PRO:HG3	1.71	0.71
2:M:387:TYR:CE1	2:M:433:MET:CG	2.74	0.71
1:C:267:CYS:SG	1:C:276:TRP:HD1	2.14	0.70
2:F:387:TYR:CE1	2:F:433:MET:CG	2.74	0.70
2:M:453:TYR:HE1	2:M:623:LYS:HD3	1.56	0.70
2:I:387:TYR:CE1	2:I:433:MET:CG	2.74	0.70
1:C:465:TRP:HB3	1:C:466:PRO:HD2	1.74	0.70
1:C:184:VAL:O	1:C:190:HIS:HB3	1.92	0.70
2:F:453:TYR:HE1	2:F:623:LYS:HD3	1.56	0.70
2:G:387:TYR:CE1	2:G:433:MET:CG	2.74	0.70
2:G:453:TYR:HE1	2:G:623:LYS:HD3	1.56	0.70
1:A:247:VAL:HG22	1:H:409:VAL:HG11	1.72	0.69
1:A:426:VAL:HG12	1:H:226:MET:CE	2.14	0.69
1:K:278:LEU:CD1	2:L:641:SER:CB	2.22	0.69
1:H:465:TRP:HB3	1:H:466:PRO:HD2	1.74	0.69
1:J:219:GLY:CA	3:J:601:TW3:C1	2.70	0.69
1:A:221:ALA:O	1:A:224:PRO:HD2	1.93	0.69
1:H:184:VAL:O	1:H:190:HIS:HB3	1.92	0.69
2:M:614:LEU:HG	2:M:615:GLU:HG2	1.76	0.68
2:I:453:TYR:HE1	2:I:623:LYS:HD3	1.56	0.68
1:J:221:ALA:O	1:J:224:PRO:HD2	1.93	0.68
1:E:219:GLY:CA	3:E:601:TW3:C1	2.70	0.68
2:G:614:LEU:HG	2:G:615:GLU:HG2	1.75	0.68
1:K:221:ALA:O	1:K:224:PRO:HD2	1.93	0.68
2:I:170:MET:HG3	2:I:333:PHE:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:614:LEU:HG	2:I:615:GLU:HG2	1.75	0.67
2:M:170:MET:HG3	2:M:333:PHE:CE2	2.29	0.67
1:E:221:ALA:O	1:E:224:PRO:HD2	1.93	0.67
2:F:614:LEU:HG	2:F:615:GLU:HG2	1.75	0.67
2:F:170:MET:HG3	2:F:333:PHE:CE2	2.29	0.67
2:G:170:MET:HG3	2:G:333:PHE:CE2	2.29	0.67
2:I:662:VAL:HG21	2:I:694:VAL:HG21	1.77	0.67
2:M:662:VAL:HG21	2:M:694:VAL:HG21	1.77	0.67
2:B:323:PHE:HB3	2:B:331:PHE:HB2	1.77	0.67
1:K:426:VAL:HG12	1:C:226:MET:CE	2.13	0.66
2:G:662:VAL:HG21	2:G:694:VAL:HG21	1.77	0.66
1:E:426:VAL:HG12	1:J:226:MET:HE2	1.77	0.66
1:E:421:ASP:HA	1:E:424:LYS:HD2	1.77	0.66
2:B:662:VAL:HG21	2:B:694:VAL:CG1	2.16	0.66
2:F:662:VAL:HG21	2:F:694:VAL:HG21	1.77	0.66
2:B:325:MET:HA	2:B:330:ASN:O	1.96	0.66
1:C:237:GLY:O	1:C:263:ALA:HB2	1.96	0.66
2:L:255:HIS:HD1	2:L:276:CYS:HB3	1.61	0.66
1:E:241:LEU:HB2	1:J:419:ALA:HB2	1.77	0.66
1:K:247:VAL:HG22	1:C:409:VAL:HG11	1.72	0.66
2:M:513:LEU:HD22	2:M:585:VAL:HG12	1.77	0.66
1:A:239:ILE:CB	1:A:266:HIS:CE1	2.79	0.66
2:B:252:THR:HA	2:B:326:ASP:HA	1.78	0.66
1:A:282:HIS:CD2	2:B:636:TYR:CG	2.83	0.66
1:K:147:PRO:O	1:K:150:VAL:CG1	2.45	0.66
1:K:241:LEU:HD13	1:C:419:ALA:HB1	1.78	0.66
2:L:253:PRO:HB2	2:L:486:THR:H	1.61	0.66
1:C:147:PRO:O	1:C:150:VAL:CG1	2.44	0.66
2:F:513:LEU:HD22	2:F:585:VAL:HG12	1.77	0.66
1:H:409:VAL:HG21	4:H:601:BTI:HN3	1.60	0.66
1:E:184:VAL:O	1:E:190:HIS:HB3	1.96	0.66
2:I:150:ILE:HD13	2:I:360:LEU:HD23	1.78	0.65
1:J:147:PRO:O	1:J:150:VAL:CG1	2.45	0.65
1:K:184:VAL:O	1:K:190:HIS:HB3	1.96	0.65
1:K:265:LEU:HD22	1:K:266:HIS:CD2	2.32	0.65
2:L:286:ILE:HD11	2:L:470:LEU:HD22	1.79	0.65
1:C:201:MET:CE	1:C:208:GLN:HE22	2.09	0.65
1:H:147:PRO:O	1:H:150:VAL:CG1	2.44	0.65
2:L:323:PHE:HB3	2:L:331:PHE:HB2	1.77	0.65
2:L:325:MET:HA	2:L:330:ASN:O	1.96	0.65
2:B:255:HIS:HD1	2:B:276:CYS:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:ILE:HD11	2:B:470:LEU:HD22	1.79	0.65
1:E:265:LEU:HD22	1:E:266:HIS:CD2	2.32	0.65
1:A:184:VAL:O	1:A:190:HIS:HB3	1.96	0.65
2:F:150:ILE:HD13	2:F:360:LEU:HD23	1.78	0.65
2:I:513:LEU:HD22	2:I:585:VAL:HG12	1.77	0.65
1:J:239:ILE:CB	1:J:266:HIS:CE1	2.79	0.65
2:L:662:VAL:HG21	2:L:694:VAL:CG1	2.16	0.65
1:J:184:VAL:O	1:J:190:HIS:HB3	1.96	0.65
1:K:239:ILE:CB	1:K:266:HIS:CE1	2.79	0.65
1:C:421:ASP:HA	1:C:424:LYS:HD2	1.78	0.65
2:M:150:ILE:HD13	2:M:360:LEU:HD23	1.78	0.65
1:E:226:MET:HE2	1:J:426:VAL:HG12	1.77	0.65
2:B:253:PRO:HB2	2:B:486:THR:H	1.61	0.65
1:C:372:ASN:OD1	1:C:404:ILE:HG23	1.96	0.65
2:G:513:LEU:HD22	2:G:585:VAL:HG12	1.77	0.65
1:H:201:MET:CE	1:H:208:GLN:HE22	2.09	0.65
2:B:304:GLU:O	2:B:307:VAL:CG1	2.44	0.65
2:G:150:ILE:HD13	2:G:360:LEU:HD23	1.78	0.65
1:K:282:HIS:CD2	2:L:636:TYR:CG	2.83	0.64
2:L:304:GLU:O	2:L:307:VAL:CG1	2.44	0.64
1:A:241:LEU:HD13	1:H:419:ALA:HB1	1.76	0.64
1:E:239:ILE:CB	1:E:266:HIS:CE1	2.79	0.64
2:L:252:THR:HA	2:L:326:ASP:HA	1.78	0.64
2:L:276:CYS:HG	2:L:284:LYS:HG2	1.62	0.64
2:M:272:PHE:CD1	2:M:299:ARG:NH2	2.66	0.64
1:J:224:PRO:HG3	1:J:239:ILE:HD11	1.80	0.64
2:F:272:PHE:CD1	2:F:299:ARG:NH2	2.66	0.64
1:H:372:ASN:OD1	1:H:404:ILE:HG23	1.96	0.64
2:L:280:ARG:HB2	2:L:489:ILE:CD1	2.27	0.64
1:E:224:PRO:HG3	1:E:239:ILE:HD11	1.80	0.64
1:K:247:VAL:CG2	1:C:409:VAL:CG1	2.72	0.63
2:I:272:PHE:CD1	2:I:299:ARG:NH2	2.66	0.63
2:L:324:ILE:N	2:L:332:CYS:O	2.30	0.63
1:A:212:VAL:HG21	1:A:239:ILE:HD11	1.81	0.63
1:A:224:PRO:HG3	1:A:239:ILE:CD1	2.29	0.63
1:J:265:LEU:HD22	1:J:266:HIS:CD2	2.32	0.63
1:K:224:PRO:HG3	1:K:239:ILE:HD11	1.80	0.63
1:A:265:LEU:HD22	1:A:266:HIS:CD2	2.32	0.63
2:B:280:ARG:HB2	2:B:489:ILE:CD1	2.27	0.63
2:G:272:PHE:CD1	2:G:299:ARG:NH2	2.66	0.63
1:A:147:PRO:O	1:A:150:VAL:CG1	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:PRO:O	1:E:150:VAL:CG1	2.44	0.63
1:J:224:PRO:HG3	1:J:239:ILE:CD1	2.29	0.63
1:K:259:ASP:HB3	1:C:411:ARG:CZ	2.29	0.63
2:B:324:ILE:N	2:B:332:CYS:O	2.29	0.63
1:E:241:LEU:CB	1:J:419:ALA:HB2	2.29	0.63
1:A:278:LEU:HD21	2:B:641:SER:CB	2.29	0.63
2:B:317:GLY:HA2	2:B:362:ILE:HD13	1.81	0.63
1:H:201:MET:HE2	1:H:208:GLN:HE22	1.64	0.63
1:H:201:MET:HE2	1:H:208:GLN:NE2	2.14	0.63
1:K:224:PRO:HG3	1:K:239:ILE:CD1	2.29	0.62
2:L:317:GLY:HA2	2:L:362:ILE:HD13	1.81	0.62
1:C:201:MET:HE2	1:C:208:GLN:NE2	2.14	0.62
1:E:241:LEU:HD22	1:J:419:ALA:H	1.53	0.62
2:L:285:ILE:C	2:L:286:ILE:HD13	2.24	0.62
2:B:660:VAL:HG23	2:B:675:MET:CG	2.30	0.62
2:G:170:MET:HG3	2:G:333:PHE:CE1	2.35	0.62
1:E:212:VAL:HG21	1:E:239:ILE:HD11	1.81	0.62
2:L:660:VAL:HG23	2:L:675:MET:CG	2.30	0.62
1:A:224:PRO:HG3	1:A:239:ILE:HD11	1.80	0.62
1:A:259:ASP:HB3	1:H:411:ARG:CZ	2.29	0.62
2:B:660:VAL:HA	2:B:675:MET:HG2	1.80	0.62
1:E:224:PRO:HG3	1:E:239:ILE:CD1	2.29	0.62
1:K:222:TYR:CE1	1:K:241:LEU:HD11	2.35	0.62
1:K:242:ALA:CB	1:C:409:VAL:HG11	2.29	0.62
1:C:201:MET:HE2	1:C:208:GLN:HE22	1.64	0.62
1:K:278:LEU:HD21	2:L:641:SER:CB	2.29	0.62
2:L:660:VAL:HA	2:L:675:MET:HG2	1.80	0.62
1:K:195:PHE:HB3	1:K:226:MET:SD	2.40	0.62
1:J:219:GLY:HA3	3:J:601:TW3:C1	2.30	0.62
1:K:212:VAL:HG21	1:K:239:ILE:HD11	1.81	0.61
2:B:285:ILE:C	2:B:286:ILE:HD13	2.24	0.61
2:B:343:GLU:O	2:B:346:VAL:HG22	2.00	0.61
1:E:219:GLY:HA3	3:E:601:TW3:C1	2.30	0.61
1:A:242:ALA:CB	1:H:409:VAL:HG11	2.30	0.61
1:E:49:MET:HG2	1:E:318:TYR:CD1	2.35	0.61
1:J:212:VAL:HG21	1:J:239:ILE:HD11	1.81	0.61
1:C:404:ILE:HD12	1:C:448:GLY:HA3	1.82	0.61
2:L:285:ILE:O	2:L:286:ILE:HD13	2.01	0.61
1:A:195:PHE:HB3	1:A:226:MET:SD	2.40	0.61
1:A:222:TYR:CE1	1:A:241:LEU:HD11	2.35	0.61
2:B:276:CYS:SG	2:B:284:LYS:CD	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:PHE:HB3	1:J:226:MET:SD	2.40	0.61
2:B:285:ILE:O	2:B:286:ILE:HD13	2.01	0.61
2:F:170:MET:HG3	2:F:333:PHE:CE1	2.35	0.61
1:H:49:MET:HG2	1:H:318:TYR:CD1	2.36	0.61
1:E:222:TYR:CE1	1:E:241:LEU:HD11	2.35	0.61
2:F:508:LEU:HD13	2:F:562:VAL:HG11	1.83	0.61
2:M:170:MET:HG3	2:M:333:PHE:CE1	2.35	0.61
1:K:49:MET:HG2	1:K:318:TYR:CD1	2.36	0.61
1:E:195:PHE:HB3	1:E:226:MET:SD	2.40	0.61
2:B:348:GLU:CG	2:B:355:LEU:HD13	2.09	0.61
2:L:348:GLU:CG	2:L:355:LEU:HD13	2.09	0.61
1:A:226:MET:HE2	1:H:426:VAL:HG12	1.81	0.61
2:B:681:LYS:HE2	1:C:477:GLN:HG3	1.82	0.61
2:I:170:MET:HG3	2:I:333:PHE:CE1	2.35	0.61
1:C:267:CYS:HG	1:C:276:TRP:HD1	1.48	0.61
1:J:49:MET:HG2	1:J:318:TYR:CD1	2.35	0.61
1:C:267:CYS:HG	1:C:276:TRP:CD1	2.18	0.60
2:F:541:SER:HB2	2:F:543:ARG:HG3	1.83	0.60
2:G:416:ILE:HG22	2:G:418:THR:HG22	1.83	0.60
2:M:541:SER:HB2	2:M:543:ARG:HG3	1.83	0.60
1:A:49:MET:HG2	1:A:318:TYR:CD1	2.35	0.60
1:H:404:ILE:HD12	1:H:448:GLY:HA3	1.82	0.60
2:M:508:LEU:HD13	2:M:562:VAL:HG11	1.83	0.60
2:L:276:CYS:SG	2:L:284:LYS:CD	2.89	0.60
1:C:60:VAL:HG12	2:F:547:ILE:HG23	1.83	0.60
2:G:508:LEU:HD13	2:G:562:VAL:HG11	1.83	0.60
1:H:267:CYS:HG	1:H:276:TRP:HD1	1.49	0.60
2:M:416:ILE:HG22	2:M:418:THR:HG22	1.83	0.60
1:C:49:MET:HG2	1:C:318:TYR:CD1	2.36	0.60
1:C:372:ASN:CG	1:C:404:ILE:HG22	2.27	0.60
1:H:543:LEU:HD23	2:I:536:PRO:HB2	1.84	0.60
2:I:508:LEU:HD13	2:I:562:VAL:HG11	1.83	0.60
1:H:60:VAL:HG12	2:I:547:ILE:HG23	1.83	0.60
1:C:404:ILE:HD12	1:C:448:GLY:CA	2.32	0.60
2:G:541:SER:HB2	2:G:543:ARG:HG3	1.82	0.60
1:H:421:ASP:HA	1:H:424:LYS:HD2	1.84	0.60
1:J:239:ILE:O	1:J:266:HIS:HE1	1.85	0.60
2:B:533:GLN:N	2:B:533:GLN:OE1	2.35	0.60
2:L:533:GLN:N	2:L:533:GLN:OE1	2.35	0.59
2:M:536:PRO:HB2	1:E:543:LEU:HD23	1.84	0.59
1:A:239:ILE:O	1:A:266:HIS:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:678:ILE:HG22	2:B:683:GLU:HG2	1.84	0.59
1:C:404:ILE:CD1	1:C:449:ASN:N	2.65	0.59
1:C:543:LEU:CD2	2:F:536:PRO:HB2	2.32	0.59
1:A:282:HIS:HD2	2:B:636:TYR:CG	2.21	0.59
1:C:187:ASP:HB3	1:C:190:HIS:HB2	1.85	0.59
1:H:372:ASN:CG	1:H:404:ILE:HG22	2.27	0.59
1:H:543:LEU:CD2	2:I:536:PRO:HB2	2.32	0.59
1:H:404:ILE:HD12	1:H:448:GLY:CA	2.32	0.59
1:K:278:LEU:HD11	2:L:641:SER:HB3	0.61	0.59
2:L:343:GLU:O	2:L:346:VAL:HG22	2.00	0.59
2:B:160:MET:SD	2:B:336:MET:O	2.61	0.59
2:F:160:MET:HB2	2:F:338:THR:HG21	1.85	0.59
1:H:404:ILE:CD1	1:H:449:ASN:N	2.65	0.59
2:I:416:ILE:HG22	2:I:418:THR:HG22	1.83	0.59
2:F:416:ILE:HG22	2:F:418:THR:HG22	1.83	0.59
2:I:272:PHE:CD1	2:I:299:ARG:CZ	2.86	0.59
2:I:160:MET:HB2	2:I:338:THR:HG21	1.85	0.59
2:I:541:SER:HB2	2:I:543:ARG:HG3	1.82	0.59
1:A:216:CYS:SG	1:A:239:ILE:HA	2.43	0.59
1:K:239:ILE:HB	1:K:266:HIS:HE1	1.68	0.58
2:G:636:TYR:CD1	1:J:282:HIS:HD2	2.20	0.58
2:M:272:PHE:CD1	2:M:299:ARG:CZ	2.86	0.58
2:G:649:PRO:HD3	2:G:689:PRO:HD3	1.85	0.58
2:M:649:PRO:HD3	2:M:689:PRO:HD3	1.85	0.58
1:C:372:ASN:OD1	1:C:404:ILE:HG22	2.03	0.58
1:E:216:CYS:SG	1:E:239:ILE:HA	2.43	0.58
2:L:660:VAL:HG23	2:L:675:MET:HG2	1.86	0.58
2:L:678:ILE:HG22	2:L:683:GLU:HG2	1.84	0.58
1:A:242:ALA:HB3	1:H:409:VAL:HG13	1.85	0.58
2:B:359:GLN:O	2:B:362:ILE:HG13	2.04	0.58
1:C:543:LEU:HD23	2:F:536:PRO:HB2	1.84	0.58
2:G:536:PRO:HB2	1:J:543:LEU:HD23	1.84	0.58
2:M:160:MET:HB2	2:M:338:THR:HG21	1.85	0.58
2:L:160:MET:SD	2:L:336:MET:O	2.61	0.58
2:L:348:GLU:HG2	2:L:355:LEU:CD1	2.10	0.58
2:F:649:PRO:HD3	2:F:689:PRO:HD3	1.85	0.58
1:H:187:ASP:HB3	1:H:190:HIS:HB2	1.85	0.58
1:K:216:CYS:SG	1:K:239:ILE:HA	2.43	0.58
1:A:247:VAL:CG2	1:H:409:VAL:CG1	2.72	0.58
2:F:272:PHE:CD1	2:F:299:ARG:CZ	2.86	0.58
1:E:239:ILE:HB	1:E:266:HIS:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:282:HIS:HD2	2:L:636:TYR:CG	2.21	0.58
2:L:456:ARG:HD3	2:L:623:LYS:O	2.04	0.58
2:M:636:TYR:CD1	1:E:282:HIS:HD2	2.20	0.58
2:L:359:GLN:O	2:L:362:ILE:HG13	2.04	0.58
2:B:456:ARG:HD3	2:B:623:LYS:O	2.04	0.58
2:G:272:PHE:CD1	2:G:299:ARG:CZ	2.86	0.58
2:M:536:PRO:HB2	1:E:543:LEU:CD2	2.34	0.58
2:B:487:ASP:C	2:B:490:PRO:HD2	2.29	0.57
2:G:536:PRO:HB2	1:J:543:LEU:CD2	2.34	0.57
2:M:636:TYR:HB3	1:E:282:HIS:CD2	2.39	0.57
1:J:216:CYS:SG	1:J:239:ILE:HA	2.43	0.57
1:J:239:ILE:HB	1:J:266:HIS:HE1	1.68	0.57
1:K:233:VAL:O	1:K:263:ALA:HB2	2.04	0.57
1:A:278:LEU:HD11	2:B:641:SER:HB3	0.61	0.57
1:C:112:GLU:OE1	1:C:146:TYR:OH	2.21	0.57
1:K:176:ALA:O	3:K:601:TW3:N5	2.37	0.57
2:G:160:MET:HB2	2:G:338:THR:HG21	1.85	0.57
2:I:649:PRO:HD3	2:I:689:PRO:HD3	1.85	0.57
1:A:176:ALA:O	3:A:601:TW3:N5	2.37	0.57
2:G:636:TYR:HB2	1:J:282:HIS:NE2	2.20	0.57
2:L:487:ASP:C	2:L:490:PRO:HD2	2.29	0.57
1:C:490:ARG:HD2	1:C:497:PHE:HB2	1.87	0.57
1:H:490:ARG:HD2	1:H:497:PHE:HB2	1.87	0.57
1:C:410:GLY:O	1:C:414:GLU:HG2	2.05	0.57
1:K:242:ALA:HB3	1:C:409:VAL:HG13	1.85	0.57
1:A:233:VAL:O	1:A:263:ALA:HB2	2.04	0.57
1:A:239:ILE:HB	1:A:266:HIS:HE1	1.68	0.57
2:L:294:ILE:HB	2:L:299:ARG:NH2	2.20	0.57
2:F:272:PHE:HD1	2:F:299:ARG:NE	2.03	0.57
2:F:299:ARG:HH22	2:F:377:LEU:HD22	1.70	0.57
2:G:299:ARG:HH22	2:G:377:LEU:HD22	1.70	0.57
1:J:233:VAL:O	1:J:263:ALA:HB2	2.04	0.57
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.86	0.56
2:I:272:PHE:HD1	2:I:299:ARG:NE	2.03	0.56
2:L:662:VAL:HG11	2:L:712:VAL:CG2	2.36	0.56
1:A:64:LYS:HD2	2:B:547:ILE:HG21	1.87	0.56
1:E:239:ILE:O	1:E:266:HIS:HE1	1.85	0.56
1:H:112:GLU:OE1	1:H:146:TYR:OH	2.21	0.56
2:M:299:ARG:HH22	2:M:377:LEU:HD22	1.70	0.56
1:K:244:PRO:HB2	1:K:245:PRO:HD3	1.86	0.56
2:L:371:SER:O	2:L:375:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:SER:O	2:B:375:ILE:HG13	2.05	0.56
2:B:660:VAL:HG23	2:B:675:MET:HG2	1.85	0.56
1:K:64:LYS:HD2	2:L:547:ILE:HG21	1.87	0.56
2:B:61:ALA:O	2:B:65:MET:HG3	2.06	0.56
2:M:272:PHE:HD1	2:M:299:ARG:NE	2.03	0.56
1:E:233:VAL:O	1:E:263:ALA:HB2	2.04	0.56
1:E:241:LEU:CD2	1:J:419:ALA:HA	2.35	0.56
2:L:675:MET:HE3	2:L:711:LEU:CD2	2.36	0.56
1:H:410:GLY:O	1:H:414:GLU:HG2	2.05	0.56
1:K:178:LEU:HD12	1:C:482:LEU:HD23	1.85	0.56
1:A:239:ILE:CB	1:A:266:HIS:HE1	2.18	0.56
2:B:662:VAL:HG11	2:B:712:VAL:CG2	2.35	0.56
1:H:372:ASN:OD1	1:H:404:ILE:HG22	2.03	0.56
1:K:195:PHE:HB3	1:K:226:MET:HE1	1.88	0.56
2:L:655:GLY:HA3	2:L:679:ALA:HB2	1.87	0.56
1:A:543:LEU:CD2	2:B:536:PRO:HB2	2.36	0.56
2:B:675:MET:HE3	2:B:711:LEU:CD2	2.36	0.56
2:I:299:ARG:HH22	2:I:377:LEU:HD22	1.70	0.56
1:K:239:ILE:O	1:K:266:HIS:HE1	1.85	0.56
1:K:278:LEU:CD2	2:L:641:SER:HB3	2.36	0.56
1:K:543:LEU:CD2	2:L:536:PRO:HB2	2.36	0.56
2:L:61:ALA:O	2:L:65:MET:HG3	2.05	0.56
2:B:655:GLY:HA3	2:B:679:ALA:HB2	1.87	0.56
2:G:272:PHE:HD1	2:G:299:ARG:NE	2.03	0.56
1:H:267:CYS:HG	1:H:276:TRP:CD1	2.24	0.56
2:B:288:GLU:HB3	2:B:382:PHE:CE1	2.41	0.55
2:B:294:ILE:HB	2:B:299:ARG:NH2	2.20	0.55
2:M:180:GLY:HA3	2:M:249:PHE:HA	1.87	0.55
1:J:239:ILE:CB	1:J:266:HIS:HE1	2.19	0.55
2:L:288:GLU:HB3	2:L:382:PHE:CE1	2.41	0.55
2:B:659:LYS:HA	2:B:701:GLU:CG	2.36	0.55
2:B:321:VAL:HG22	2:B:336:MET:SD	2.47	0.55
2:L:65:MET:O	2:L:69:LYS:HG2	2.06	0.55
2:L:662:VAL:HG11	2:L:712:VAL:HG22	1.88	0.55
2:B:347:THR:HA	2:B:350:ILE:HG12	1.88	0.55
1:H:266:HIS:HA	1:H:270:SER:HB2	1.87	0.55
2:L:304:GLU:C	2:L:307:VAL:HG12	2.31	0.55
2:L:321:VAL:HG22	2:L:336:MET:SD	2.47	0.55
2:B:152:PRO:HG3	2:B:338:THR:CB	2.37	0.55
2:G:273:GLU:CD	2:G:294:ILE:HD12	2.32	0.55
2:L:344:HIS:O	2:L:347:THR:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:347:THR:HA	2:L:350:ILE:HG12	1.88	0.55
1:A:178:LEU:HD12	1:H:482:LEU:HD23	1.86	0.55
1:A:195:PHE:HB3	1:A:226:MET:HE1	1.88	0.55
2:B:65:MET:O	2:B:69:LYS:HG2	2.06	0.55
1:C:282:HIS:HD2	2:F:636:TYR:CD1	2.25	0.55
2:M:636:TYR:HB2	1:E:282:HIS:NE2	2.20	0.55
1:K:239:ILE:CB	1:K:266:HIS:HE1	2.19	0.55
2:L:265:HIS:CD2	2:L:367:LYS:HG2	2.42	0.55
1:E:226:MET:CE	1:J:426:VAL:HG12	2.36	0.55
2:B:265:HIS:CD2	2:B:367:LYS:HG2	2.42	0.55
2:B:304:GLU:C	2:B:307:VAL:HG12	2.31	0.55
2:B:380:HIS:N	2:B:441:ALA:O	2.35	0.55
2:B:628:GLU:O	2:B:629:ILE:HD13	2.06	0.55
2:B:662:VAL:HG11	2:B:712:VAL:HG22	1.88	0.55
2:L:272:PHE:HD1	2:L:299:ARG:HD3	1.72	0.54
2:L:628:GLU:O	2:L:629:ILE:HD13	2.06	0.54
1:A:278:LEU:CD2	2:B:641:SER:HB3	2.36	0.54
1:H:462:LEU:O	1:H:529:ASP:HB2	2.07	0.54
1:K:178:LEU:HB2	1:K:179:PRO:HD3	1.89	0.54
1:E:239:ILE:CB	1:E:266:HIS:HE1	2.19	0.54
2:L:152:PRO:HG3	2:L:338:THR:CB	2.37	0.54
1:C:426:VAL:HG22	1:C:451:GLY:HA2	1.88	0.54
1:J:421:ASP:HA	1:J:424:LYS:HD2	1.89	0.54
2:L:468:ASP:N	2:L:468:ASP:OD1	2.41	0.54
2:B:272:PHE:HD1	2:B:299:ARG:HD3	1.72	0.54
2:I:273:GLU:CD	2:I:294:ILE:HD12	2.32	0.54
1:A:178:LEU:HB2	1:A:179:PRO:HD3	1.90	0.54
2:F:402:LEU:HD13	2:F:405:LEU:HD22	1.90	0.54
1:K:177:TYR:HA	3:K:601:TW3:N5	2.23	0.54
1:A:278:LEU:CG	2:B:641:SER:CB	2.80	0.54
2:B:270:TYR:CD2	2:B:303:GLY:HA3	2.43	0.54
1:A:177:TYR:HA	3:A:601:TW3:N5	2.22	0.54
1:J:195:PHE:HB3	1:J:226:MET:HE1	1.88	0.54
1:K:278:LEU:CG	2:L:641:SER:CB	2.80	0.54
2:B:274:ARG:HD2	2:B:346:VAL:CG2	2.38	0.54
2:B:653:MET:HA	2:B:707:ARG:HD2	1.90	0.54
2:F:273:GLU:CD	2:F:294:ILE:HD12	2.32	0.54
2:M:273:GLU:CD	2:M:294:ILE:HD12	2.32	0.54
1:J:178:LEU:HB2	1:J:179:PRO:HD3	1.89	0.54
1:J:479:ALA:HB1	1:J:506:LYS:HG2	1.90	0.54
2:L:270:TYR:CD2	2:L:303:GLY:HA3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:ASP:N	2:B:468:ASP:OD1	2.41	0.54
1:C:462:LEU:O	1:C:529:ASP:HB2	2.08	0.54
2:L:678:ILE:CG2	2:L:683:GLU:HG2	2.38	0.54
1:E:195:PHE:HB3	1:E:226:MET:HE1	1.88	0.54
1:K:479:ALA:HB1	1:K:506:LYS:HG2	1.90	0.53
1:H:282:HIS:HD2	2:I:636:TYR:CD1	2.25	0.53
2:M:547:ILE:HG22	1:E:61:GLU:OE2	2.08	0.53
1:E:497:PHE:CE2	1:E:502:GLU:HG2	2.43	0.53
1:A:479:ALA:HB1	1:A:506:LYS:HG2	1.90	0.53
2:B:127:PRO:HG3	2:B:149:PHE:CZ	2.44	0.53
2:B:276:CYS:SG	2:B:284:LYS:HD2	2.49	0.53
2:B:344:HIS:O	2:B:347:THR:HG22	2.07	0.53
2:G:402:LEU:HD13	2:G:405:LEU:HD22	1.90	0.53
2:G:547:ILE:HG22	1:J:61:GLU:OE2	2.08	0.53
2:L:127:PRO:HG3	2:L:149:PHE:CZ	2.43	0.53
2:L:274:ARG:HD2	2:L:346:VAL:CG2	2.38	0.53
2:B:60:ILE:HG12	2:B:129:CYS:H	1.73	0.53
1:H:268:ARG:HH22	1:H:276:TRP:NE1	2.07	0.53
2:M:402:LEU:HD13	2:M:405:LEU:HD22	1.90	0.53
2:L:653:MET:HB2	1:H:408:MET:HE3	1.90	0.53
2:B:348:GLU:HG2	2:B:355:LEU:CD1	2.10	0.53
2:B:678:ILE:CG2	2:B:683:GLU:HG2	2.38	0.53
2:F:649:PRO:HB2	2:F:686:ILE:HG23	1.91	0.53
1:K:497:PHE:CE2	1:K:502:GLU:HG2	2.43	0.53
1:A:497:PHE:CE2	1:A:502:GLU:HG2	2.44	0.53
2:M:649:PRO:HB2	2:M:686:ILE:HG23	1.90	0.53
1:H:472:VAL:HG13	1:H:473:MET:HG2	1.91	0.53
2:I:402:LEU:HD13	2:I:405:LEU:HD22	1.90	0.53
1:E:456:ALA:HA	1:J:188:ARG:HA	1.90	0.53
2:L:653:MET:HA	2:L:707:ARG:HD2	1.89	0.53
1:C:377:PHE:CE2	1:C:408:MET:HG2	2.43	0.53
1:H:505:LEU:O	1:H:508:PRO:HD2	2.08	0.53
1:J:239:ILE:CA	1:J:266:HIS:HE1	2.22	0.53
2:B:441:ALA:HB3	2:B:447:ALA:HB2	1.91	0.53
1:H:377:PHE:CE2	1:H:408:MET:HG2	2.43	0.53
1:E:178:LEU:HB2	1:E:179:PRO:HD3	1.90	0.53
1:E:479:ALA:HB1	1:E:506:LYS:HG2	1.90	0.53
2:B:469:PHE:CE1	2:B:496:LEU:HD13	2.44	0.53
2:B:666:ASP:O	2:B:693:THR:HG23	2.09	0.53
1:E:188:ARG:HA	1:J:456:ALA:HA	1.90	0.53
2:L:441:ALA:HB3	2:L:447:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:636:TYR:HB3	1:J:282:HIS:CD2	2.39	0.53
1:H:267:CYS:SG	1:H:276:TRP:HD1	2.32	0.53
2:I:594:ASP:OD1	2:I:594:ASP:N	2.39	0.53
2:M:249:PHE:HB2	2:M:252:THR:HB	1.91	0.53
1:E:221:ALA:C	1:E:224:PRO:HD2	2.34	0.53
2:L:469:PHE:CE1	2:L:496:LEU:HD13	2.44	0.52
2:L:653:MET:O	2:L:677:MET:CE	2.54	0.52
1:A:260:LEU:HD12	1:H:411:ARG:HA	1.92	0.52
2:B:285:ILE:HG22	2:B:286:ILE:CD1	2.39	0.52
1:E:239:ILE:CA	1:E:266:HIS:HE1	2.22	0.52
1:J:497:PHE:CE2	1:J:502:GLU:HG2	2.44	0.52
1:K:221:ALA:C	1:K:224:PRO:HD2	2.34	0.52
2:L:284:LYS:HD2	2:L:343:GLU:OE2	2.09	0.52
1:C:472:VAL:HG13	1:C:473:MET:HG2	1.91	0.52
2:L:619:TYR:CD1	2:L:628:GLU:HG2	2.45	0.52
1:C:505:LEU:O	1:C:508:PRO:HD2	2.08	0.52
2:L:285:ILE:HG22	2:L:286:ILE:CD1	2.39	0.52
1:C:268:ARG:HH22	1:C:276:TRP:NE1	2.07	0.52
1:K:239:ILE:CA	1:K:266:HIS:HE1	2.22	0.52
2:L:285:ILE:CG2	2:L:470:LEU:HD21	2.40	0.52
2:L:666:ASP:O	2:L:693:THR:HG23	2.09	0.52
2:I:649:PRO:HB2	2:I:686:ILE:HG23	1.90	0.52
1:E:241:LEU:HD13	1:J:419:ALA:CA	2.34	0.52
1:K:260:LEU:HD12	1:C:411:ARG:HA	1.91	0.52
2:B:653:MET:HG3	2:B:679:ALA:HB3	1.92	0.52
1:H:176:ALA:O	3:H:602:TW3:N5	2.43	0.52
2:L:60:ILE:HG12	2:L:129:CYS:H	1.73	0.52
2:L:377:LEU:HD12	2:L:377:LEU:C	2.35	0.52
2:L:659:LYS:HA	2:L:701:GLU:CG	2.37	0.52
2:B:284:LYS:HD2	2:B:343:GLU:OE2	2.09	0.52
2:G:66:ARG:HG3	2:G:91:MET:HE1	1.92	0.52
2:M:175:VAL:HG12	2:M:333:PHE:CB	2.39	0.52
1:E:241:LEU:HD22	1:J:419:ALA:CB	2.40	0.52
2:L:639:SER:O	2:L:642:SER:OG	2.26	0.52
2:L:653:MET:HG3	2:L:679:ALA:HB3	1.92	0.52
1:C:61:GLU:OE2	2:F:547:ILE:HG22	2.10	0.52
1:C:268:ARG:HH22	1:C:276:TRP:HE1	1.58	0.52
2:G:649:PRO:HB2	2:G:686:ILE:HG23	1.90	0.52
1:A:265:LEU:HA	1:A:269:LYS:CE	2.40	0.52
2:B:254:ARG:HB2	2:B:325:MET:O	2.10	0.52
2:B:388:ALA:HB3	2:B:432:PRO:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:66:ARG:HG3	2:I:91:MET:HE1	1.92	0.52
2:I:273:GLU:HG2	2:I:299:ARG:CD	2.40	0.52
1:J:221:ALA:C	1:J:224:PRO:HD2	2.34	0.52
1:K:456:ALA:HA	1:C:188:ARG:HA	1.92	0.52
2:L:276:CYS:SG	2:L:284:LYS:HD2	2.49	0.52
2:B:653:MET:O	2:B:677:MET:CE	2.54	0.52
1:H:119:ILE:HD11	1:H:134:ILE:HG22	1.92	0.52
2:M:273:GLU:HG2	2:M:299:ARG:CD	2.40	0.52
2:M:513:LEU:HD22	2:M:585:VAL:CG1	2.40	0.52
1:A:239:ILE:CA	1:A:266:HIS:HE1	2.22	0.51
2:B:619:TYR:CD1	2:B:628:GLU:HG2	2.44	0.51
1:H:404:ILE:HD13	1:H:448:GLY:C	2.34	0.51
2:L:380:HIS:N	2:L:441:ALA:O	2.35	0.51
2:L:388:ALA:HB3	2:L:432:PRO:HB2	1.92	0.51
2:B:170:MET:CE	2:B:175:VAL:HG21	2.41	0.51
1:C:266:HIS:HA	1:C:270:SER:HB2	1.91	0.51
1:C:404:ILE:HD13	1:C:448:GLY:C	2.34	0.51
2:F:513:LEU:HD22	2:F:585:VAL:CG1	2.40	0.51
1:E:265:LEU:HA	1:E:269:LYS:CE	2.40	0.51
2:L:324:ILE:O	2:L:331:PHE:HA	2.11	0.51
2:B:653:MET:HB2	1:C:408:MET:HE3	1.91	0.51
2:G:273:GLU:HG2	2:G:299:ARG:CD	2.40	0.51
2:M:456:ARG:HD3	2:M:623:LYS:O	2.11	0.51
1:C:176:ALA:O	3:C:602:TW3:N5	2.43	0.51
2:G:286:ILE:HD12	2:G:473:LEU:HD22	1.93	0.51
2:I:456:ARG:HD3	2:I:623:LYS:O	2.11	0.51
2:L:513:LEU:HD22	2:L:585:VAL:HG12	1.93	0.51
2:B:285:ILE:CG2	2:B:470:LEU:HD21	2.40	0.51
2:F:273:GLU:HG2	2:F:299:ARG:CD	2.40	0.51
1:J:265:LEU:HA	1:J:269:LYS:CE	2.40	0.51
1:A:221:ALA:C	1:A:224:PRO:HD2	2.34	0.51
1:A:543:LEU:HD23	2:B:536:PRO:HB2	1.93	0.51
2:B:272:PHE:CD1	2:B:377:LEU:HD23	2.44	0.51
1:C:119:ILE:HD11	1:C:134:ILE:HG22	1.92	0.51
2:G:456:ARG:HD3	2:G:623:LYS:O	2.11	0.51
2:M:547:ILE:HG23	1:E:60:VAL:HG12	1.92	0.51
2:L:681:LYS:HE2	1:H:477:GLN:HE21	1.75	0.51
2:B:377:LEU:HD12	2:B:377:LEU:C	2.35	0.51
1:E:119:ILE:HD11	1:E:134:ILE:HG22	1.92	0.51
1:A:119:ILE:HD11	1:A:134:ILE:HG22	1.92	0.51
1:K:265:LEU:HA	1:K:269:LYS:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:ARG:HG3	2:F:91:MET:HE1	1.92	0.51
1:H:268:ARG:HH22	1:H:276:TRP:HE1	1.58	0.51
2:M:66:ARG:HG3	2:M:91:MET:HE1	1.92	0.51
1:K:119:ILE:HD11	1:K:134:ILE:HG22	1.92	0.51
2:B:655:GLY:HA3	2:B:679:ALA:CB	2.41	0.51
1:C:223:VAL:HB	1:C:224:PRO:HD3	1.93	0.51
1:J:265:LEU:HA	1:J:269:LYS:HE2	1.93	0.51
2:B:513:LEU:HD22	2:B:585:VAL:HG12	1.93	0.50
1:K:241:LEU:CD1	1:C:419:ALA:HB2	2.28	0.50
1:A:265:LEU:HA	1:A:269:LYS:HE2	1.93	0.50
2:F:273:GLU:OE2	2:F:294:ILE:HG21	2.12	0.50
2:F:286:ILE:HD12	2:F:473:LEU:HD22	1.93	0.50
2:I:513:LEU:HD22	2:I:585:VAL:CG1	2.40	0.50
2:M:273:GLU:OE2	2:M:294:ILE:HG21	2.12	0.50
1:E:265:LEU:HA	1:E:269:LYS:HE2	1.93	0.50
1:A:167:CYS:SG	1:A:201:MET:HE1	2.52	0.50
2:B:639:SER:O	2:B:642:SER:OG	2.27	0.50
2:F:456:ARG:HD3	2:F:623:LYS:O	2.11	0.50
2:G:408:PRO:O	2:G:416:ILE:HD11	2.12	0.50
2:M:286:ILE:HD12	2:M:473:LEU:HD22	1.93	0.50
1:K:167:CYS:SG	1:K:201:MET:HE1	2.52	0.50
2:L:670:ALA:HA	2:L:688:SER:HB3	1.93	0.50
1:A:456:ALA:HA	1:H:188:ARG:HA	1.92	0.50
2:B:324:ILE:O	2:B:331:PHE:HA	2.11	0.50
2:B:670:ALA:HA	2:B:688:SER:HB3	1.93	0.50
2:F:408:PRO:O	2:F:416:ILE:HD11	2.12	0.50
2:G:547:ILE:HG23	1:J:60:VAL:HG12	1.93	0.50
2:I:272:PHE:HD1	2:I:299:ARG:CZ	2.25	0.50
2:I:286:ILE:HD12	2:I:473:LEU:HD22	1.93	0.50
1:J:167:CYS:SG	1:J:201:MET:HE1	2.52	0.50
2:L:254:ARG:HB2	2:L:325:MET:O	2.10	0.50
2:L:256:VAL:O	2:L:323:PHE:N	2.30	0.50
2:L:590:TYR:OH	2:L:608:LYS:HD3	2.11	0.50
1:A:259:ASP:HB3	1:H:411:ARG:NH2	2.25	0.50
2:B:463:LEU:HD12	2:B:463:LEU:C	2.37	0.50
2:L:285:ILE:HG22	2:L:286:ILE:HD13	1.93	0.50
2:L:653:MET:HA	2:L:707:ARG:CD	2.42	0.50
2:M:272:PHE:HD1	2:M:299:ARG:CZ	2.25	0.50
1:J:147:PRO:C	1:J:150:VAL:HG12	2.37	0.50
1:H:223:VAL:HB	1:H:224:PRO:HD3	1.94	0.50
1:K:178:LEU:CD1	1:C:482:LEU:HD21	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:239:ILE:HB	1:K:266:HIS:ND1	2.27	0.50
1:K:259:ASP:HB3	1:C:411:ARG:NH2	2.26	0.50
1:K:543:LEU:HD23	2:L:536:PRO:HB2	1.93	0.50
2:L:170:MET:CE	2:L:175:VAL:HG21	2.41	0.50
2:B:657:ILE:HD12	2:B:699:TYR:HB3	1.94	0.50
1:C:147:PRO:C	1:C:150:VAL:HG12	2.37	0.50
1:C:177:TYR:HA	3:C:602:TW3:N5	2.27	0.50
1:H:61:GLU:OE2	2:I:547:ILE:HG22	2.10	0.50
1:E:147:PRO:C	1:E:150:VAL:HG12	2.37	0.50
2:B:345:PRO:HB2	2:B:438:VAL:HG21	1.94	0.50
2:F:349:MET:SD	2:F:415:ARG:HD3	2.52	0.50
2:B:590:TYR:OH	2:B:608:LYS:HD3	2.11	0.49
2:M:717:GLU:O	2:M:717:GLU:HG2	2.12	0.49
1:J:119:ILE:HD11	1:J:134:ILE:HG22	1.92	0.49
2:G:513:LEU:HD22	2:G:585:VAL:CG1	2.40	0.49
1:H:498:SER:O	1:H:502:GLU:HG3	2.13	0.49
2:M:349:MET:SD	2:M:415:ARG:HD3	2.52	0.49
1:K:334:VAL:O	1:K:338:ILE:HG23	2.13	0.49
2:L:463:LEU:HD12	2:L:463:LEU:C	2.37	0.49
2:L:655:GLY:HA3	2:L:679:ALA:CB	2.41	0.49
2:B:653:MET:HA	2:B:707:ARG:CD	2.42	0.49
2:F:717:GLU:O	2:F:717:GLU:HG2	2.12	0.49
2:G:349:MET:SD	2:G:415:ARG:HD3	2.52	0.49
1:K:265:LEU:HA	1:K:269:LYS:HE2	1.93	0.49
2:G:273:GLU:OE2	2:G:294:ILE:HG21	2.12	0.49
2:I:349:MET:SD	2:I:415:ARG:HD3	2.52	0.49
2:L:160:MET:CE	2:L:338:THR:HG23	2.37	0.49
2:G:717:GLU:O	2:G:717:GLU:HG2	2.12	0.49
1:H:177:TYR:HA	3:H:602:TW3:N5	2.27	0.49
2:L:345:PRO:HB2	2:L:438:VAL:HG21	1.94	0.49
2:L:657:ILE:HD12	2:L:699:TYR:HB3	1.94	0.49
1:C:378:SER:HB3	1:C:421:ASP:OD2	2.12	0.49
2:G:272:PHE:HD1	2:G:299:ARG:CZ	2.25	0.49
1:E:239:ILE:HB	1:E:266:HIS:ND1	2.27	0.49
1:J:239:ILE:HB	1:J:266:HIS:ND1	2.27	0.49
1:A:239:ILE:HB	1:A:266:HIS:ND1	2.27	0.49
1:H:334:VAL:O	1:H:338:ILE:HG23	2.13	0.49
2:B:272:PHE:CZ	2:B:377:LEU:HB3	2.48	0.49
1:H:378:SER:HB3	1:H:421:ASP:OD2	2.12	0.49
1:E:167:CYS:SG	1:E:201:MET:HE1	2.52	0.49
1:E:334:VAL:O	1:E:338:ILE:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:MET:CE	2:B:338:THR:HG23	2.37	0.49
1:C:498:SER:O	1:C:502:GLU:HG3	2.13	0.49
2:F:253:PRO:HB2	2:F:485:HIS:CB	2.38	0.49
2:I:273:GLU:OE2	2:I:294:ILE:HG21	2.12	0.49
1:A:334:VAL:O	1:A:338:ILE:HG23	2.13	0.49
2:B:399:ALA:HB1	2:B:426:VAL:O	2.13	0.49
2:I:408:PRO:O	2:I:416:ILE:HD11	2.12	0.49
1:K:303:THR:HG23	1:E:295:ASN:OD1	2.13	0.48
2:L:408:PRO:HG3	2:L:454:SER:HB3	1.95	0.48
2:L:590:TYR:HE1	2:L:599:LYS:HB2	1.78	0.48
2:B:285:ILE:HG22	2:B:286:ILE:HD13	1.93	0.48
2:F:272:PHE:HD1	2:F:299:ARG:CZ	2.25	0.48
2:F:273:GLU:OE2	2:F:294:ILE:HD12	2.13	0.48
2:B:382:PHE:O	2:B:438:VAL:HA	2.13	0.48
1:C:416:GLU:OE2	1:C:416:GLU:HA	2.13	0.48
1:K:55:GLN:O	1:K:58:GLU:HG2	2.14	0.48
2:L:382:PHE:O	2:L:438:VAL:HA	2.13	0.48
2:L:383:GLU:HG3	2:L:438:VAL:HG22	1.94	0.48
2:B:590:TYR:HE1	2:B:599:LYS:HB2	1.78	0.48
1:C:141:LYS:NZ	3:C:602:TW3:O15	2.35	0.48
2:I:717:GLU:HG2	2:I:717:GLU:O	2.12	0.48
2:M:273:GLU:OE2	2:M:294:ILE:HD12	2.13	0.48
2:M:408:PRO:O	2:M:416:ILE:HD11	2.12	0.48
1:K:278:LEU:CD2	2:L:641:SER:CB	2.92	0.48
2:B:176:PRO:HB2	2:B:332:CYS:HA	1.95	0.48
2:B:383:GLU:HG3	2:B:438:VAL:HG22	1.94	0.48
2:B:681:LYS:HZ3	4:C:601:BTI:C11	2.08	0.48
1:C:55:GLN:O	1:C:58:GLU:HG2	2.14	0.48
1:C:334:VAL:O	1:C:338:ILE:HG23	2.13	0.48
1:H:416:GLU:OE2	1:H:416:GLU:HA	2.13	0.48
1:J:269:LYS:HE3	1:J:269:LYS:HB2	1.62	0.48
1:J:334:VAL:O	1:J:338:ILE:HG23	2.13	0.48
1:K:421:ASP:HA	1:K:424:LYS:HD2	1.94	0.48
1:H:55:GLN:O	1:H:58:GLU:HG2	2.14	0.48
1:A:278:LEU:CD2	2:B:641:SER:CB	2.92	0.48
2:G:273:GLU:OE2	2:G:294:ILE:HD12	2.13	0.48
1:J:366:PRO:O	1:J:397:PRO:HG2	2.14	0.48
1:A:147:PRO:C	1:A:150:VAL:HG12	2.37	0.48
2:I:273:GLU:OE2	2:I:294:ILE:HD12	2.13	0.48
2:I:653:MET:HE2	2:I:679:ALA:HB1	1.96	0.48
2:L:272:PHE:CZ	2:L:377:LEU:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:272:PHE:CD1	2:L:377:LEU:HD23	2.44	0.48
1:A:366:PRO:O	1:A:397:PRO:HG2	2.14	0.48
2:M:160:MET:HB2	2:M:338:THR:CG2	2.44	0.48
2:B:408:PRO:HG3	2:B:454:SER:HB3	1.95	0.48
2:B:681:LYS:HZ2	4:C:601:BTI:H11	0.65	0.48
2:I:601:SER:HA	2:I:605:VAL:O	2.14	0.48
1:J:89:ASN:HB2	1:J:284:LEU:HD13	1.96	0.48
2:L:165:THR:O	2:L:169:ILE:HG13	2.14	0.47
2:B:639:SER:OG	2:B:642:SER:OG	2.27	0.47
2:G:160:MET:HB2	2:G:338:THR:CG2	2.44	0.47
1:H:89:ASN:HB2	1:H:284:LEU:HD13	1.96	0.47
1:H:237:GLY:O	1:H:263:ALA:HB2	2.14	0.47
2:I:160:MET:HB2	2:I:338:THR:CG2	2.44	0.47
2:I:175:VAL:HG12	2:I:333:PHE:CB	2.39	0.47
1:K:366:PRO:O	1:K:397:PRO:CG	2.62	0.47
2:L:654:THR:HA	2:L:705:ALA:O	2.15	0.47
1:A:55:GLN:O	1:A:58:GLU:HG2	2.14	0.47
1:A:178:LEU:CD1	1:H:482:LEU:CD2	2.88	0.47
2:B:165:THR:O	2:B:169:ILE:HG13	2.14	0.47
1:C:473:MET:HG3	1:C:478:ALA:HB2	1.96	0.47
2:G:601:SER:HA	2:G:605:VAL:O	2.14	0.47
1:E:366:PRO:O	1:E:397:PRO:HG2	2.14	0.47
1:J:366:PRO:O	1:J:397:PRO:CG	2.62	0.47
1:K:60:VAL:HG11	2:L:546:ASN:HB2	1.96	0.47
1:A:60:VAL:HG11	2:B:546:ASN:HB2	1.96	0.47
1:A:303:THR:HG23	1:J:295:ASN:OD1	2.14	0.47
2:M:653:MET:HE2	2:M:679:ALA:HB1	1.96	0.47
2:B:326:ASP:OD1	2:B:326:ASP:N	2.47	0.47
2:B:675:MET:CE	2:B:711:LEU:HD23	2.44	0.47
2:F:653:MET:HE2	2:F:679:ALA:HB1	1.96	0.47
1:E:89:ASN:HB2	1:E:284:LEU:HD13	1.96	0.47
1:J:55:GLN:O	1:J:58:GLU:HG2	2.14	0.47
2:L:399:ALA:HB1	2:L:426:VAL:O	2.13	0.47
2:B:601:SER:HA	2:B:605:VAL:O	2.15	0.47
1:H:404:ILE:HD13	1:H:448:GLY:O	2.15	0.47
2:I:63:ARG:NH2	2:I:354:ASP:OD1	2.40	0.47
2:M:601:SER:HA	2:M:605:VAL:O	2.14	0.47
1:K:234:ARG:NH2	2:L:644:GLU:OE1	2.46	0.47
1:A:248:LYS:NZ	1:A:254:GLU:HB2	2.30	0.47
1:A:366:PRO:O	1:A:397:PRO:CG	2.62	0.47
1:E:55:GLN:O	1:E:58:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:366:PRO:O	1:K:397:PRO:HG2	2.14	0.47
2:L:176:PRO:HB2	2:L:332:CYS:HA	1.95	0.47
2:B:346:VAL:CG1	2:B:383:GLU:HB2	2.45	0.47
2:B:487:ASP:OD1	2:B:490:PRO:HG2	2.15	0.47
2:B:654:THR:HA	2:B:705:ALA:O	2.15	0.47
2:F:63:ARG:NH2	2:F:354:ASP:OD1	2.40	0.47
2:F:601:SER:HA	2:F:605:VAL:O	2.14	0.47
1:H:147:PRO:C	1:H:150:VAL:HG12	2.37	0.47
2:L:272:PHE:CE2	2:L:377:LEU:HB3	2.50	0.47
2:L:302:LEU:HD11	2:L:323:PHE:CD1	2.50	0.47
2:L:326:ASP:OD1	2:L:326:ASP:N	2.47	0.47
2:L:675:MET:CE	2:L:711:LEU:HD23	2.44	0.47
2:L:675:MET:HE3	2:L:711:LEU:HD22	1.97	0.47
2:G:413:SER:O	2:G:439:VAL:HA	2.15	0.47
2:G:653:MET:HE2	2:G:679:ALA:HB1	1.96	0.47
1:K:89:ASN:HB2	1:K:284:LEU:HD13	1.96	0.47
1:K:248:LYS:NZ	1:K:254:GLU:HB2	2.30	0.47
1:K:282:HIS:HD2	2:L:636:TYR:CD2	2.33	0.47
2:L:346:VAL:CG1	2:L:383:GLU:HB2	2.45	0.47
1:A:94:GLY:O	2:B:542:GLY:N	2.48	0.47
2:M:63:ARG:NH2	2:M:354:ASP:OD1	2.40	0.47
2:L:671:GLY:HA2	2:L:687:LYS:HB3	1.97	0.47
2:B:393:ASN:HB2	2:B:396:MET:HG2	1.97	0.47
2:B:687:LYS:HE2	2:B:687:LYS:HA	1.97	0.47
1:C:267:CYS:SG	1:C:276:TRP:CD1	3.02	0.47
1:C:404:ILE:HD13	1:C:448:GLY:O	2.15	0.47
2:I:253:PRO:HB3	2:I:486:THR:OG1	2.15	0.47
1:K:94:GLY:O	2:L:542:GLY:N	2.48	0.46
1:K:216:CYS:SG	1:K:239:ILE:HG12	2.55	0.46
2:L:687:LYS:HE2	2:L:687:LYS:HA	1.97	0.46
1:C:60:VAL:CG1	2:F:547:ILE:HG23	2.43	0.46
1:J:563:MET:H	1:J:563:MET:HG3	1.43	0.46
1:K:147:PRO:C	1:K:150:VAL:HG12	2.37	0.46
2:L:393:ASN:HB2	2:L:396:MET:HG2	1.97	0.46
1:A:89:ASN:HB2	1:A:284:LEU:HD13	1.96	0.46
1:A:234:ARG:NH2	2:B:644:GLU:OE1	2.46	0.46
1:A:282:HIS:HD2	2:B:636:TYR:CD2	2.32	0.46
2:B:259:GLN:HE21	2:B:261:PHE:HE1	1.63	0.46
2:B:681:LYS:HZ2	2:B:681:LYS:HB2	1.79	0.46
2:F:160:MET:HB2	2:F:338:THR:CG2	2.44	0.46
2:F:273:GLU:HG2	2:F:299:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:472:VAL:HG12	1:C:181:GLN:OE1	2.16	0.46
2:L:259:GLN:HE21	2:L:261:PHE:HE1	1.63	0.46
2:B:256:VAL:O	2:B:323:PHE:N	2.30	0.46
2:M:413:SER:O	2:M:439:VAL:HA	2.15	0.46
1:E:366:PRO:O	1:E:397:PRO:CG	2.63	0.46
2:L:344:HIS:CG	2:L:345:PRO:HD3	2.50	0.46
2:L:601:SER:HA	2:L:605:VAL:O	2.15	0.46
2:L:660:VAL:HG22	2:L:662:VAL:H	1.80	0.46
1:A:236:GLN:H	1:A:236:GLN:HG3	1.58	0.46
2:F:413:SER:O	2:F:439:VAL:HA	2.15	0.46
2:G:254:ARG:HB3	2:G:485:HIS:HA	1.97	0.46
2:I:434:ILE:HD11	2:I:463:LEU:HD11	1.98	0.46
2:M:273:GLU:HG2	2:M:299:ARG:HD3	1.97	0.46
1:E:216:CYS:SG	1:E:239:ILE:HG12	2.55	0.46
1:J:216:CYS:SG	1:J:239:ILE:HG12	2.55	0.46
1:C:282:HIS:NE2	2:F:636:TYR:HB2	2.30	0.46
2:F:434:ILE:HD11	2:F:463:LEU:HD11	1.98	0.46
2:F:559:LYS:HB2	2:F:559:LYS:HE2	1.74	0.46
2:G:253:PRO:O	2:G:485:HIS:HB2	2.15	0.46
1:H:213:MET:HE2	1:H:213:MET:HB3	1.81	0.46
1:H:490:ARG:HD2	1:H:497:PHE:CB	2.46	0.46
2:L:487:ASP:OD1	2:L:490:PRO:HG2	2.15	0.46
1:A:472:VAL:HG12	1:H:181:GLN:OE1	2.15	0.46
2:B:302:LEU:HD11	2:B:323:PHE:CD1	2.50	0.46
1:C:89:ASN:HB2	1:C:284:LEU:HD13	1.96	0.46
1:C:274:ASP:OD1	1:J:348:LYS:HE3	2.15	0.46
1:H:60:VAL:CG1	2:I:547:ILE:HG23	2.43	0.46
1:K:295:ASN:OD1	1:H:303:THR:HG23	2.16	0.46
2:L:359:GLN:HA	2:L:362:ILE:HG12	1.98	0.46
2:L:556:LYS:HG3	2:L:561:ASN:OD1	2.16	0.46
1:A:226:MET:CE	1:H:426:VAL:HG12	2.42	0.46
1:A:260:LEU:CD1	1:H:411:ARG:HA	2.46	0.46
2:B:272:PHE:CE2	2:B:377:LEU:HB3	2.50	0.46
2:B:660:VAL:HG22	2:B:662:VAL:H	1.80	0.46
1:C:497:PHE:CZ	1:C:502:GLU:HG2	2.51	0.46
1:H:274:ASP:OD1	1:E:348:LYS:HE3	2.16	0.46
1:H:452:MET:HE3	1:H:452:MET:HB3	1.88	0.46
1:H:497:PHE:CZ	1:H:502:GLU:HG2	2.51	0.46
2:I:413:SER:O	2:I:439:VAL:HA	2.15	0.46
2:M:494:LYS:HE2	2:M:494:LYS:HB3	1.51	0.46
2:B:344:HIS:CG	2:B:345:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:GLN:HA	2:B:362:ILE:HG12	1.98	0.46
2:G:273:GLU:HG2	2:G:299:ARG:HD3	1.97	0.46
2:L:639:SER:OG	2:L:642:SER:OG	2.27	0.46
1:A:421:ASP:HA	1:A:424:LYS:HD3	1.97	0.46
1:C:413:TYR:O	1:C:418:ILE:HG22	2.16	0.46
2:G:150:ILE:HD13	2:G:360:LEU:CD2	2.46	0.46
2:G:678:ILE:O	2:G:678:ILE:HG13	2.16	0.46
2:I:273:GLU:HG2	2:I:299:ARG:HD3	1.97	0.46
2:I:302:LEU:HA	2:I:331:PHE:CZ	2.51	0.46
2:I:345:PRO:HB2	2:I:438:VAL:HG21	1.98	0.46
1:K:178:LEU:CD1	1:C:482:LEU:CD2	2.88	0.45
1:A:295:ASN:OD1	1:C:303:THR:HG23	2.16	0.45
2:B:358:TRP:O	2:B:362:ILE:HG23	2.16	0.45
2:B:556:LYS:HG3	2:B:561:ASN:OD1	2.16	0.45
1:C:280:ASP:O	1:C:284:LEU:HG	2.16	0.45
1:C:504:ALA:O	1:C:508:PRO:HD3	2.16	0.45
2:F:651:ALA:CB	2:F:677:MET:HE1	2.47	0.45
2:I:494:LYS:HE2	2:I:494:LYS:HB3	1.51	0.45
2:M:302:LEU:HA	2:M:331:PHE:CZ	2.51	0.45
2:M:651:ALA:CB	2:M:677:MET:HE1	2.47	0.45
1:J:236:GLN:H	1:J:236:GLN:HG3	1.58	0.45
1:J:528:ASP:O	1:J:529:ASP:C	2.59	0.45
1:K:280:ASP:O	1:K:284:LEU:HG	2.16	0.45
1:A:216:CYS:SG	1:A:239:ILE:HG12	2.55	0.45
1:A:112:GLU:OE1	1:A:146:TYR:OH	2.21	0.45
2:F:678:ILE:O	2:F:678:ILE:HG13	2.16	0.45
1:K:269:LYS:HE3	1:K:269:LYS:HB2	1.62	0.45
2:B:383:GLU:HA	2:B:437:LEU:O	2.16	0.45
2:B:675:MET:HE3	2:B:711:LEU:HD22	1.97	0.45
1:E:280:ASP:O	1:E:284:LEU:HG	2.16	0.45
1:K:452:MET:HE3	1:K:452:MET:HB3	1.88	0.45
2:B:671:GLY:HA2	2:B:687:LYS:HB3	1.97	0.45
1:C:424:LYS:HB3	1:C:424:LYS:HE3	1.63	0.45
1:H:282:HIS:NE2	2:I:636:TYR:HB2	2.30	0.45
2:I:270:TYR:OH	2:I:300:LYS:HA	2.17	0.45
2:M:434:ILE:HD11	2:M:463:LEU:HD11	1.98	0.45
2:L:317:GLY:HA2	2:L:362:ILE:CD1	2.46	0.45
2:L:383:GLU:HA	2:L:437:LEU:O	2.16	0.45
2:B:272:PHE:HE1	2:B:377:LEU:HD23	1.70	0.45
2:M:555:LEU:HD13	2:M:629:ILE:HG21	1.99	0.45
1:E:269:LYS:HE3	1:E:269:LYS:HB2	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:81:LEU:N	1:J:280:ASP:OD2	2.49	0.45
2:L:359:GLN:HA	2:L:362:ILE:CG1	2.47	0.45
2:L:460:ILE:HD12	2:L:465:THR:HG21	1.99	0.45
1:C:528:ASP:O	1:C:529:ASP:C	2.59	0.45
2:G:614:LEU:HG	2:G:615:GLU:CG	2.45	0.45
1:H:280:ASP:O	1:H:284:LEU:HG	2.16	0.45
1:H:504:ALA:O	1:H:508:PRO:HD3	2.16	0.45
2:I:441:ALA:HB3	2:I:447:ALA:HB2	1.99	0.45
2:M:651:ALA:HB1	2:M:677:MET:HE1	1.99	0.45
1:K:195:PHE:HB3	1:K:226:MET:CE	2.47	0.45
1:K:289:LYS:HD2	1:H:28:VAL:HG22	1.99	0.45
2:F:302:LEU:HA	2:F:331:PHE:CZ	2.51	0.45
2:G:302:LEU:HA	2:G:331:PHE:CZ	2.52	0.45
2:G:555:LEU:HD13	2:G:629:ILE:HG21	1.99	0.45
1:H:528:ASP:O	1:H:529:ASP:C	2.59	0.45
2:L:358:TRP:O	2:L:362:ILE:HG23	2.16	0.45
1:A:280:ASP:O	1:A:284:LEU:HG	2.16	0.45
2:F:594:ASP:OD1	2:F:594:ASP:N	2.39	0.45
2:I:614:LEU:HG	2:I:615:GLU:CG	2.45	0.45
1:E:195:PHE:HB3	1:E:226:MET:CE	2.47	0.45
2:B:638:SER:OG	2:B:640:VAL:HG23	2.17	0.45
1:C:60:VAL:HG12	2:F:547:ILE:CG2	2.47	0.45
1:C:490:ARG:HD2	1:C:497:PHE:CB	2.46	0.45
2:G:63:ARG:NH2	2:G:354:ASP:OD1	2.40	0.45
1:H:60:VAL:HG12	2:I:547:ILE:CG2	2.47	0.45
1:H:413:TYR:O	1:H:418:ILE:HG22	2.16	0.45
2:I:264:HIS:CE1	2:I:316:VAL:HG11	2.52	0.45
2:I:555:LEU:HD13	2:I:629:ILE:HG21	1.99	0.45
2:M:270:TYR:OH	2:M:300:LYS:HA	2.17	0.45
1:E:528:ASP:O	1:E:529:ASP:C	2.59	0.45
1:J:195:PHE:HB3	1:J:226:MET:CE	2.47	0.45
2:B:175:VAL:HG11	2:B:333:PHE:HB2	1.99	0.44
1:C:282:HIS:CD2	2:F:636:TYR:HB3	2.48	0.44
2:G:252:THR:HG23	2:G:324:ILE:HG21	1.99	0.44
2:I:680:MET:HE3	2:I:680:MET:HB2	1.78	0.44
2:M:453:TYR:HE1	2:M:623:LYS:CD	2.28	0.44
1:K:260:LEU:CD1	1:C:411:ARG:HA	2.46	0.44
2:B:359:GLN:HA	2:B:362:ILE:CG1	2.47	0.44
2:B:654:THR:O	2:B:679:ALA:HB1	2.17	0.44
2:F:264:HIS:CE1	2:F:316:VAL:HG11	2.52	0.44
2:G:434:ILE:HD11	2:G:463:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:651:ALA:CB	2:G:677:MET:HE1	2.46	0.44
1:H:182:ALA:O	1:H:186:PRO:HD2	2.17	0.44
2:B:487:ASP:O	2:B:490:PRO:HD2	2.18	0.44
2:F:150:ILE:HD13	2:F:360:LEU:CD2	2.46	0.44
2:G:651:ALA:HB1	2:G:677:MET:HE1	1.99	0.44
2:I:651:ALA:CB	2:I:677:MET:HE1	2.47	0.44
2:I:651:ALA:HB1	2:I:677:MET:HE1	1.99	0.44
2:M:345:PRO:HB2	2:M:438:VAL:HG21	1.98	0.44
1:J:280:ASP:O	1:J:284:LEU:HG	2.16	0.44
1:K:528:ASP:O	1:K:529:ASP:C	2.59	0.44
1:K:563:MET:HE2	1:J:563:MET:HB3	1.98	0.44
2:B:682:MET:HE2	1:C:405:THR:HG21	1.99	0.44
2:F:453:TYR:HE1	2:F:623:LYS:CD	2.28	0.44
1:H:121:THR:HG22	1:H:134:ILE:HG23	2.00	0.44
2:M:264:HIS:CE1	2:M:316:VAL:HG11	2.52	0.44
1:A:188:ARG:HA	1:H:456:ALA:HA	2.00	0.44
1:A:563:MET:HE2	1:A:563:MET:HB2	1.77	0.44
1:C:182:ALA:O	1:C:186:PRO:HD2	2.17	0.44
2:G:264:HIS:CE1	2:G:316:VAL:HG11	2.52	0.44
2:G:270:TYR:OH	2:G:300:LYS:HA	2.17	0.44
2:G:594:ASP:OD1	2:G:594:ASP:N	2.39	0.44
1:H:25:GLY:O	1:H:26:ASP:C	2.59	0.44
2:I:678:ILE:O	2:I:678:ILE:HG13	2.16	0.44
2:M:678:ILE:HG13	2:M:678:ILE:O	2.16	0.44
1:E:112:GLU:OE1	1:E:146:TYR:OH	2.21	0.44
1:E:121:THR:HG22	1:E:134:ILE:HG23	2.00	0.44
1:E:241:LEU:HD23	1:J:418:ILE:HB	1.98	0.44
1:J:413:TYR:HE1	1:J:418:ILE:HG13	1.82	0.44
2:L:673:SER:HA	2:L:686:ILE:O	2.17	0.44
1:C:191:PHE:HE2	3:C:602:TW3:C1	2.31	0.44
1:C:236:GLN:H	1:C:236:GLN:HG3	1.58	0.44
2:F:345:PRO:HB2	2:F:438:VAL:HG21	1.98	0.44
2:F:555:LEU:HD13	2:F:629:ILE:HG21	1.99	0.44
2:I:134:GLU:CD	2:I:339:ARG:HD3	2.43	0.44
2:M:134:GLU:CD	2:M:339:ARG:HD3	2.43	0.44
1:J:408:MET:HE3	1:J:408:MET:HB3	1.87	0.44
2:L:175:VAL:HG11	2:L:333:PHE:HB2	1.99	0.44
2:L:522:MET:HB3	2:L:522:MET:HE2	1.70	0.44
2:L:682:MET:SD	2:L:684:HIS:NE2	2.90	0.44
1:A:195:PHE:HB3	1:A:226:MET:CE	2.47	0.44
1:A:278:LEU:HD21	2:B:641:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ILE:HD12	2:B:465:THR:HG21	1.99	0.44
2:L:387:TYR:CE1	2:L:433:MET:HE2	2.53	0.44
1:A:121:THR:HG22	1:A:134:ILE:HG23	2.00	0.44
2:B:387:TYR:CE1	2:B:433:MET:HE2	2.53	0.44
2:F:270:TYR:OH	2:F:300:LYS:HA	2.17	0.44
2:G:134:GLU:CD	2:G:339:ARG:HD3	2.43	0.44
1:H:191:PHE:HE2	3:H:602:TW3:C1	2.31	0.44
1:H:404:ILE:HD11	1:H:449:ASN:N	2.33	0.44
2:M:614:LEU:HG	2:M:615:GLU:CG	2.46	0.44
2:L:653:MET:SD	1:H:408:MET:CE	3.06	0.44
1:A:289:LYS:HD2	1:C:28:VAL:HG22	1.99	0.44
2:B:280:ARG:HD2	2:B:395:PHE:CD1	2.53	0.44
2:B:485:HIS:CE1	2:B:488:PHE:HA	2.53	0.44
2:B:673:SER:HA	2:B:686:ILE:O	2.17	0.44
1:C:404:ILE:HD11	1:C:449:ASN:N	2.33	0.44
2:F:441:ALA:HB3	2:F:447:ALA:HB2	1.99	0.44
2:I:258:VAL:HG13	2:I:272:PHE:O	2.18	0.44
2:I:533:GLN:H	2:I:533:GLN:HG2	1.59	0.44
1:K:236:GLN:H	1:K:236:GLN:HG3	1.58	0.43
1:K:413:TYR:HE1	1:K:418:ILE:HG13	1.82	0.43
1:A:178:LEU:CD1	1:H:482:LEU:HD21	2.40	0.43
1:A:326:LYS:HA	1:A:326:LYS:HD3	1.80	0.43
2:B:675:MET:CE	2:B:711:LEU:CD2	2.96	0.43
1:C:389:GLN:HE22	1:H:561:PHE:H	1.65	0.43
1:C:561:PHE:H	1:H:389:GLN:HE22	1.65	0.43
2:L:160:MET:HA	2:L:166:SER:HB3	1.99	0.43
2:L:638:SER:OG	2:L:640:VAL:HG23	2.17	0.43
2:L:675:MET:CE	2:L:711:LEU:CD2	2.96	0.43
2:B:280:ARG:HD2	2:B:395:PHE:CE1	2.53	0.43
1:J:217:THR:O	1:J:221:ALA:N	2.48	0.43
2:L:255:HIS:ND1	2:L:276:CYS:HB3	2.31	0.43
2:L:280:ARG:HD2	2:L:395:PHE:CE1	2.53	0.43
2:L:654:THR:O	2:L:679:ALA:HB1	2.17	0.43
1:A:413:TYR:HE1	1:A:418:ILE:HG13	1.82	0.43
2:B:513:LEU:HD22	2:B:585:VAL:CG1	2.49	0.43
1:C:121:THR:HG22	1:C:134:ILE:HG23	2.00	0.43
2:G:258:VAL:HG13	2:G:272:PHE:O	2.18	0.43
1:J:121:THR:HG22	1:J:134:ILE:HG23	2.00	0.43
1:A:213:MET:HE2	1:A:213:MET:HB3	1.91	0.43
2:B:653:MET:SD	1:C:408:MET:CE	3.06	0.43
2:F:667:LYS:HG2	2:F:693:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:667:LYS:HG2	2:G:693:THR:OG1	2.19	0.43
1:H:376:LEU:HD23	1:H:376:LEU:HA	1.89	0.43
2:I:252:THR:HG23	2:I:324:ILE:HG21	1.99	0.43
2:I:662:VAL:HG23	2:I:666:ASP:HB3	2.00	0.43
1:E:466:PRO:O	1:E:519:PRO:HG2	2.19	0.43
1:E:473:MET:HG3	1:E:478:ALA:HB2	2.00	0.43
1:K:473:MET:HG3	1:K:478:ALA:HB2	2.00	0.43
2:L:280:ARG:HD2	2:L:395:PHE:CD1	2.53	0.43
2:G:345:PRO:HB2	2:G:438:VAL:HG21	1.98	0.43
1:E:219:GLY:HA2	3:E:601:TW3:C1	2.48	0.43
1:J:224:PRO:CG	1:J:239:ILE:CD1	2.96	0.43
2:L:274:ARG:HD2	2:L:346:VAL:HG23	1.99	0.43
2:L:476:HIS:NE2	2:L:495:GLN:OE1	2.52	0.43
2:L:601:SER:HA	2:L:606:ALA:HA	2.00	0.43
2:L:682:MET:HE2	1:H:405:THR:HG21	1.99	0.43
2:B:391:PRO:HA	2:B:395:PHE:CD1	2.54	0.43
2:F:258:VAL:HG13	2:F:272:PHE:O	2.18	0.43
1:E:413:TYR:HE1	1:E:418:ILE:HG13	1.82	0.43
1:J:112:GLU:OE1	1:J:146:TYR:OH	2.21	0.43
1:J:213:MET:HE2	1:J:213:MET:HB3	1.91	0.43
1:K:121:THR:HG22	1:K:134:ILE:HG23	2.00	0.43
2:L:522:MET:HE1	1:H:25:GLY:N	2.33	0.43
2:B:317:GLY:HA2	2:B:362:ILE:CD1	2.46	0.43
2:B:601:SER:HA	2:B:606:ALA:HA	2.00	0.43
2:B:653:MET:HG3	2:B:679:ALA:CB	2.49	0.43
2:F:614:LEU:HG	2:F:615:GLU:CG	2.46	0.43
2:G:542:GLY:N	1:J:94:GLY:O	2.52	0.43
1:H:476:GLU:OE2	1:H:477:GLN:NE2	2.51	0.43
1:E:408:MET:HE3	1:E:408:MET:HB3	1.87	0.43
1:J:563:MET:HE2	1:J:563:MET:HB2	1.68	0.43
1:K:247:VAL:CG2	1:C:409:VAL:HG11	2.45	0.43
2:L:662:VAL:O	2:L:662:VAL:HG13	2.18	0.43
2:L:681:LYS:HZ2	2:L:681:LYS:HB2	1.83	0.43
2:B:160:MET:HA	2:B:166:SER:HB3	1.99	0.43
2:B:381:ALA:HA	2:B:439:VAL:O	2.19	0.43
1:H:201:MET:CE	1:H:208:GLN:NE2	2.78	0.43
4:H:601:BTI:HN2	4:H:601:BTI:H72	1.71	0.43
2:I:529:GLN:H	2:I:529:GLN:HG3	1.56	0.43
2:M:150:ILE:HD13	2:M:360:LEU:CD2	2.46	0.43
1:E:147:PRO:HA	1:E:150:VAL:HG12	2.01	0.43
1:J:466:PRO:O	1:J:519:PRO:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:ARG:HA	1:C:456:ALA:HA	2.00	0.43
2:L:391:PRO:HA	2:L:395:PHE:CD1	2.54	0.43
2:L:485:HIS:CE1	2:L:488:PHE:HA	2.53	0.43
2:B:393:ASN:CB	2:B:396:MET:HG2	2.49	0.43
2:B:676:VAL:HA	2:B:684:HIS:O	2.19	0.43
2:M:637:LEU:HD23	2:M:637:LEU:HA	1.88	0.43
2:M:667:LYS:HG2	2:M:693:THR:OG1	2.19	0.43
1:K:563:MET:OXT	1:J:563:MET:SD	2.77	0.43
1:A:147:PRO:HA	1:A:150:VAL:HG12	2.01	0.43
1:A:473:MET:HG3	1:A:478:ALA:HB2	2.00	0.43
2:B:637:LEU:HD23	2:B:637:LEU:HA	1.84	0.43
2:B:661:PHE:HB2	2:B:673:SER:O	2.19	0.43
2:B:662:VAL:O	2:B:662:VAL:HG13	2.18	0.43
1:C:404:ILE:HG13	1:C:444:SER:HA	2.00	0.43
2:F:662:VAL:HG23	2:F:666:ASP:HB3	2.00	0.43
2:G:662:VAL:HG23	2:G:666:ASP:HB3	2.00	0.43
1:H:487:LYS:HA	1:H:497:PHE:HD2	1.84	0.43
2:M:281:ARG:HH22	2:M:394:ASN:HD21	1.67	0.43
2:M:382:PHE:O	2:M:438:VAL:HA	2.19	0.43
1:K:147:PRO:HA	1:K:150:VAL:HG12	2.01	0.42
1:K:408:MET:HE3	1:K:408:MET:HB3	1.87	0.42
2:L:487:ASP:O	2:L:490:PRO:HD2	2.18	0.42
1:A:241:LEU:CD1	1:H:419:ALA:HB2	2.27	0.42
2:B:274:ARG:HD3	2:B:347:THR:HB	2.01	0.42
1:C:81:LEU:N	1:C:280:ASP:OD2	2.49	0.42
2:M:258:VAL:HG13	2:M:272:PHE:O	2.18	0.42
2:M:273:GLU:OE1	2:M:302:LEU:CD2	2.67	0.42
2:M:441:ALA:HB3	2:M:447:ALA:HB2	2.01	0.42
2:M:680:MET:HE3	2:M:680:MET:HB2	1.78	0.42
1:E:223:VAL:N	1:E:224:PRO:HD2	2.34	0.42
1:J:452:MET:HE3	1:J:452:MET:HB3	1.88	0.42
1:J:473:MET:HG3	1:J:478:ALA:HB2	2.00	0.42
2:B:696:LYS:HG2	2:B:697:VAL:N	2.35	0.42
1:C:487:LYS:HA	1:C:497:PHE:HD2	1.84	0.42
2:I:248:LYS:HD2	2:I:248:LYS:HA	1.47	0.42
2:I:382:PHE:O	2:I:438:VAL:HA	2.19	0.42
2:I:667:LYS:HG2	2:I:693:THR:OG1	2.19	0.42
2:M:271:LEU:HD23	2:M:351:THR:HG21	2.01	0.42
2:L:253:PRO:HB2	2:L:486:THR:N	2.32	0.42
2:B:476:HIS:NE2	2:B:495:GLN:OE1	2.52	0.42
2:B:675:MET:HE3	2:B:711:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:134:GLU:CD	2:F:339:ARG:HD3	2.43	0.42
2:G:387:TYR:CE1	2:G:433:MET:HG3	2.54	0.42
2:I:273:GLU:OE1	2:I:302:LEU:CD2	2.67	0.42
2:I:559:LYS:HE2	2:I:559:LYS:HB2	1.74	0.42
1:K:466:PRO:O	1:K:519:PRO:HG2	2.19	0.42
2:L:393:ASN:CB	2:L:396:MET:HG2	2.49	0.42
2:L:653:MET:HG3	2:L:679:ALA:CB	2.49	0.42
2:B:517:LEU:HD12	2:B:598:LEU:CD1	2.50	0.42
2:F:273:GLU:OE1	2:F:302:LEU:CD2	2.67	0.42
2:G:386:ILE:HD12	2:G:467:ILE:HG12	2.00	0.42
2:I:254:ARG:HB2	2:I:325:MET:O	2.18	0.42
2:M:542:GLY:N	1:E:94:GLY:O	2.52	0.42
1:K:376:LEU:HD23	1:K:376:LEU:HA	1.89	0.42
2:L:411:ASP:OD2	2:L:412:PRO:HD2	2.16	0.42
2:L:517:LEU:HD12	2:L:598:LEU:CD1	2.50	0.42
2:L:659:LYS:HD3	2:L:661:PHE:CE1	2.54	0.42
2:L:681:LYS:HZ3	4:H:601:BTI:C11	2.11	0.42
2:B:274:ARG:HD2	2:B:346:VAL:HG23	1.99	0.42
2:G:382:PHE:O	2:G:438:VAL:HA	2.19	0.42
2:G:407:THR:HB	2:G:416:ILE:HD13	2.01	0.42
1:H:404:ILE:HG13	1:H:444:SER:HA	2.00	0.42
2:I:407:THR:HB	2:I:416:ILE:HD13	2.01	0.42
1:K:278:LEU:HD21	2:L:641:SER:HB2	2.00	0.42
1:A:224:PRO:CG	1:A:239:ILE:CD1	2.96	0.42
1:C:477:GLN:H	1:C:477:GLN:HG2	1.68	0.42
1:H:81:LEU:N	1:H:280:ASP:OD2	2.49	0.42
2:I:265:HIS:CD2	2:I:265:HIS:H	2.38	0.42
2:M:254:ARG:H	2:M:486:THR:H	1.67	0.42
1:J:219:GLY:HA2	3:J:601:TW3:C1	2.48	0.42
2:L:682:MET:HE2	2:L:682:MET:HB3	1.91	0.42
1:A:97:PHE:CZ	1:A:122:GLY:HA3	2.55	0.42
2:B:443:ASP:OD2	2:B:446:ALA:N	2.44	0.42
2:B:659:LYS:HD3	2:B:661:PHE:CE1	2.54	0.42
2:F:651:ALA:HB1	2:F:677:MET:HE1	1.99	0.42
1:H:147:PRO:HA	1:H:150:VAL:HG12	2.01	0.42
2:M:290:PRO:HB3	2:M:299:ARG:NH1	2.35	0.42
1:K:224:PRO:CG	1:K:239:ILE:CD1	2.96	0.42
2:L:513:LEU:HD22	2:L:585:VAL:CG1	2.49	0.42
1:A:241:LEU:HD22	1:H:419:ALA:CA	2.49	0.42
1:H:97:PHE:CZ	1:H:122:GLY:HA3	2.55	0.42
1:H:326:LYS:HA	1:H:326:LYS:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:313:VAL:HG23	2:M:315:TYR:HB2	2.02	0.42
2:M:662:VAL:HG23	2:M:666:ASP:HB3	2.00	0.42
1:K:201:MET:HE3	1:K:208:GLN:HE22	1.85	0.42
2:L:274:ARG:HD3	2:L:347:THR:HB	2.01	0.42
2:L:623:LYS:HE2	2:L:623:LYS:H	1.85	0.42
2:L:661:PHE:HB2	2:L:673:SER:O	2.19	0.42
2:L:696:LYS:HG2	2:L:697:VAL:N	2.35	0.42
2:B:344:HIS:O	2:B:348:GLU:HG3	2.20	0.42
2:F:265:HIS:CD2	2:F:265:HIS:H	2.38	0.42
2:F:271:LEU:HD23	2:F:351:THR:HG21	2.01	0.42
2:F:382:PHE:O	2:F:438:VAL:HA	2.19	0.42
2:F:494:LYS:H	2:F:494:LYS:HG2	1.36	0.42
2:G:453:TYR:HE1	2:G:623:LYS:CD	2.28	0.42
1:E:81:LEU:N	1:E:280:ASP:OD2	2.49	0.42
1:E:426:VAL:HG12	1:J:226:MET:CE	2.36	0.42
1:J:97:PHE:CZ	1:J:122:GLY:HA3	2.55	0.42
1:J:223:VAL:N	1:J:224:PRO:HD2	2.34	0.42
1:A:83:PRO:HA	1:A:86:ARG:HD2	2.02	0.42
1:A:179:PRO:O	1:A:180:ARG:HB2	2.20	0.42
1:A:223:VAL:N	1:A:224:PRO:HD2	2.34	0.42
2:B:463:LEU:HD12	2:B:464:HIS:O	2.20	0.42
2:B:682:MET:HE2	2:B:682:MET:HB3	1.90	0.42
2:G:313:VAL:HG23	2:G:315:TYR:HB2	2.02	0.42
1:H:390:LEU:HD23	1:H:390:LEU:HA	1.92	0.42
2:M:386:ILE:HD12	2:M:467:ILE:HG12	2.02	0.42
2:M:407:THR:HB	2:M:416:ILE:HD13	2.01	0.42
1:J:62:HIS:O	1:J:65:LEU:HB2	2.20	0.42
1:K:62:HIS:O	1:K:65:LEU:HB2	2.20	0.41
2:L:676:VAL:HA	2:L:684:HIS:O	2.19	0.41
1:A:201:MET:HE3	1:A:208:GLN:HE22	1.85	0.41
1:A:492:ARG:HD2	1:A:492:ARG:HA	1.82	0.41
2:B:522:MET:HB3	2:B:522:MET:HE2	1.70	0.41
1:C:355:LEU:HD12	1:C:371:GLY:O	2.20	0.41
2:F:386:ILE:HD12	2:F:467:ILE:HG12	2.01	0.41
2:I:150:ILE:HD13	2:I:360:LEU:CD2	2.46	0.41
1:E:201:MET:HE3	1:E:208:GLN:HE22	1.85	0.41
1:J:201:MET:HE3	1:J:208:GLN:HE22	1.85	0.41
1:K:223:VAL:N	1:K:224:PRO:HD2	2.34	0.41
2:L:152:PRO:HG3	2:L:338:THR:HG21	2.02	0.41
2:L:637:LEU:HD23	2:L:637:LEU:HA	1.84	0.41
1:A:278:LEU:HD21	2:B:641:SER:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:HD12	1:A:371:GLY:O	2.20	0.41
1:A:389:GLN:HE22	1:E:561:PHE:H	1.67	0.41
1:A:466:PRO:O	1:A:519:PRO:HG2	2.19	0.41
1:C:147:PRO:HA	1:C:150:VAL:HG12	2.01	0.41
2:I:453:TYR:HE1	2:I:623:LYS:CD	2.28	0.41
1:J:83:PRO:HA	1:J:86:ARG:HD2	2.02	0.41
1:K:241:LEU:HD12	1:K:241:LEU:HA	1.92	0.41
1:K:241:LEU:HD22	1:C:419:ALA:CA	2.50	0.41
1:K:265:LEU:HD23	1:K:266:HIS:N	2.35	0.41
2:B:255:HIS:ND1	2:B:276:CYS:HB3	2.31	0.41
2:B:659:LYS:HA	2:B:701:GLU:OE2	2.21	0.41
2:G:265:HIS:CD2	2:G:265:HIS:H	2.38	0.41
2:G:271:LEU:HD23	2:G:351:THR:HG21	2.01	0.41
2:G:610:LYS:HB3	2:G:621:PHE:HB2	2.02	0.41
1:H:62:HIS:O	1:H:65:LEU:HB2	2.20	0.41
2:I:290:PRO:HB3	2:I:299:ARG:NH1	2.35	0.41
1:E:65:LEU:HD23	1:E:65:LEU:HA	1.81	0.41
1:E:411:ARG:H	1:E:411:ARG:HG2	1.61	0.41
2:L:344:HIS:O	2:L:348:GLU:HG3	2.20	0.41
2:L:659:LYS:HA	2:L:701:GLU:OE2	2.20	0.41
1:A:81:LEU:N	1:A:280:ASP:OD2	2.49	0.41
2:B:682:MET:SD	2:B:684:HIS:NE2	2.90	0.41
2:F:407:THR:HB	2:F:416:ILE:HD13	2.01	0.41
2:G:259:GLN:HB3	2:G:271:LEU:HB2	2.03	0.41
2:G:290:PRO:HB3	2:G:299:ARG:NH1	2.35	0.41
2:I:386:ILE:HD12	2:I:467:ILE:HG12	2.02	0.41
2:M:259:GLN:HB3	2:M:271:LEU:HB2	2.02	0.41
1:K:65:LEU:HD23	1:K:65:LEU:HA	1.81	0.41
1:K:83:PRO:HA	1:K:86:ARG:HD2	2.02	0.41
1:K:97:PHE:CZ	1:K:122:GLY:HA3	2.55	0.41
1:K:179:PRO:O	1:K:180:ARG:HB2	2.20	0.41
1:A:462:LEU:O	1:A:529:ASP:HB2	2.20	0.41
2:B:623:LYS:H	2:B:623:LYS:HE2	1.85	0.41
1:C:97:PHE:CZ	1:C:122:GLY:HA3	2.55	0.41
1:C:452:MET:HE3	1:C:452:MET:HB3	1.88	0.41
2:G:273:GLU:OE1	2:G:302:LEU:CD2	2.67	0.41
1:E:179:PRO:O	1:E:180:ARG:HB2	2.20	0.41
1:J:147:PRO:HA	1:J:150:VAL:HG12	2.01	0.41
1:K:25:GLY:O	1:K:26:ASP:C	2.63	0.41
1:A:265:LEU:HD23	1:A:266:HIS:N	2.35	0.41
1:A:361:ARG:NH1	1:A:366:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:ILE:HD13	2:B:621:PHE:HE2	1.86	0.41
1:C:62:HIS:O	1:C:65:LEU:HB2	2.20	0.41
2:M:265:HIS:CD2	2:M:265:HIS:H	2.38	0.41
1:E:83:PRO:HA	1:E:86:ARG:HD2	2.02	0.41
2:L:257:GLU:HA	2:L:321:VAL:O	2.20	0.41
2:L:261:PHE:CZ	2:L:318:ALA:HB2	2.56	0.41
2:L:381:ALA:HA	2:L:439:VAL:O	2.19	0.41
2:B:257:GLU:HA	2:B:322:GLU:HA	2.03	0.41
2:M:653:MET:HE1	2:M:680:MET:HE2	2.03	0.41
1:J:355:LEU:HD12	1:J:371:GLY:O	2.20	0.41
1:K:361:ARG:NH1	1:K:366:PRO:HD3	2.36	0.41
2:L:463:LEU:HD12	2:L:464:HIS:O	2.20	0.41
1:A:62:HIS:O	1:A:65:LEU:HB2	2.20	0.41
1:A:269:LYS:HE3	1:A:269:LYS:HB2	1.62	0.41
2:B:258:VAL:O	2:B:320:THR:HA	2.21	0.41
2:B:343:GLU:HG2	2:B:385:ARG:NH2	2.35	0.41
2:G:590:TYR:OH	2:G:608:LYS:HD3	2.21	0.41
2:G:637:LEU:HD23	2:G:637:LEU:HA	1.88	0.41
2:I:271:LEU:HD23	2:I:351:THR:HG21	2.01	0.41
1:E:97:PHE:CZ	1:E:122:GLY:HA3	2.55	0.41
1:E:265:LEU:HD23	1:E:266:HIS:N	2.35	0.41
1:E:355:LEU:HD12	1:E:371:GLY:O	2.20	0.41
1:J:179:PRO:O	1:J:180:ARG:HB2	2.20	0.41
1:J:221:ALA:O	1:J:224:PRO:CD	2.67	0.41
1:J:265:LEU:HD23	1:J:266:HIS:N	2.35	0.41
1:K:561:PHE:HB3	1:J:563:MET:HE1	2.02	0.41
2:L:257:GLU:HA	2:L:322:GLU:HA	2.03	0.41
2:L:660:VAL:HG23	2:L:675:MET:HG3	2.03	0.41
2:L:675:MET:HE3	2:L:711:LEU:HD23	2.01	0.41
2:B:257:GLU:HA	2:B:321:VAL:O	2.20	0.41
1:C:83:PRO:HA	1:C:86:ARG:HD2	2.02	0.41
1:C:473:MET:HE2	1:C:473:MET:HB3	1.93	0.41
2:F:290:PRO:HB3	2:F:299:ARG:NH1	2.35	0.41
2:F:313:VAL:HG23	2:F:315:TYR:HB2	2.02	0.41
2:F:590:TYR:OH	2:F:608:LYS:HD3	2.21	0.41
2:G:441:ALA:HB3	2:G:447:ALA:HB2	2.02	0.41
2:G:453:TYR:CE1	2:G:623:LYS:HD3	2.47	0.41
2:G:635:LYS:H	2:G:635:LYS:HG3	1.63	0.41
1:H:83:PRO:HA	1:H:86:ARG:HD2	2.02	0.41
1:H:355:LEU:HD12	1:H:371:GLY:O	2.20	0.41
2:I:590:TYR:OH	2:I:608:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:610:LYS:HB3	2:I:621:PHE:HB2	2.02	0.41
2:M:63:ARG:HH22	2:M:354:ASP:CG	2.28	0.41
2:L:253:PRO:HB3	2:L:486:THR:HG22	2.03	0.41
2:L:280:ARG:HH22	2:L:466:ASN:HD22	1.69	0.41
2:L:343:GLU:HG2	2:L:385:ARG:NH2	2.36	0.41
1:A:344:PHE:CZ	1:A:358:GLY:HA3	2.56	0.41
2:B:261:PHE:CZ	2:B:318:ALA:HB2	2.56	0.41
2:B:469:PHE:CZ	2:B:496:LEU:HD13	2.55	0.41
2:I:176:PRO:O	2:I:333:PHE:HB3	2.21	0.41
2:I:586:LEU:O	2:I:586:LEU:HD12	2.21	0.41
1:J:49:MET:CG	1:J:318:TYR:CD1	3.04	0.41
1:J:344:PHE:CZ	1:J:358:GLY:HA3	2.56	0.41
1:K:213:MET:HE2	1:K:213:MET:HB3	1.92	0.40
2:L:469:PHE:CZ	2:L:496:LEU:HD13	2.55	0.40
2:B:280:ARG:HH22	2:B:466:ASN:HD22	1.69	0.40
2:G:66:ARG:CG	2:G:91:MET:HE1	2.51	0.40
1:H:344:PHE:CZ	1:H:358:GLY:HA3	2.56	0.40
2:I:259:GLN:HB3	2:I:271:LEU:HB2	2.03	0.40
1:E:62:HIS:O	1:E:65:LEU:HB2	2.20	0.40
1:E:525:ARG:H	1:E:525:ARG:HG2	1.68	0.40
1:J:64:LYS:O	1:J:64:LYS:HG2	2.21	0.40
1:K:344:PHE:CZ	1:K:358:GLY:HA3	2.56	0.40
1:K:543:LEU:HD21	2:L:536:PRO:HB2	2.04	0.40
2:L:532:ASP:CG	2:L:535:SER:HB3	2.47	0.40
2:B:675:MET:CE	2:B:711:LEU:CB	2.89	0.40
1:C:64:LYS:O	1:C:64:LYS:HG2	2.21	0.40
1:C:117:GLY:O	1:C:149:THR:OG1	2.31	0.40
1:C:221:ALA:O	1:C:224:PRO:HD2	2.21	0.40
1:H:221:ALA:O	1:H:224:PRO:HD2	2.21	0.40
2:M:248:LYS:HA	2:M:248:LYS:HD2	1.49	0.40
1:E:326:LYS:HA	1:E:326:LYS:HD3	1.80	0.40
1:J:361:ARG:NH1	1:J:366:PRO:HD3	2.36	0.40
1:K:98:LEU:HD12	2:L:545:LEU:HD11	2.03	0.40
1:K:134:ILE:HD12	1:K:169:TYR:CE2	2.56	0.40
2:L:612:ILE:HD13	2:L:621:PHE:HE2	1.86	0.40
1:A:134:ILE:HD12	1:A:169:TYR:CE2	2.57	0.40
1:A:301:ASP:OD1	1:A:301:ASP:N	2.55	0.40
2:B:681:LYS:HE2	1:C:477:GLN:CG	2.49	0.40
1:C:274:ASP:HA	1:J:348:LYS:HG2	2.03	0.40
1:H:271:GLY:O	1:H:272:VAL:C	2.65	0.40
2:I:66:ARG:CG	2:I:91:MET:HE1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:590:TYR:OH	2:M:608:LYS:HD3	2.21	0.40
1:E:224:PRO:CG	1:E:239:ILE:CD1	2.96	0.40
1:E:301:ASP:OD1	1:E:301:ASP:N	2.55	0.40
1:E:361:ARG:NH1	1:E:366:PRO:HD3	2.36	0.40
1:J:177:TYR:HA	3:J:601:TW3:N5	2.36	0.40
1:K:355:LEU:HD12	1:K:371:GLY:O	2.21	0.40
1:K:490:ARG:HB3	1:K:495:LYS:O	2.22	0.40
2:L:612:ILE:HD13	2:L:621:PHE:CE2	2.56	0.40
2:L:711:LEU:HD12	2:L:711:LEU:N	2.37	0.40
1:A:221:ALA:O	1:A:224:PRO:CD	2.67	0.40
1:A:490:ARG:HB3	1:A:495:LYS:O	2.22	0.40
2:B:126:HIS:CD2	2:B:150:ILE:HG21	2.56	0.40
2:G:653:MET:HE1	2:G:680:MET:HE2	2.03	0.40
1:H:49:MET:CG	1:H:318:TYR:CD1	3.04	0.40
1:H:412:GLU:HG2	1:H:413:TYR:N	2.37	0.40
2:I:313:VAL:HG23	2:I:315:TYR:HB2	2.02	0.40
1:E:294:LEU:HD23	1:E:294:LEU:HA	1.95	0.40
1:E:492:ARG:HA	1:E:492:ARG:HD2	1.82	0.40
1:K:121:THR:HA	1:K:133:ILE:O	2.22	0.40
1:K:301:ASP:N	1:K:301:ASP:OD1	2.55	0.40
2:L:126:HIS:CD2	2:L:150:ILE:HG21	2.56	0.40
2:L:687:LYS:O	2:L:689:PRO:HD3	2.22	0.40
1:A:98:LEU:HD12	2:B:545:LEU:HD11	2.03	0.40
1:A:452:MET:HE3	1:A:452:MET:HB3	1.88	0.40
2:B:152:PRO:HG3	2:B:338:THR:HG21	2.02	0.40
2:B:389:GLU:HA	2:B:396:MET:O	2.22	0.40
2:B:612:ILE:HD13	2:B:621:PHE:CE2	2.56	0.40
2:B:650:LEU:HB3	2:B:708:HIS:HA	2.03	0.40
2:F:586:LEU:HD12	2:F:586:LEU:O	2.21	0.40
2:F:610:LYS:HB3	2:F:621:PHE:HB2	2.02	0.40
2:F:653:MET:HE1	2:F:680:MET:HE2	2.03	0.40
2:F:680:MET:HE3	2:F:680:MET:HB2	1.78	0.40
1:H:121:THR:HA	1:H:133:ILE:O	2.22	0.40
1:J:492:ARG:HA	1:J:492:ARG:HD2	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	539/563 (96%)	521 (97%)	18 (3%)	0	100	100
1	C	516/563 (92%)	502 (97%)	14 (3%)	0	100	100
1	E	520/563 (92%)	502 (96%)	17 (3%)	1 (0%)	43	74
1	H	516/563 (92%)	503 (98%)	12 (2%)	1 (0%)	43	74
1	J	518/563 (92%)	500 (96%)	17 (3%)	1 (0%)	43	74
1	K	539/563 (96%)	520 (96%)	17 (3%)	2 (0%)	30	62
2	B	535/725 (74%)	524 (98%)	11 (2%)	0	100	100
2	F	603/725 (83%)	585 (97%)	18 (3%)	0	100	100
2	G	603/725 (83%)	579 (96%)	24 (4%)	0	100	100
2	I	603/725 (83%)	584 (97%)	18 (3%)	1 (0%)	43	74
2	L	535/725 (74%)	524 (98%)	11 (2%)	0	100	100
2	M	603/725 (83%)	585 (97%)	18 (3%)	0	100	100
All	All	6630/7728 (86%)	6429 (97%)	195 (3%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	26	ASP
1	K	529	ASP
1	H	26	ASP
1	E	529	ASP
1	J	529	ASP
2	I	254	ARG

5.3.2 Protein sidechains

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/445 (97%)	419 (97%)	11 (3%)	40	62
1	C	415/445 (93%)	406 (98%)	9 (2%)	45	65
1	E	418/445 (94%)	410 (98%)	8 (2%)	50	68
1	H	415/445 (93%)	404 (97%)	11 (3%)	39	62
1	J	417/445 (94%)	403 (97%)	14 (3%)	32	57
1	K	430/445 (97%)	421 (98%)	9 (2%)	47	66
2	B	456/609 (75%)	456 (100%)	0	100	100
2	F	511/609 (84%)	496 (97%)	15 (3%)	37	60
2	G	511/609 (84%)	495 (97%)	16 (3%)	35	59
2	I	511/609 (84%)	494 (97%)	17 (3%)	33	58
2	L	456/609 (75%)	456 (100%)	0	100	100
2	M	511/609 (84%)	497 (97%)	14 (3%)	39	62
All	All	5481/6324 (87%)	5357 (98%)	124 (2%)	44	64

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	24	HIS
1	K	26	ASP
1	K	236	GLN
1	K	240	PHE
1	K	251	THR
1	K	409	VAL
1	K	425	MET
1	K	472	VAL
1	K	563	MET
1	A	24	HIS
1	A	26	ASP
1	A	27	SER
1	A	236	GLN
1	A	240	PHE
1	A	251	THR
1	A	292	ARG
1	A	409	VAL
1	A	424	LYS

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Mol	Chain	Res	Type
1	A	425	MET
1	A	472	VAL
1	C	26	ASP
1	C	27	SER
1	C	212	VAL
1	C	236	GLN
1	C	238	THR
1	C	265	LEU
1	C	424	LYS
1	C	515	GLU
1	C	527	TRP
2	F	175	VAL
2	F	178	VAL
2	F	248	LYS
2	F	250	VAL
2	F	251	ASP
2	F	252	THR
2	F	254	ARG
2	F	261	PHE
2	F	280	ARG
2	F	443	ASP
2	F	493	HIS
2	F	494	LYS
2	F	495	GLN
2	F	535	SER
2	F	645	THR
2	G	175	VAL
2	G	177	VAL
2	G	178	VAL
2	G	248	LYS
2	G	249	PHE
2	G	250	VAL
2	G	251	ASP
2	G	254	ARG
2	G	256	VAL
2	G	261	PHE
2	G	280	ARG
2	G	493	HIS
2	G	494	LYS
2	G	495	GLN
2	G	498	LEU
2	G	645	THR

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Mol	Chain	Res	Type
1	H	24	HIS
1	H	26	ASP
1	H	212	VAL
1	H	236	GLN
1	H	239	ILE
1	H	265	LEU
1	H	424	LYS
1	H	425	MET
1	H	476	GLU
1	H	515	GLU
1	H	527	TRP
2	I	178	VAL
2	I	247	GLU
2	I	248	LYS
2	I	249	PHE
2	I	252	THR
2	I	254	ARG
2	I	261	PHE
2	I	280	ARG
2	I	443	ASP
2	I	491	GLN
2	I	493	HIS
2	I	494	LYS
2	I	495	GLN
2	I	498	LEU
2	I	529	GLN
2	I	533	GLN
2	I	645	THR
2	M	178	VAL
2	M	248	LYS
2	M	249	PHE
2	M	250	VAL
2	M	252	THR
2	M	254	ARG
2	M	261	PHE
2	M	280	ARG
2	M	491	GLN
2	M	493	HIS
2	M	494	LYS
2	M	495	GLN
2	M	498	LEU
2	M	645	THR

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Mol	Chain	Res	Type
1	E	24	HIS
1	E	26	ASP
1	E	236	GLN
1	E	240	PHE
1	E	409	VAL
1	E	472	VAL
1	E	527	TRP
1	E	563	MET
1	J	24	HIS
1	J	26	ASP
1	J	27	SER
1	J	77	SER
1	J	78	ARG
1	J	236	GLN
1	J	240	PHE
1	J	409	VAL
1	J	425	MET
1	J	472	VAL
1	J	527	TRP
1	J	560	ILE
1	J	562	ARG
1	J	563	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	24	HIS
1	K	102	GLN
1	K	266	HIS
1	K	282	HIS
1	K	389	GLN
1	K	449	ASN
2	L	135	ASN
2	L	283	GLN
2	L	445	GLN
2	L	457	GLN
1	A	24	HIS
1	A	102	GLN
1	A	266	HIS
1	A	282	HIS
1	A	389	GLN
1	A	449	ASN

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Mol	Chain	Res	Type
2	B	135	ASN
2	B	445	GLN
2	B	457	GLN
2	B	485	HIS
1	C	136	ASN
1	C	208	GLN
1	C	282	HIS
1	C	386	HIS
1	C	389	GLN
1	C	449	ASN
1	C	477	GLN
1	C	480	ASN
2	F	85	ASN
2	F	259	GLN
2	F	264	HIS
2	F	359	GLN
2	F	372	GLN
2	F	457	GLN
2	F	493	HIS
2	F	708	HIS
2	G	85	ASN
2	G	259	GLN
2	G	264	HIS
2	G	359	GLN
2	G	429	HIS
2	G	457	GLN
2	G	708	HIS
1	H	136	ASN
1	H	208	GLN
1	H	282	HIS
1	H	389	GLN
1	H	449	ASN
1	H	477	GLN
2	I	85	ASN
2	I	259	GLN
2	I	264	HIS
2	I	359	GLN
2	I	372	GLN
2	I	429	HIS
2	I	457	GLN
2	I	708	HIS
2	M	85	ASN

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Mol	Chain	Res	Type
2	M	259	GLN
2	M	264	HIS
2	M	359	GLN
2	M	372	GLN
2	M	429	HIS
2	M	457	GLN
2	M	492	HIS
2	M	708	HIS
1	E	24	HIS
1	E	266	HIS
1	E	282	HIS
1	E	389	GLN
1	E	449	ASN
1	J	24	HIS
1	J	266	HIS
1	J	282	HIS
1	J	449	ASN
1	J	477	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	TW3	J	601	-	53,56,56	0.45	0	77,83,83	1.19	3 (3%)
4	BTI	I	801	-	15,16,16	0.55	0	20,21,21	0.78	0
4	BTI	G	801	-	15,16,16	0.55	0	20,21,21	0.77	0
3	TW3	E	601	-	53,56,56	0.45	0	77,83,83	1.19	3 (3%)
4	BTI	H	601	-	15,16,16	1.27	1 (6%)	20,21,21	1.77	6 (30%)
4	BTI	C	601	-	15,16,16	1.28	1 (6%)	20,21,21	1.92	5 (25%)
3	TW3	H	602	-	53,56,56	0.45	0	77,83,83	1.19	3 (3%)
4	BTI	M	801	-	15,16,16	0.56	0	20,21,21	0.76	0
3	TW3	K	601	-	53,56,56	0.46	0	77,83,83	1.18	3 (3%)
3	TW3	A	601	-	53,56,56	0.46	0	77,83,83	1.18	3 (3%)
4	BTI	F	801	-	15,16,16	0.57	0	20,21,21	0.77	0
3	TW3	C	602	-	53,56,56	0.45	0	77,83,83	1.19	3 (3%)

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
3	TW3	J	601	-	-	14/54/71/71	0/3/3/3
4	BTI	I	801	-	-	3/6/27/27	0/2/2/2
4	BTI	G	801	-	-	3/6/27/27	0/2/2/2
3	TW3	E	601	-	-	14/54/71/71	0/3/3/3
4	BTI	H	601	-	-	4/6/27/27	0/2/2/2
4	BTI	C	601	-	-	4/6/27/27	0/2/2/2
3	TW3	H	602	-	-	14/54/71/71	0/3/3/3
4	BTI	M	801	-	-	3/6/27/27	0/2/2/2
3	TW3	K	601	-	-	14/54/71/71	0/3/3/3
3	TW3	A	601	-	-	14/54/71/71	0/3/3/3
4	BTI	F	801	-	-	3/6/27/27	0/2/2/2
3	TW3	C	602	-	-	14/54/71/71	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	BTI	C2-S1	-3.62	1.76	1.82
4	H	601	BTI	C2-S1	-3.45	1.77	1.82

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	TW3	C4-C5-S1	7.76	121.18	111.32
3	C	602	TW3	C4-C5-S1	7.75	121.17	111.32
3	J	601	TW3	C4-C5-S1	7.72	121.13	111.32
3	H	602	TW3	C4-C5-S1	7.71	121.12	111.32
3	A	601	TW3	C4-C5-S1	7.68	121.07	111.32
3	K	601	TW3	C4-C5-S1	7.68	121.07	111.32
4	C	601	BTI	C6-C5-N3	-3.98	108.05	113.18
4	H	601	BTI	C2-C4-N2	-3.64	109.49	113.34
4	C	601	BTI	C4-C2-S1	3.59	109.11	105.03
4	C	601	BTI	C6-S1-C2	3.48	97.22	89.98
4	H	601	BTI	C4-C2-S1	3.08	108.53	105.03
3	E	601	TW3	O1-C5-C4	-2.94	121.72	125.41
3	C	602	TW3	O1-C5-C4	-2.92	121.75	125.41
3	J	601	TW3	O1-C5-C4	-2.90	121.77	125.41
3	H	602	TW3	O1-C5-C4	-2.87	121.80	125.41
3	K	601	TW3	O1-C5-C4	-2.87	121.81	125.41
3	A	601	TW3	O1-C5-C4	-2.85	121.83	125.41
4	H	601	BTI	C6-S1-C2	2.83	95.88	89.98
4	C	601	BTI	C8-C7-C2	-2.72	107.80	114.04
4	H	601	BTI	C8-C7-C2	-2.59	108.08	114.04
3	H	602	TW3	O1-C5-S1	-2.57	117.08	122.44
3	C	602	TW3	O1-C5-S1	-2.57	117.08	122.44
3	A	601	TW3	O1-C5-S1	-2.56	117.09	122.44
3	E	601	TW3	O1-C5-S1	-2.56	117.10	122.44
3	J	601	TW3	O1-C5-S1	-2.56	117.10	122.44
3	K	601	TW3	O1-C5-S1	-2.55	117.12	122.44
4	H	601	BTI	C6-C5-N3	-2.40	110.09	113.18
4	C	601	BTI	C5-C6-S1	2.16	109.04	106.06
4	H	601	BTI	C8-C9-C10	-2.04	104.06	113.86

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	601	TW3	N2-C11-C12-C13
3	K	601	TW3	N2-C11-C12-O4

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Mol	Chain	Res	Type	Atoms
3	K	601	TW3	O3-C11-C12-C13
3	K	601	TW3	O3-C11-C12-O4
3	K	601	TW3	C18-C17-O11-P2
3	K	601	TW3	C17-O11-P2-O9
3	A	601	TW3	N2-C11-C12-C13
3	A	601	TW3	N2-C11-C12-O4
3	A	601	TW3	O3-C11-C12-C13
3	A	601	TW3	O3-C11-C12-O4
3	A	601	TW3	C18-C17-O11-P2
3	A	601	TW3	C17-O11-P2-O9
3	C	602	TW3	N2-C11-C12-C13
3	C	602	TW3	N2-C11-C12-O4
3	C	602	TW3	O3-C11-C12-C13
3	C	602	TW3	O3-C11-C12-O4
3	C	602	TW3	C18-C17-O11-P2
3	C	602	TW3	C17-O11-P2-O9
3	H	602	TW3	N2-C11-C12-C13
3	H	602	TW3	N2-C11-C12-O4
3	H	602	TW3	O3-C11-C12-C13
3	H	602	TW3	O3-C11-C12-O4
3	H	602	TW3	C18-C17-O11-P2
3	H	602	TW3	C17-O11-P2-O9
3	E	601	TW3	N2-C11-C12-C13
3	E	601	TW3	N2-C11-C12-O4
3	E	601	TW3	O3-C11-C12-C13
3	E	601	TW3	O3-C11-C12-O4
3	E	601	TW3	C18-C17-O11-P2
3	E	601	TW3	C17-O11-P2-O9
3	J	601	TW3	N2-C11-C12-C13
3	J	601	TW3	N2-C11-C12-O4
3	J	601	TW3	O3-C11-C12-C13
3	J	601	TW3	O3-C11-C12-O4
3	J	601	TW3	C18-C17-O11-P2
3	J	601	TW3	C17-O11-P2-O9
4	C	601	BTI	S1-C2-C7-C8
4	C	601	BTI	C4-C2-C7-C8
4	F	801	BTI	C9-C10-C11-O11
4	G	801	BTI	C9-C10-C11-O11
4	H	601	BTI	C11-C10-C9-C8
4	H	601	BTI	S1-C2-C7-C8
4	H	601	BTI	C4-C2-C7-C8
4	I	801	BTI	C9-C10-C11-O11

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Mol	Chain	Res	Type	Atoms
4	M	801	BTI	C9-C10-C11-O11
3	K	601	TW3	O12-C19-N3-C20
3	A	601	TW3	O12-C19-N3-C20
3	C	602	TW3	O12-C19-N3-C20
3	H	602	TW3	O12-C19-N3-C20
3	E	601	TW3	O12-C19-N3-C20
3	J	601	TW3	O12-C19-N3-C20
3	K	601	TW3	C25-C26-O14-P3
3	A	601	TW3	C25-C26-O14-P3
3	C	602	TW3	C25-C26-O14-P3
3	H	602	TW3	C25-C26-O14-P3
3	E	601	TW3	C25-C26-O14-P3
3	J	601	TW3	C25-C26-O14-P3
3	K	601	TW3	O12-C19-N3-C24
3	A	601	TW3	O12-C19-N3-C24
3	C	602	TW3	O12-C19-N3-C24
3	H	602	TW3	O12-C19-N3-C24
3	E	601	TW3	O12-C19-N3-C24
3	J	601	TW3	O12-C19-N3-C24
3	K	601	TW3	O11-C17-C18-C26
3	A	601	TW3	O11-C17-C18-C26
3	C	602	TW3	O11-C17-C18-C26
3	H	602	TW3	O11-C17-C18-C26
3	E	601	TW3	O11-C17-C18-C26
3	J	601	TW3	O11-C17-C18-C26
3	K	601	TW3	C18-C26-O14-P3
3	A	601	TW3	C18-C26-O14-P3
3	C	602	TW3	C18-C26-O14-P3
3	H	602	TW3	C18-C26-O14-P3
3	E	601	TW3	C18-C26-O14-P3
3	J	601	TW3	C18-C26-O14-P3
3	K	601	TW3	O11-C17-C18-O12
3	A	601	TW3	O11-C17-C18-O12
3	C	602	TW3	O11-C17-C18-O12
3	H	602	TW3	O11-C17-C18-O12
3	E	601	TW3	O11-C17-C18-O12
3	J	601	TW3	O11-C17-C18-O12
4	F	801	BTI	C2-C7-C8-C9
4	G	801	BTI	C2-C7-C8-C9
4	H	601	BTI	C2-C7-C8-C9
4	I	801	BTI	C2-C7-C8-C9
4	M	801	BTI	C2-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	C	601	BTI	C7-C8-C9-C10
4	C	601	BTI	C11-C10-C9-C8
4	F	801	BTI	C11-C10-C9-C8
4	G	801	BTI	C11-C10-C9-C8
4	I	801	BTI	C11-C10-C9-C8
4	M	801	BTI	C11-C10-C9-C8
3	K	601	TW3	C16-O5-P1-O6
3	A	601	TW3	C16-O5-P1-O6
3	C	602	TW3	C16-O5-P1-O6
3	H	602	TW3	C16-O5-P1-O6
3	E	601	TW3	C16-O5-P1-O6
3	J	601	TW3	C16-O5-P1-O6
3	K	601	TW3	C13-C16-O5-P1
3	A	601	TW3	C13-C16-O5-P1
3	C	602	TW3	C13-C16-O5-P1
3	H	602	TW3	C13-C16-O5-P1
3	E	601	TW3	C13-C16-O5-P1
3	J	601	TW3	C13-C16-O5-P1

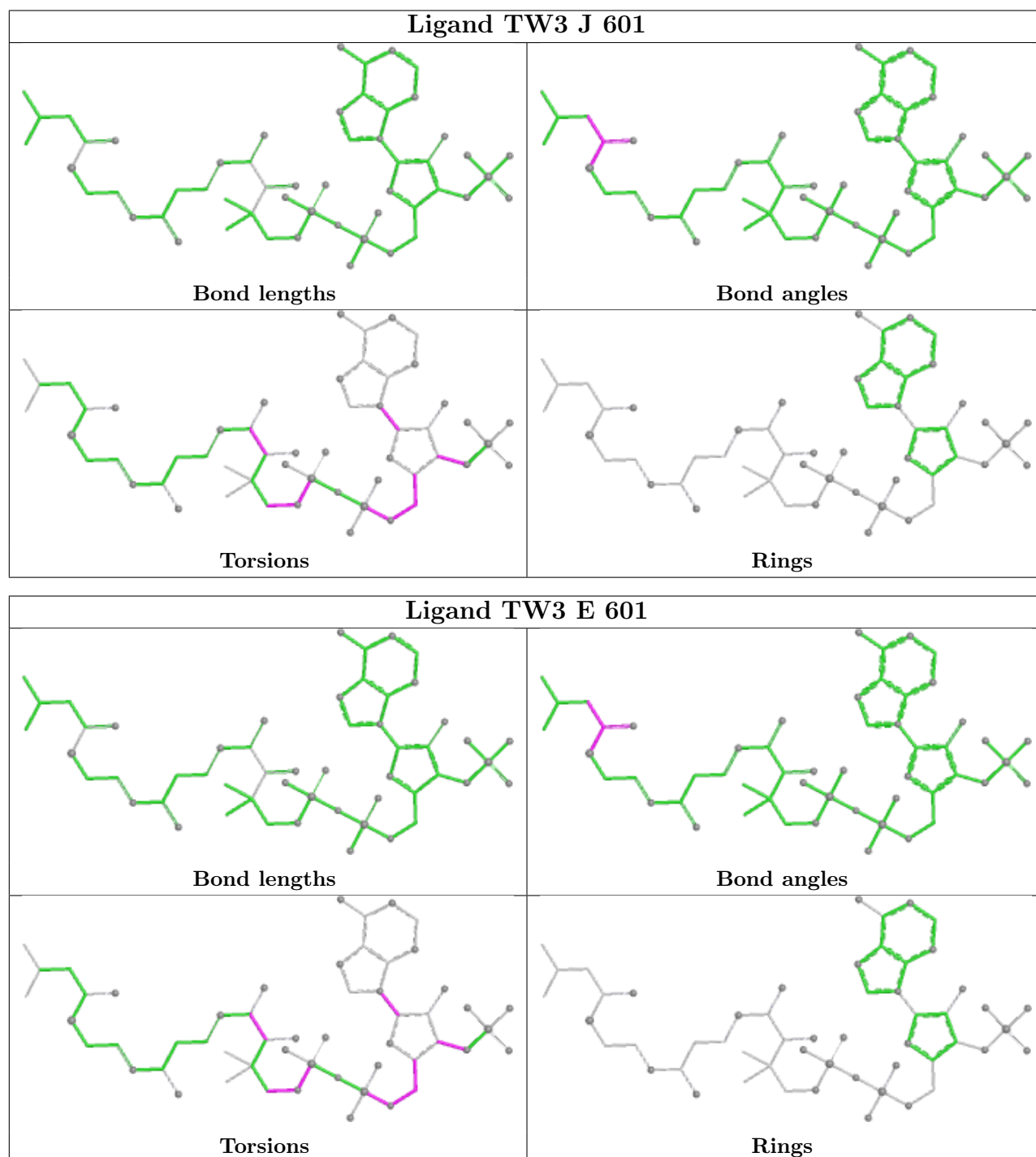
There are no ring outliers.

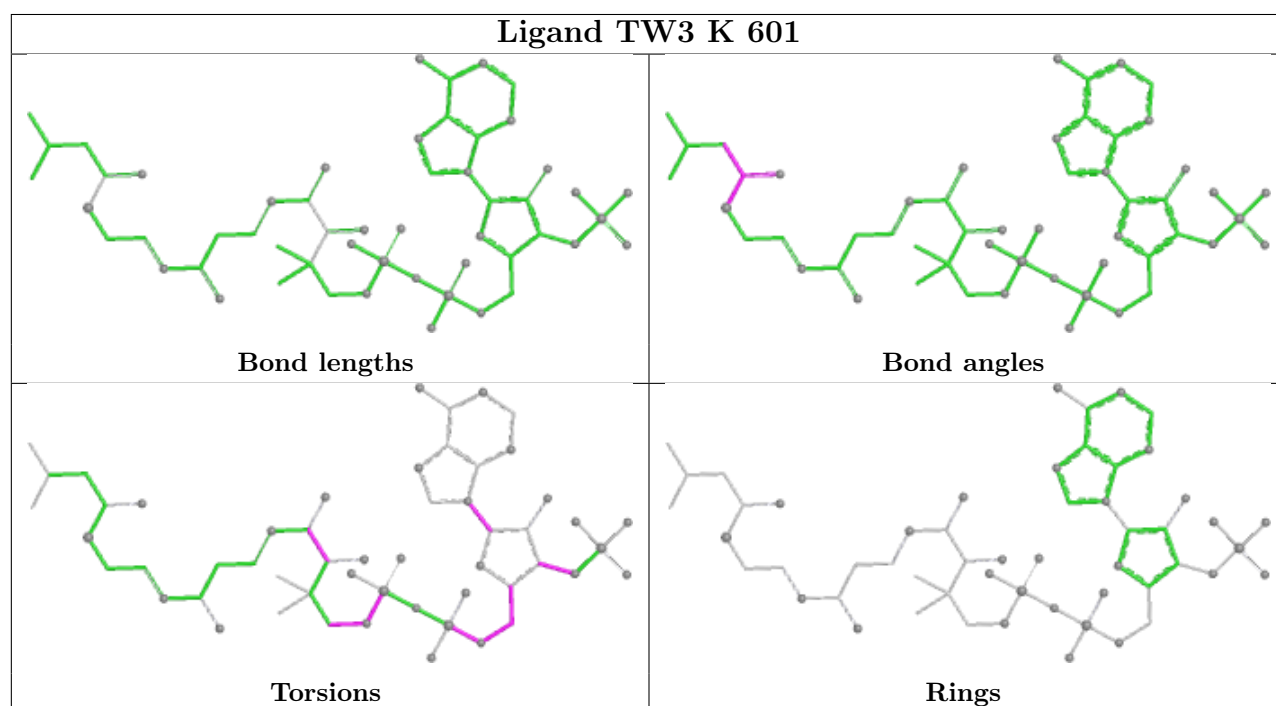
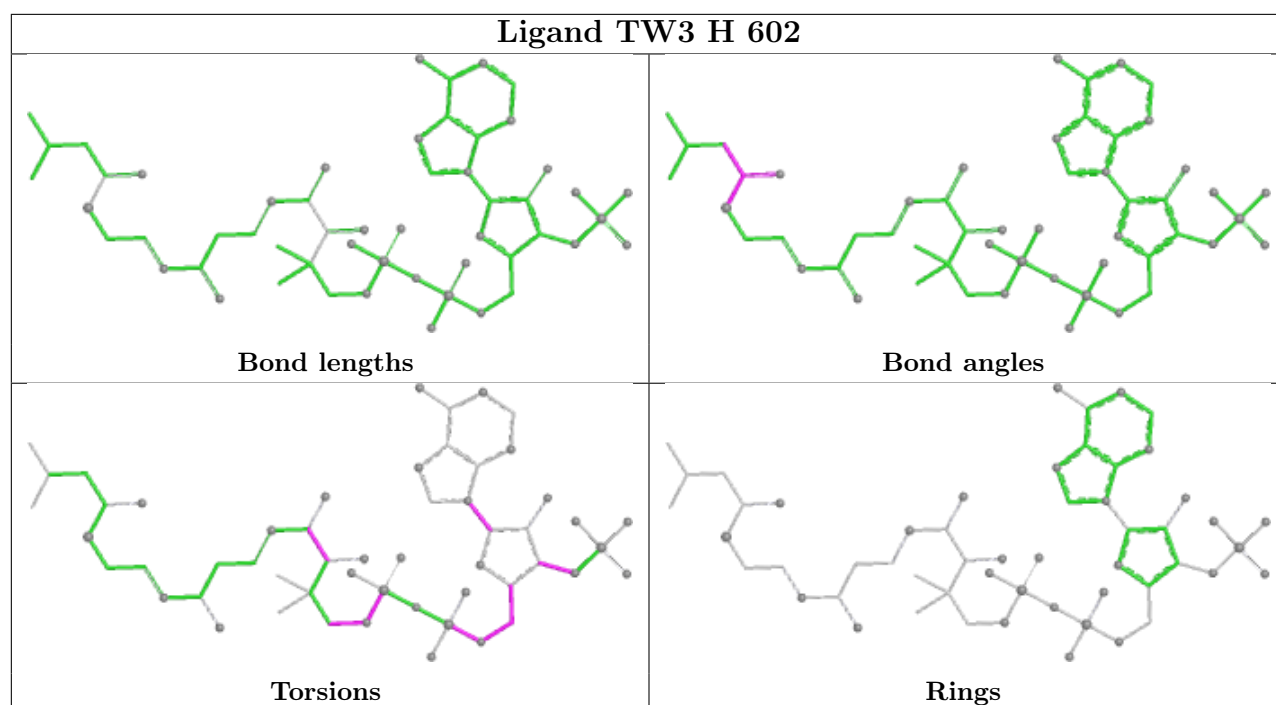
12 monomers are involved in 52 short contacts:

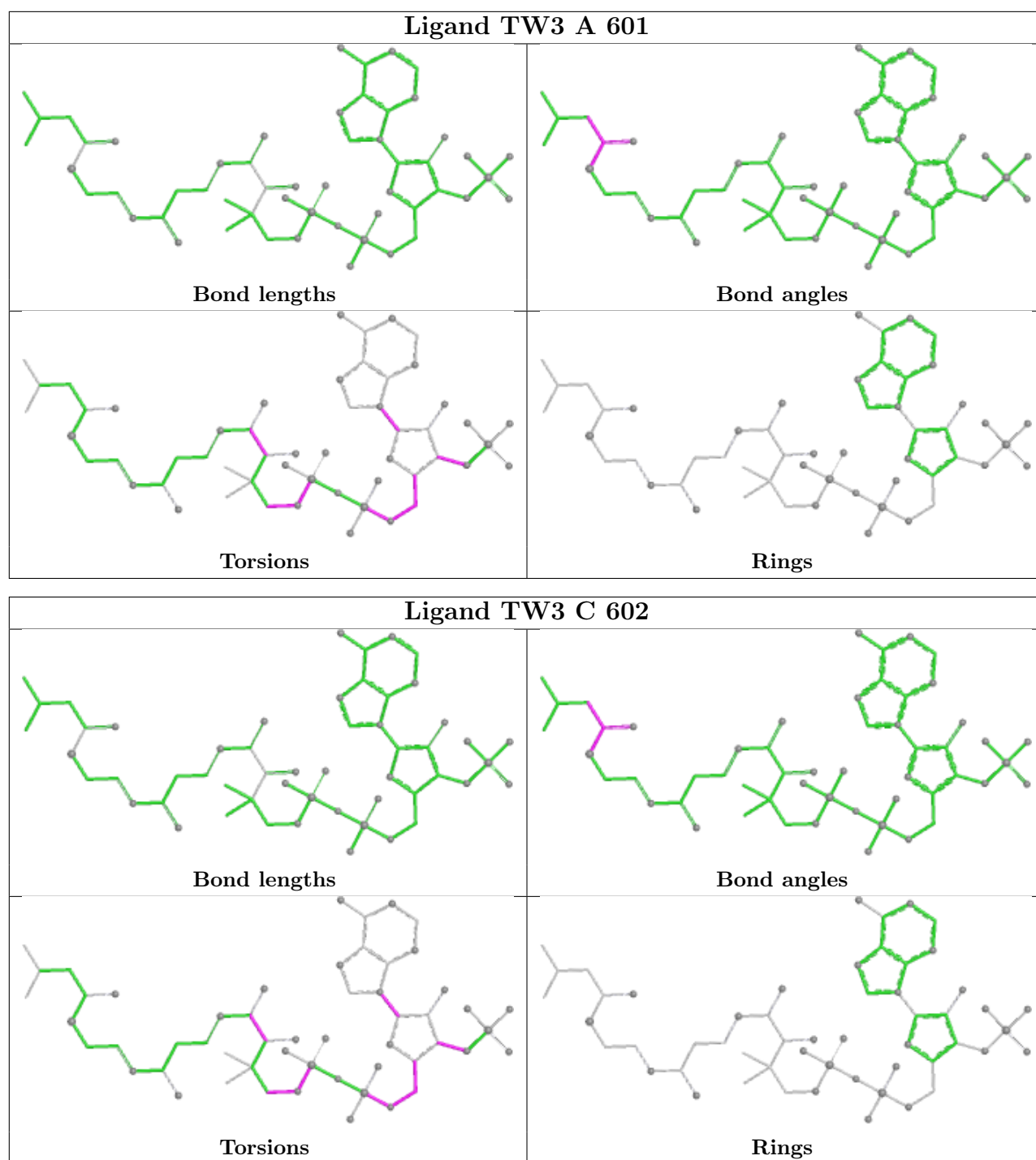
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	601	TW3	4	0
4	I	801	BTI	3	0
4	G	801	BTI	3	0
3	E	601	TW3	3	0
4	H	601	BTI	9	0
4	C	601	BTI	7	0
3	H	602	TW3	6	0
4	M	801	BTI	3	0
3	K	601	TW3	2	0
3	A	601	TW3	2	0
4	F	801	BTI	3	0
3	C	602	TW3	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

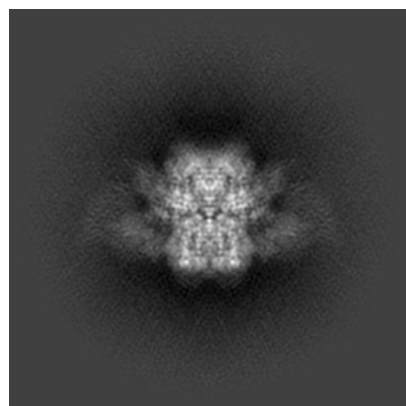
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36705. These allow visual inspection of the internal detail of the map and identification of artifacts.

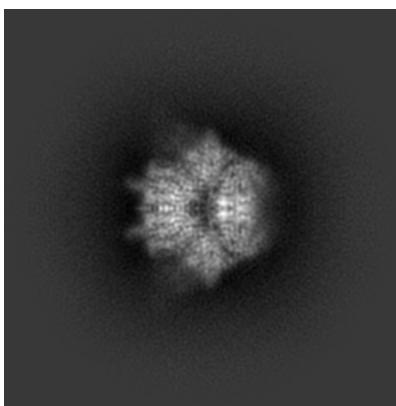
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

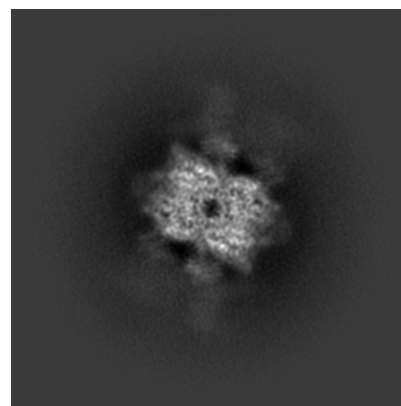
6.1.1 Primary map



X

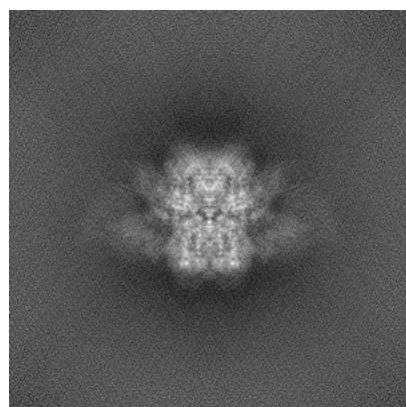


Y

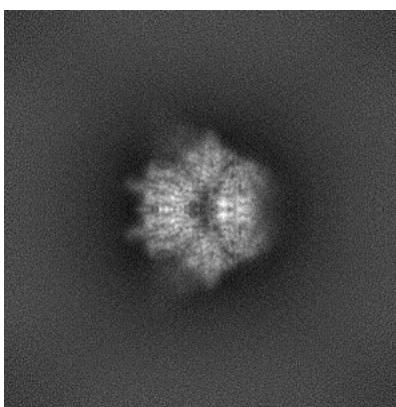


Z

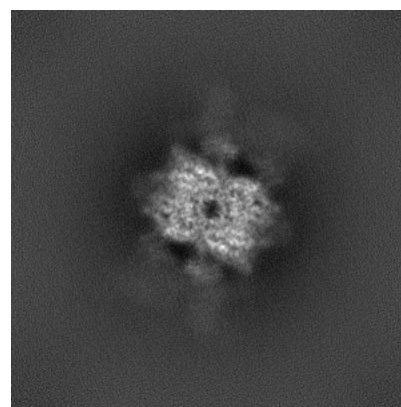
6.1.2 Raw map



X



Y

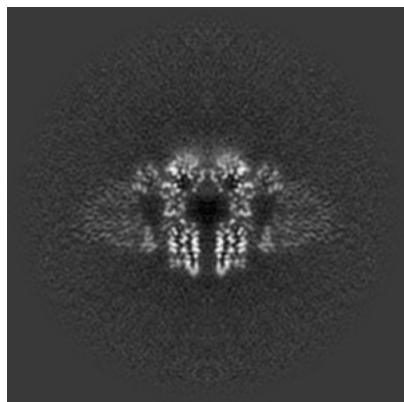


Z

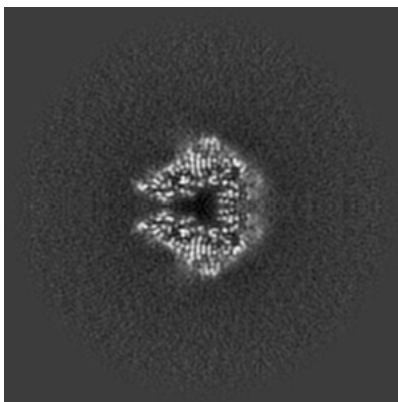
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

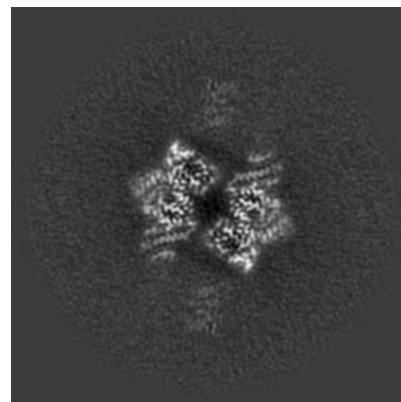
6.2.1 Primary map



X Index: 180

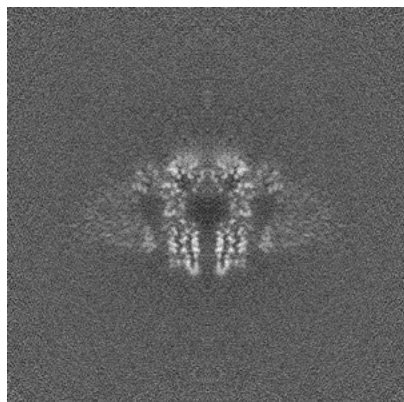


Y Index: 180

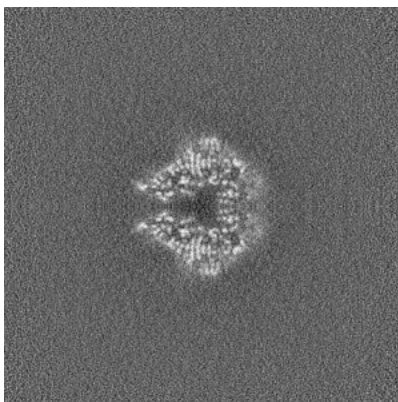


Z Index: 180

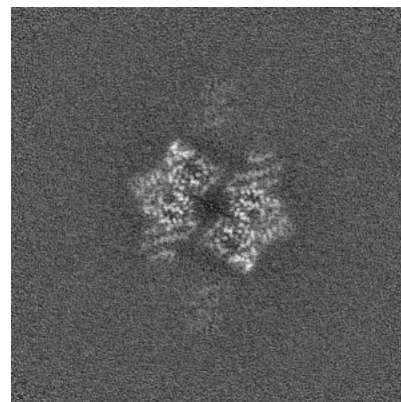
6.2.2 Raw map



X Index: 180



Y Index: 180

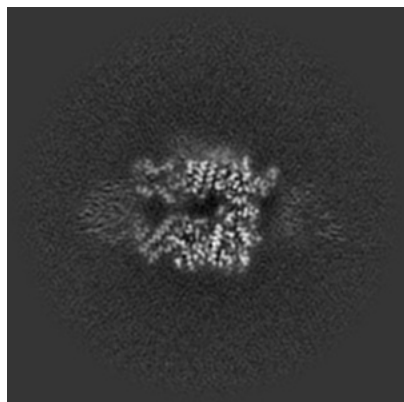


Z Index: 180

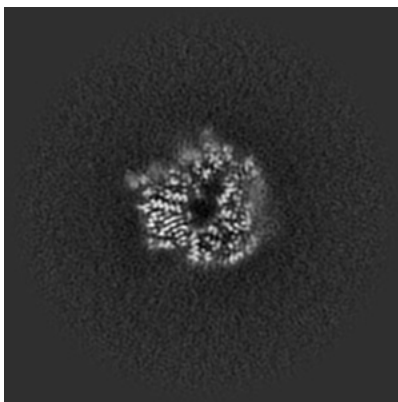
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

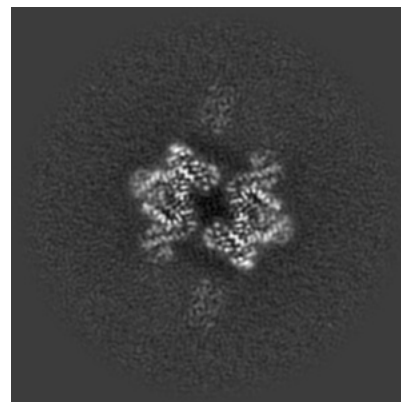
6.3.1 Primary map



X Index: 171

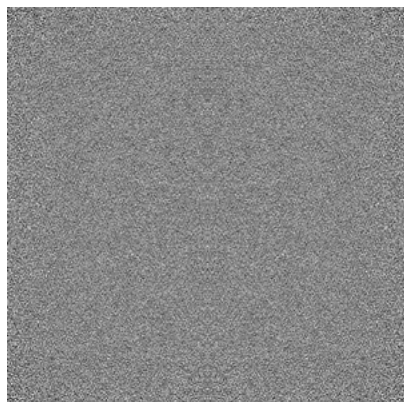


Y Index: 170

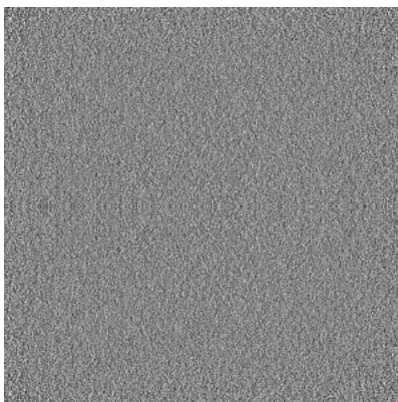


Z Index: 182

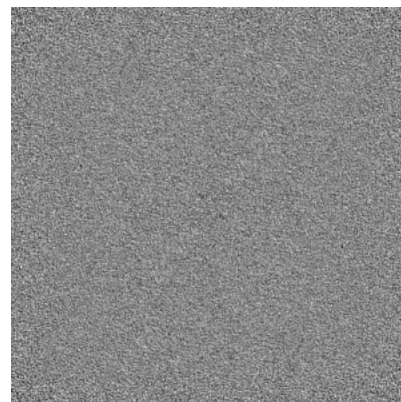
6.3.2 Raw map



X Index: 0



Y Index: 0

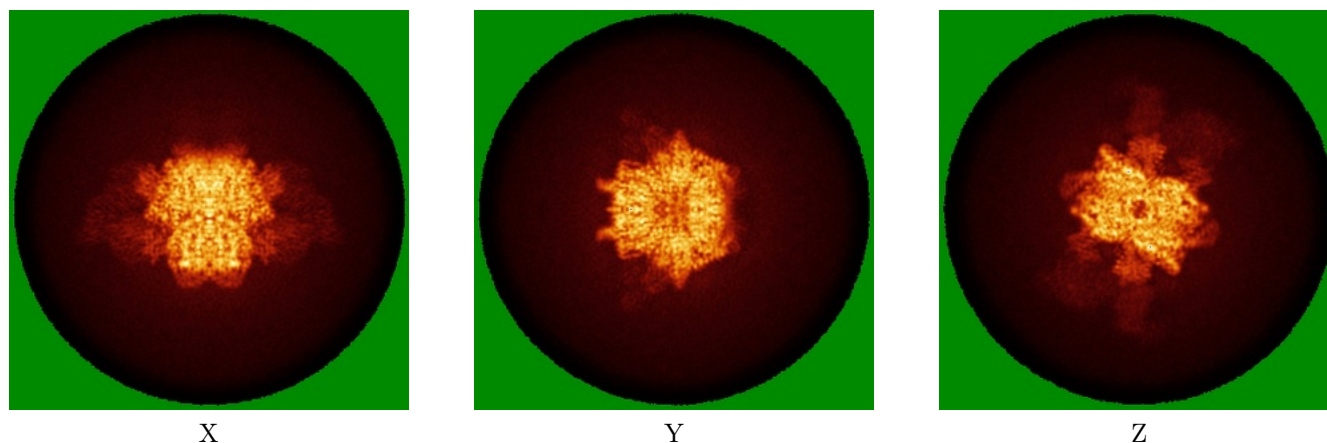


Z Index: 0

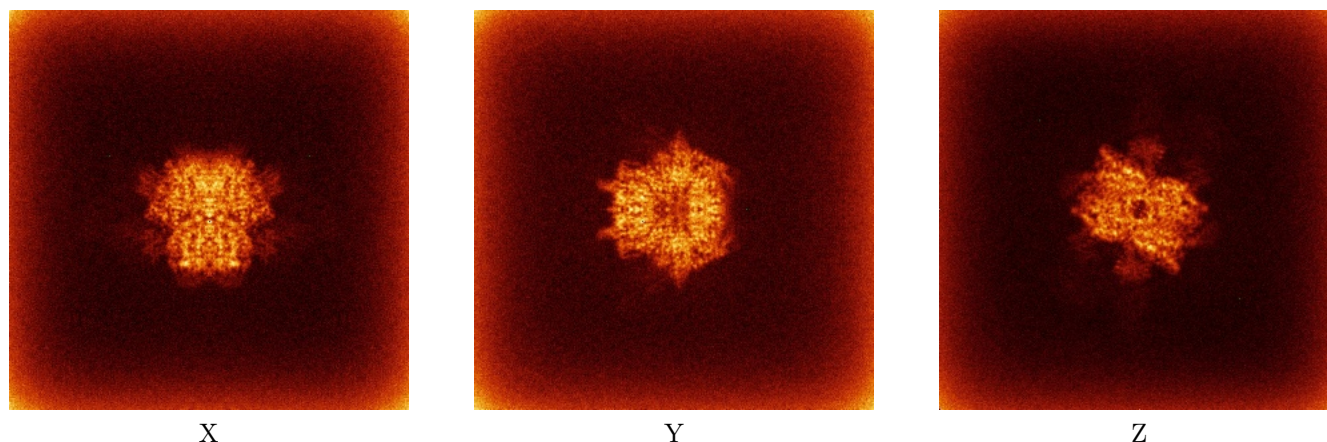
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

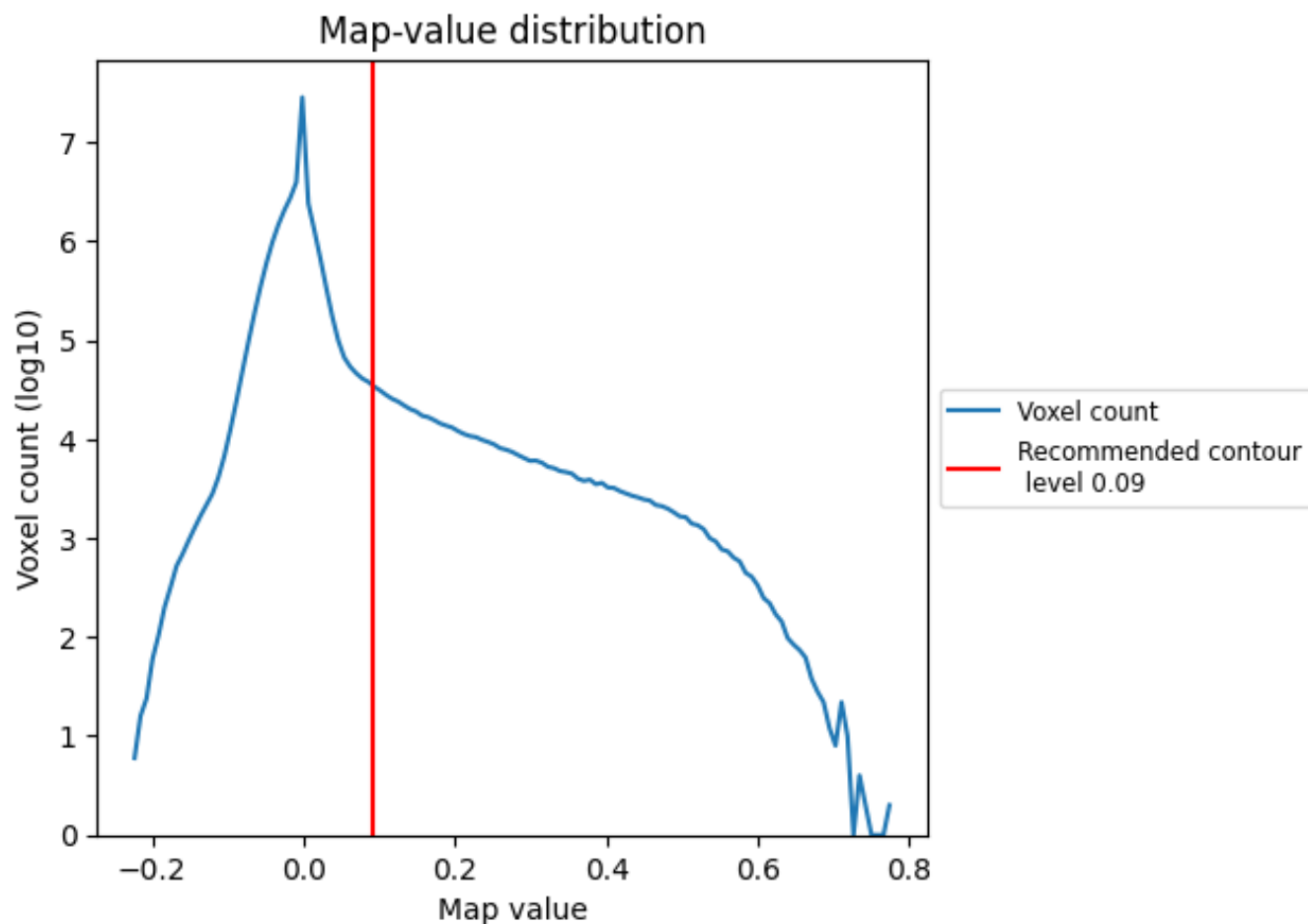
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

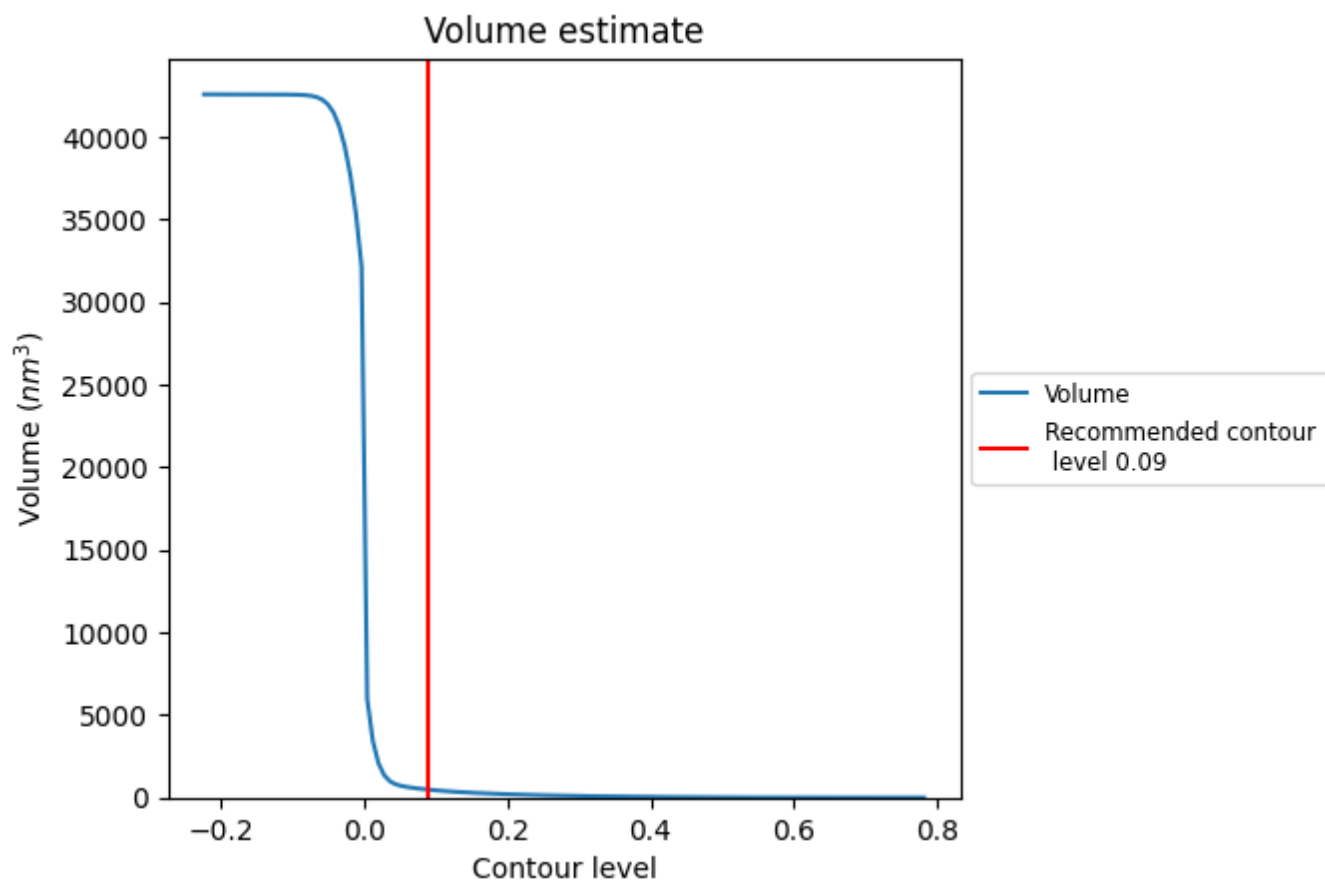
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

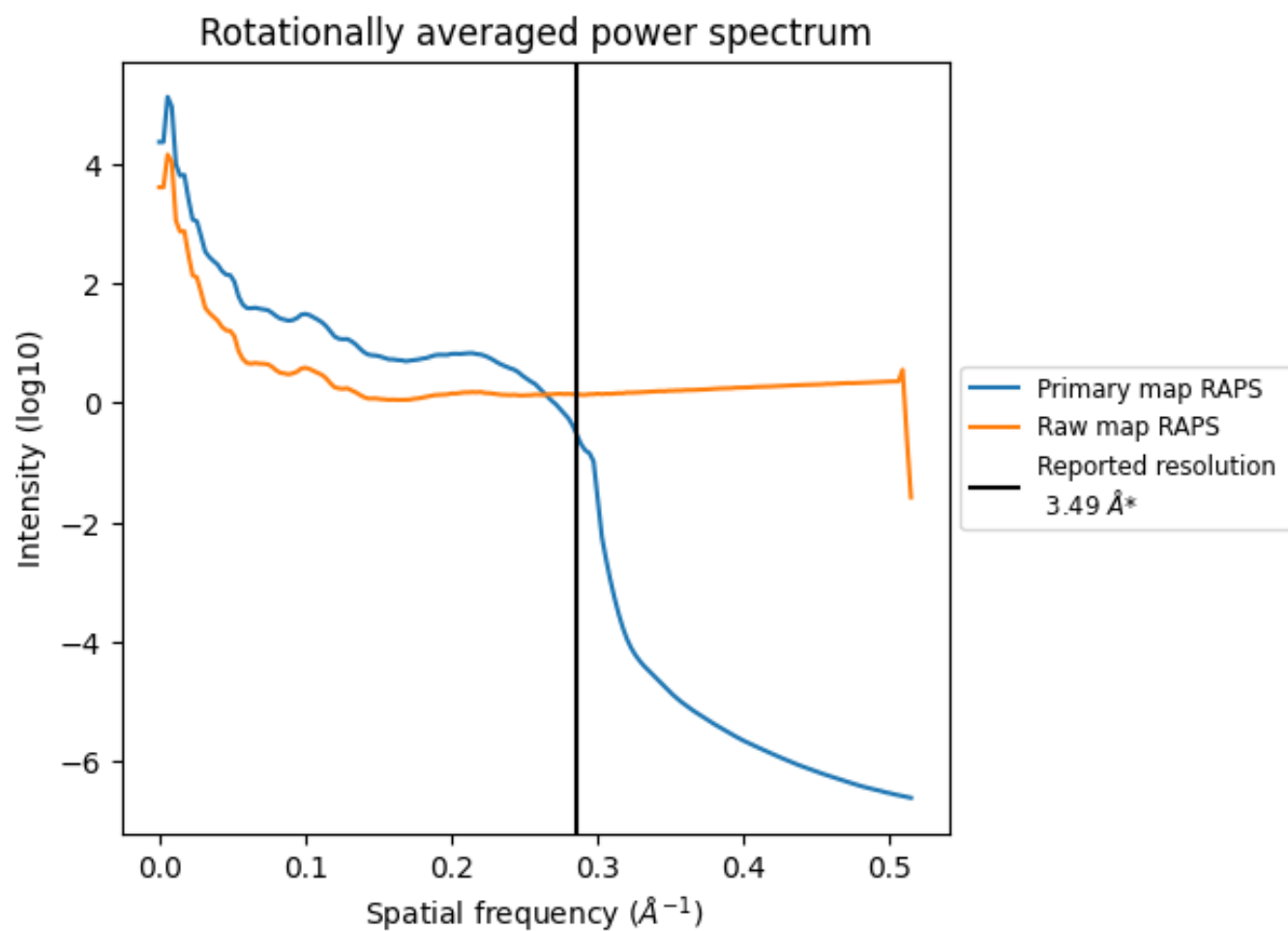
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 477 nm³; this corresponds to an approximate mass of 431 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](#)

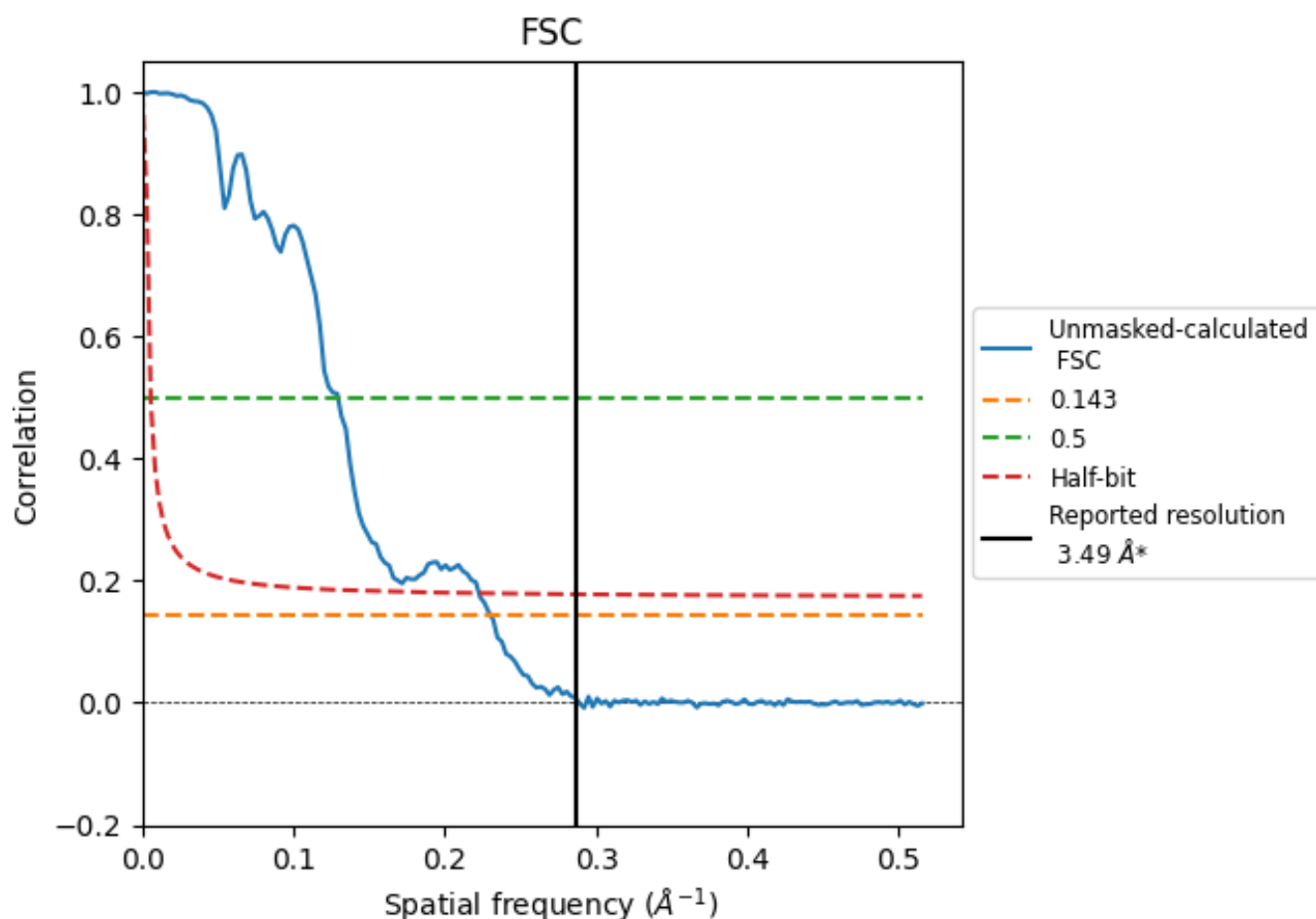


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.34	7.73	4.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.49 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36705 and PDB model 8JXM. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

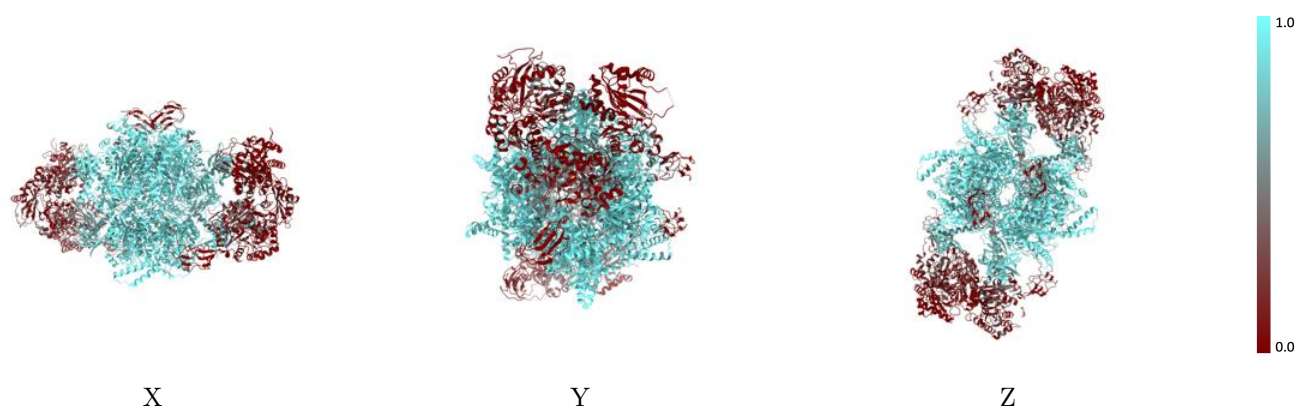
This section was not generated.

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



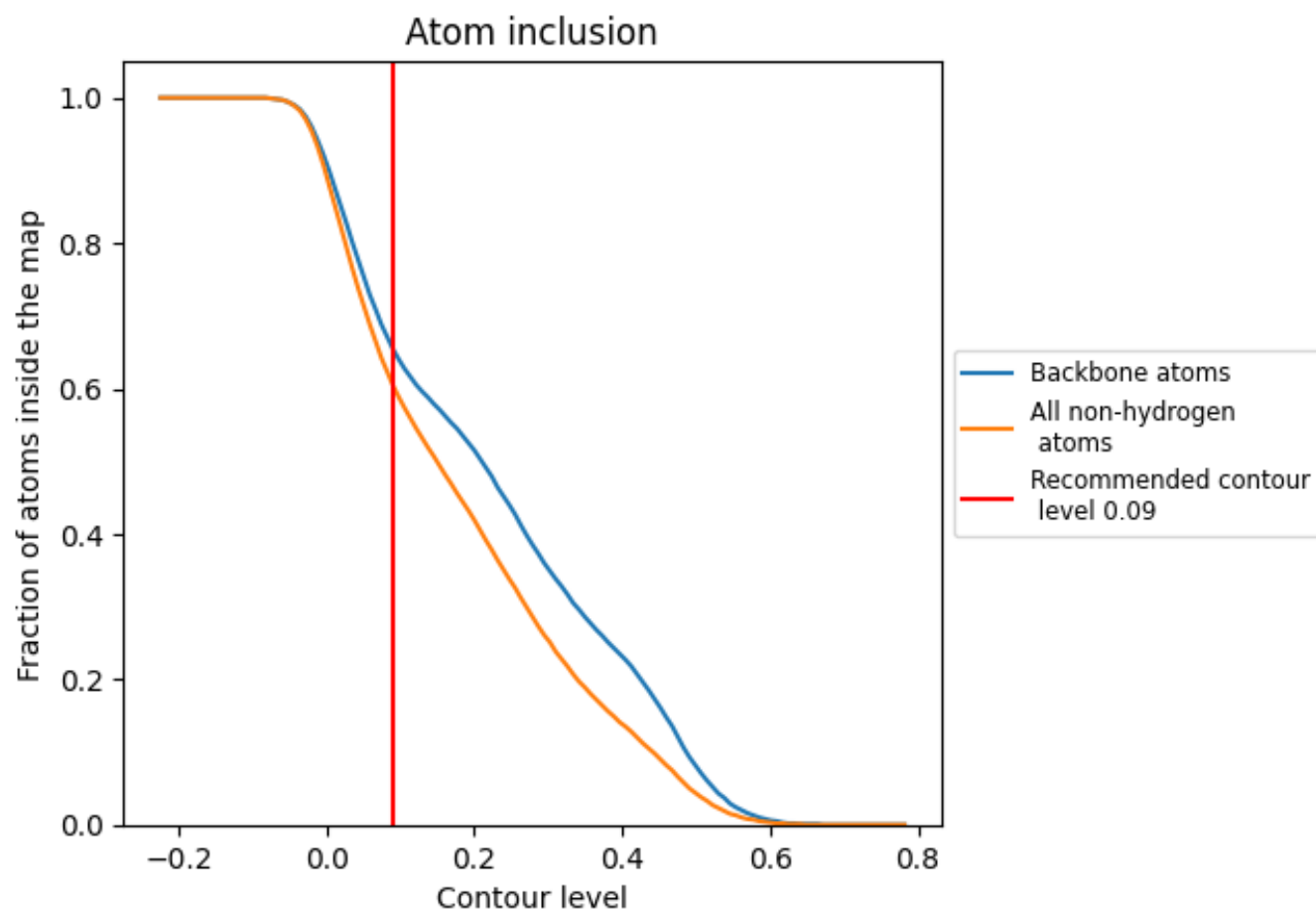
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6060	0.2890
A	0.9580	0.4320
B	0.2930	0.1610
C	0.9510	0.4320
E	0.9610	0.4420
F	0.2640	0.1550
G	0.3110	0.1530
H	0.9530	0.4310
I	0.2620	0.1540
J	0.9610	0.4430
K	0.9580	0.4330
L	0.2920	0.1600
M	0.3100	0.1510

1.0

0.0

<0.0