Full wwPDB EM Validation Report

Oct 18, 2026 – 06:20 PM JST

PDB ID	:	9WKR / pdb_00009wkr
EMDB ID	:	EMD-66037
Title	:	structure of human propionyl-coenzyme A carboxylase in BC binding state
Authors	:	Tian, X.Y.; Su, J.Y.
Deposited on	:	2025-09-01
Resolution	:	3.64 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:

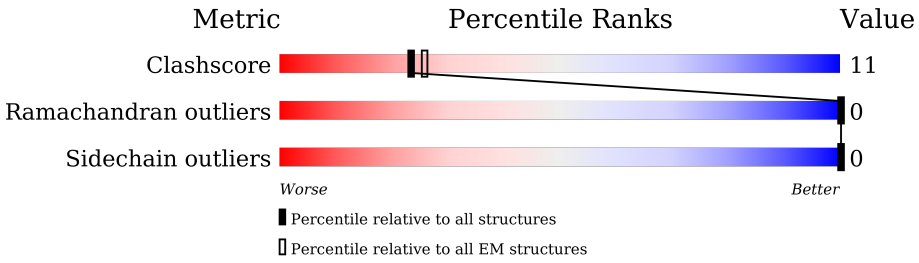
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

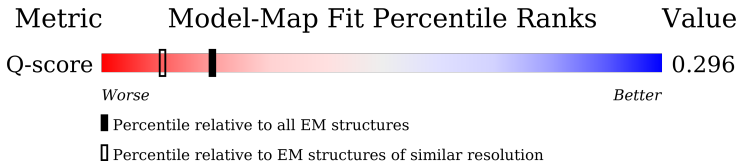
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.64 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	11633 (3.14 - 4.14)

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

Mol	Chain	Length	Quality of chain
1	A	670	66% 75% 25%
1	B	670	25% 74% 26%
1	D	670	78% 74% 26%
1	F	670	38% 73% 27%

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Mol	Chain	Length	Quality of chain
1	H	670	36% 74% 26%
1	J	670	68% 75% 25%
2	G	507	13% 74% 26%
2	I	507	15% 75% 25%
2	K	507	13% 74% 26%
2	L	507	11% 74% 26%
2	N	507	11% 74% 26%
2	O	507	11% 75% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 54318 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.

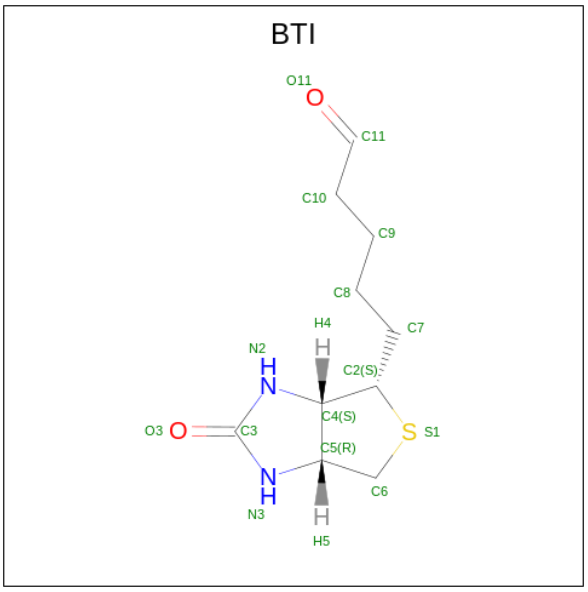
- Molecule 1 is a protein called Propionyl-CoA carboxylase alpha chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	670	Total 5164	C 3241	N 906	O 987	S 30	0	0
1	B	670	Total 5164	C 3241	N 906	O 987	S 30	0	0
1	D	670	Total 5164	C 3241	N 906	O 987	S 30	0	0
1	F	670	Total 5164	C 3241	N 906	O 987	S 30	0	0
1	H	670	Total 5164	C 3241	N 906	O 987	S 30	0	0
1	J	670	Total 5164	C 3241	N 906	O 987	S 30	0	0

- Molecule 2 is a protein called Propionyl-CoA carboxylase beta chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	507	Total 3874	C 2447	N 680	O 726	S 21	0	0
2	I	507	Total 3874	C 2447	N 680	O 726	S 21	0	0
2	K	507	Total 3874	C 2447	N 680	O 726	S 21	0	0
2	L	507	Total 3874	C 2447	N 680	O 726	S 21	0	0
2	N	507	Total 3874	C 2447	N 680	O 726	S 21	0	0
2	O	507	Total 3874	C 2447	N 680	O 726	S 21	0	0

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: $C_{10}H_{16}N_2O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	B	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	D	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	F	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	H	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	J	1	Total	C	N	O	S	0
			15	10	2	2	1	

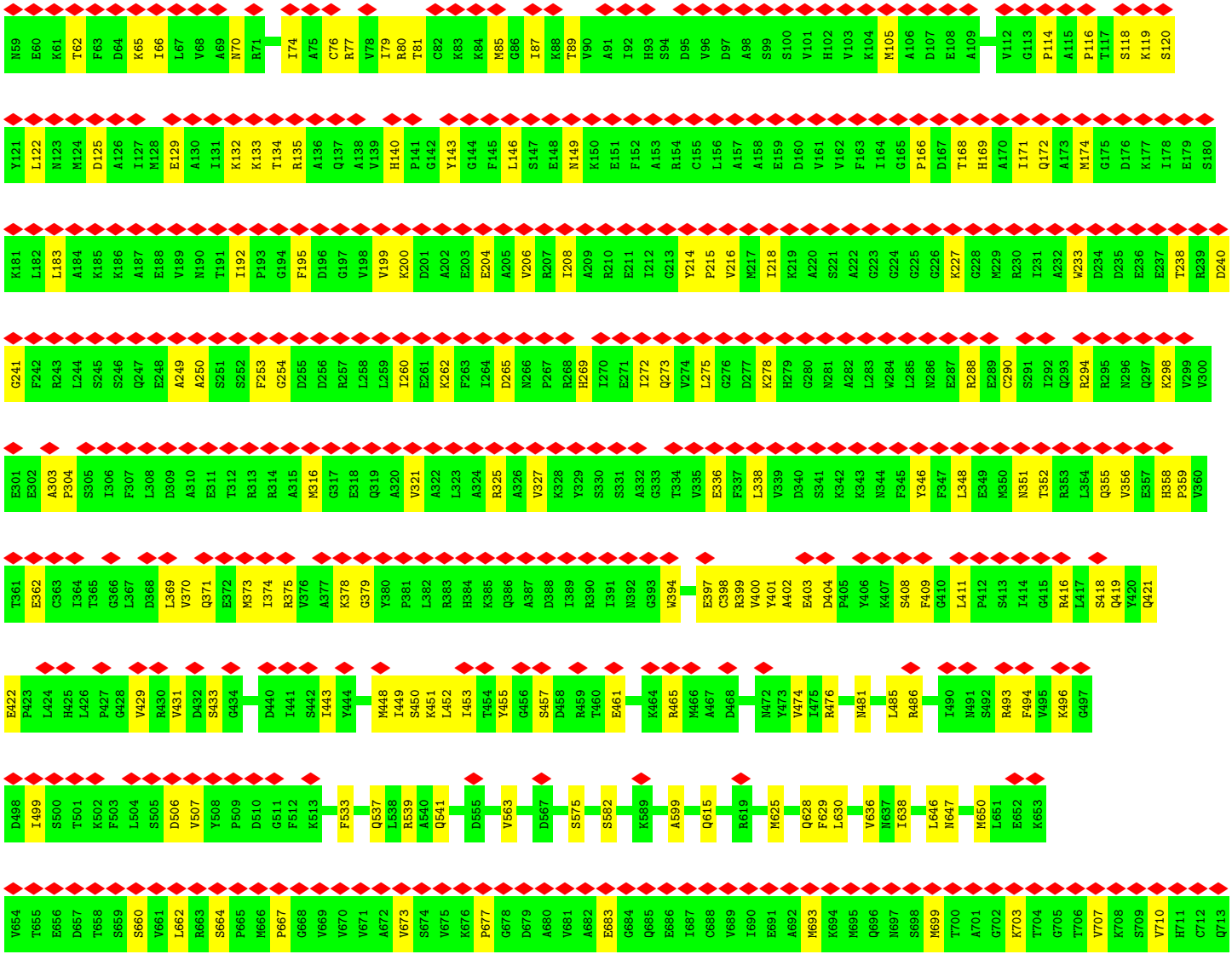
3 Residue-property plots (i)

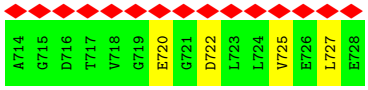
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Propionyl-CoA carboxylase alpha chain, mitochondrial

Chain A:



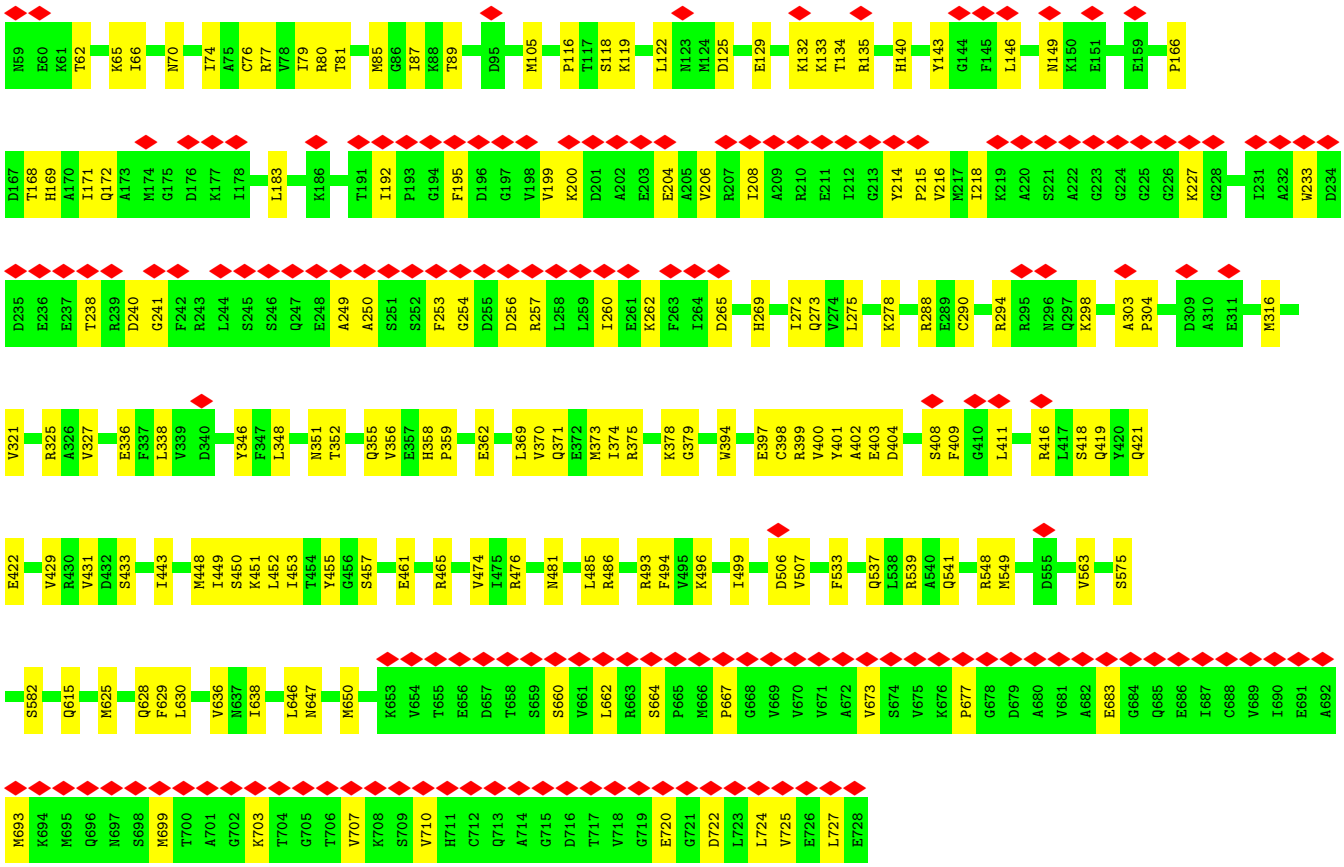




• Molecule 1: Propionyl-CoA carboxylase alpha chain, mitochondrial

Chain B:



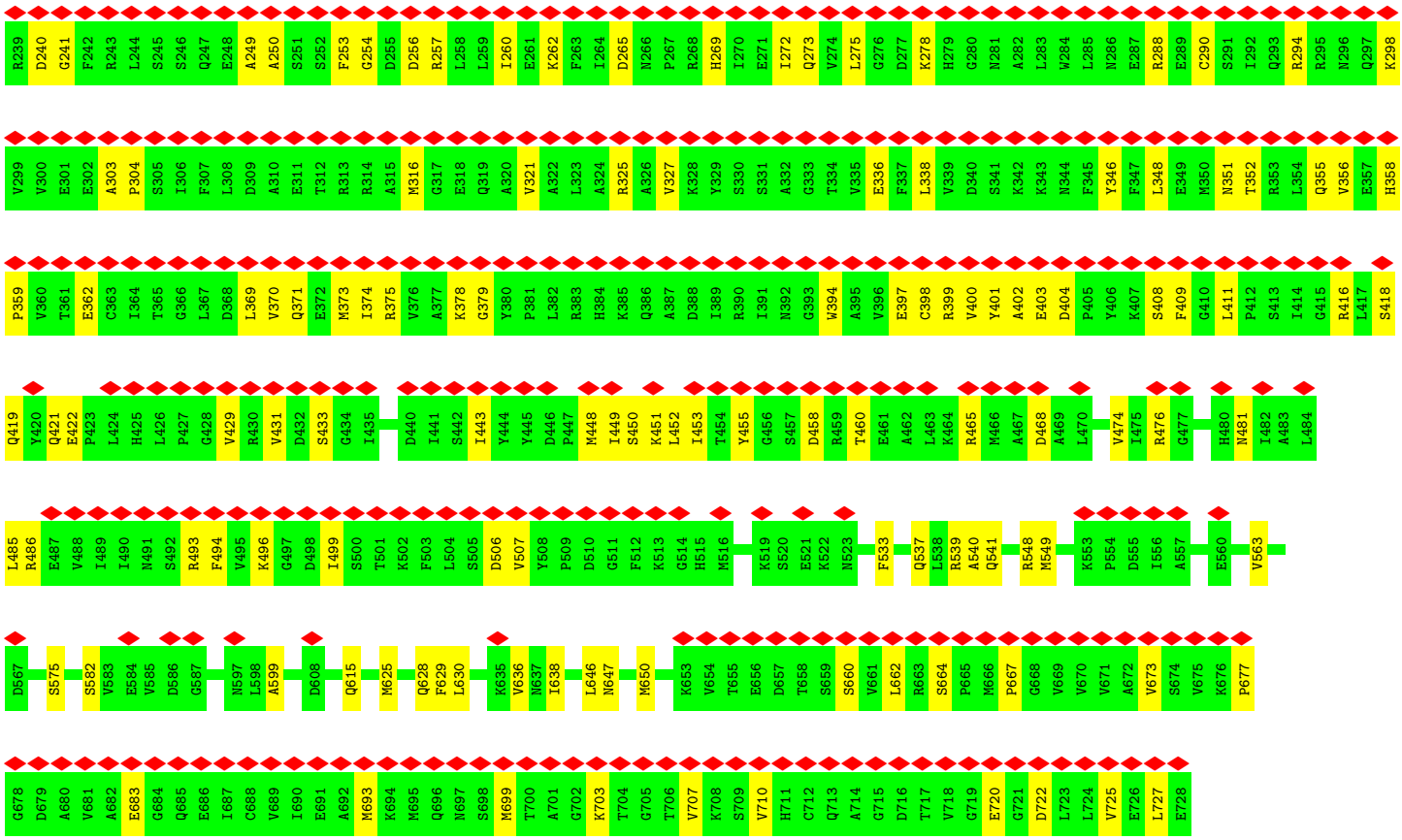


• Molecule 1: Propionyl-CoA carboxylase alpha chain, mitochondrial

Chain D:



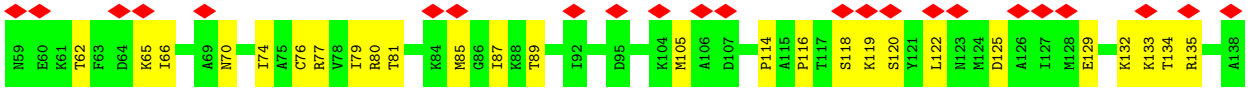


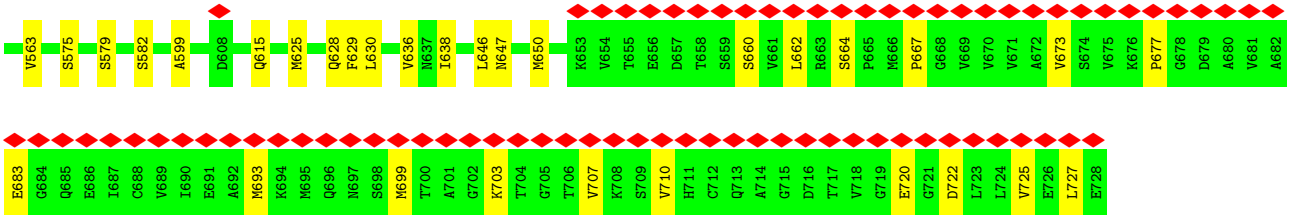


• Molecule 1: Propionyl-CoA carboxylase alpha chain, mitochondrial

Chain F:



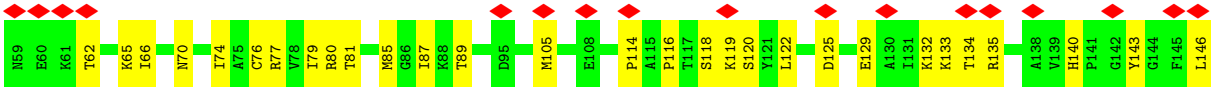


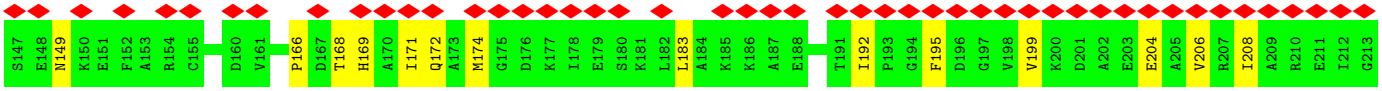


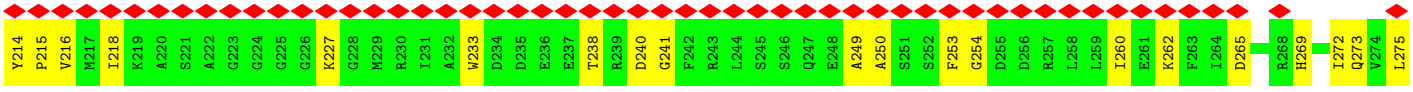
• Molecule 1: Propionyl-CoA carboxylase alpha chain, mitochondrial

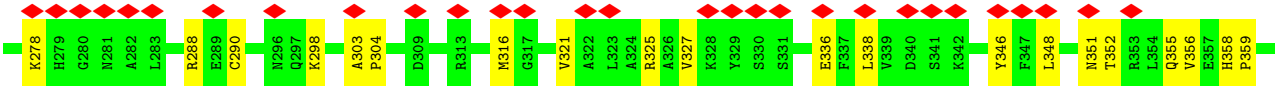
Chain H:

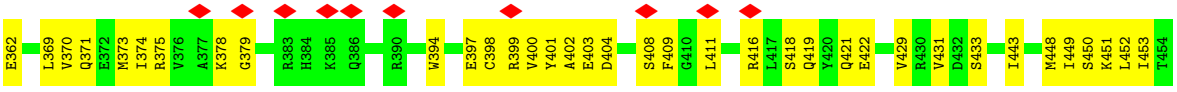


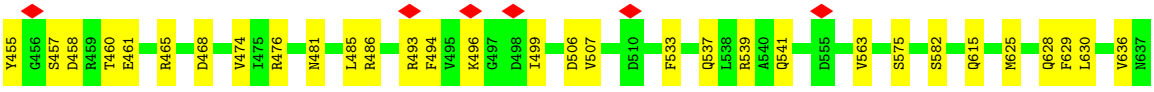


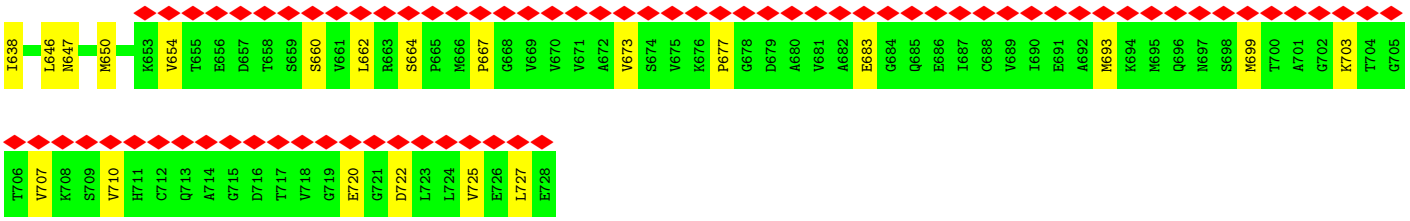








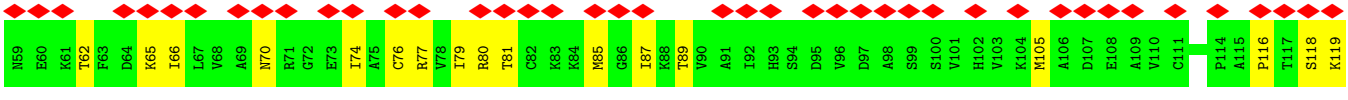


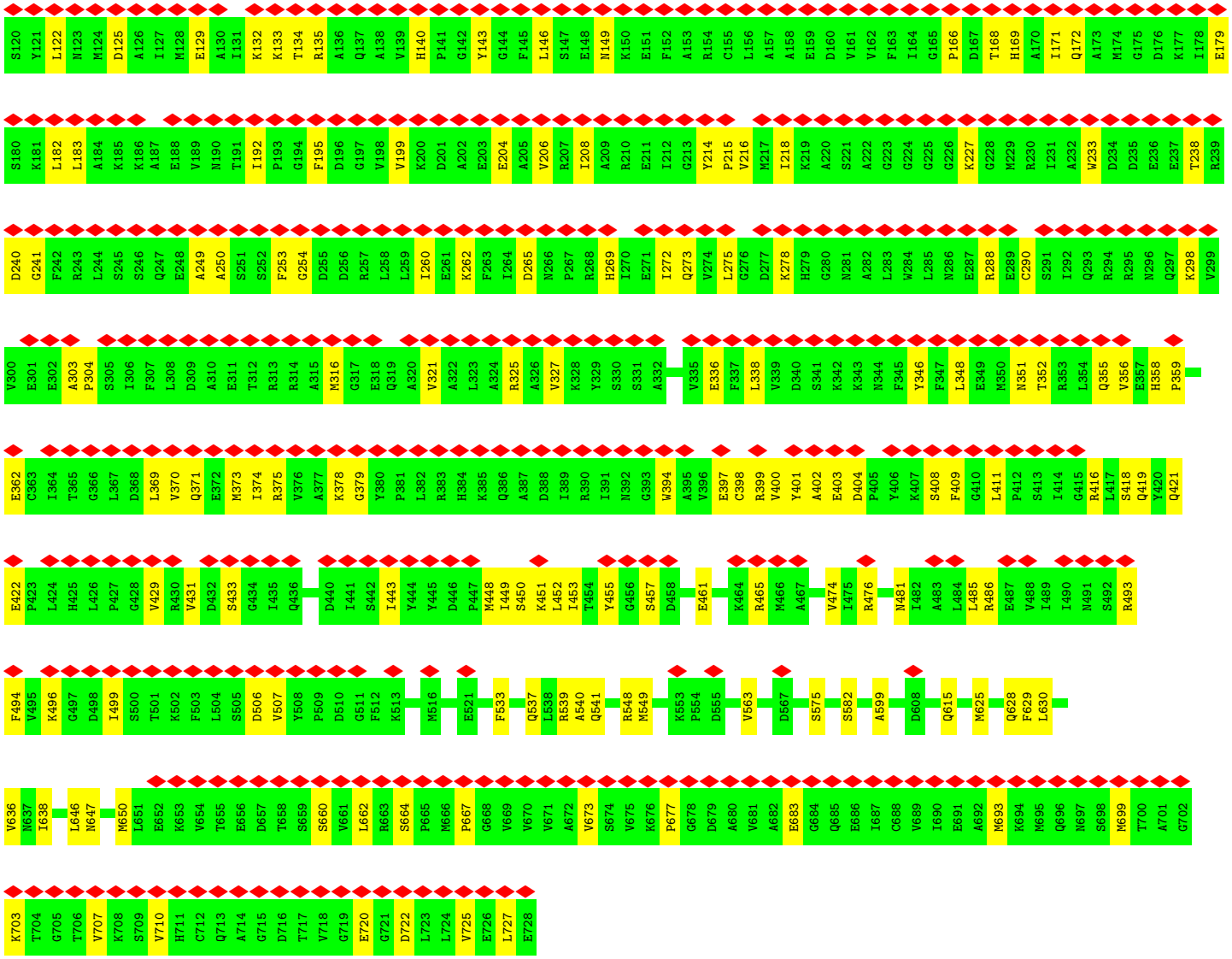


• Molecule 1: Propionyl-CoA carboxylase alpha chain, mitochondrial

Chain J:



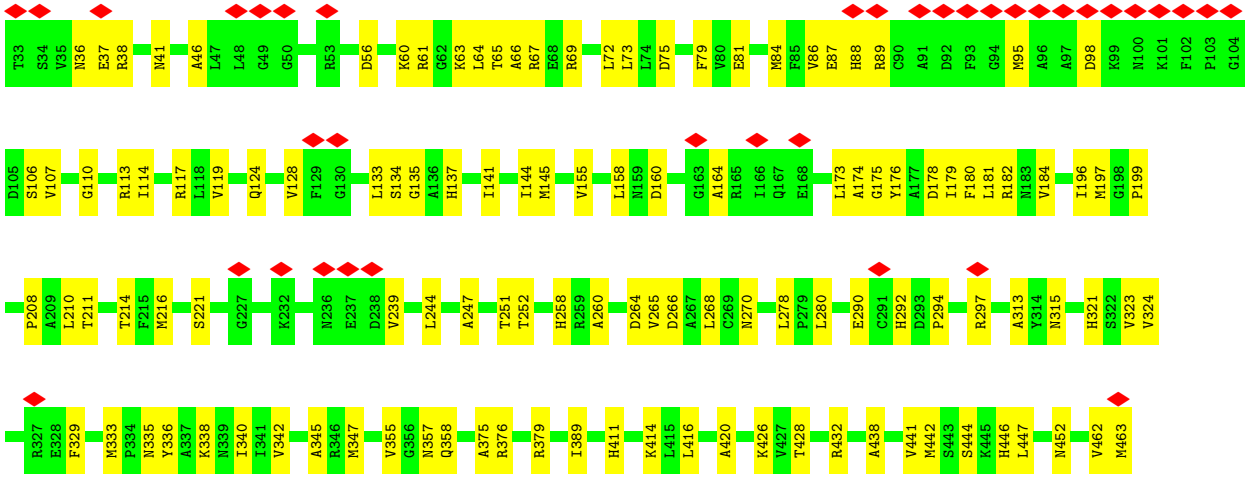


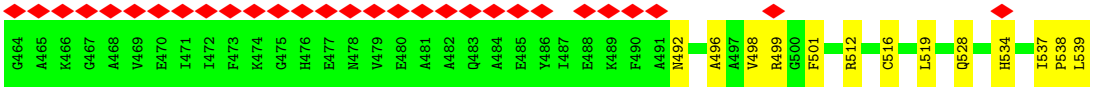


• Molecule 2: Propionyl-CoA carboxylase beta chain, mitochondrial

Chain G:



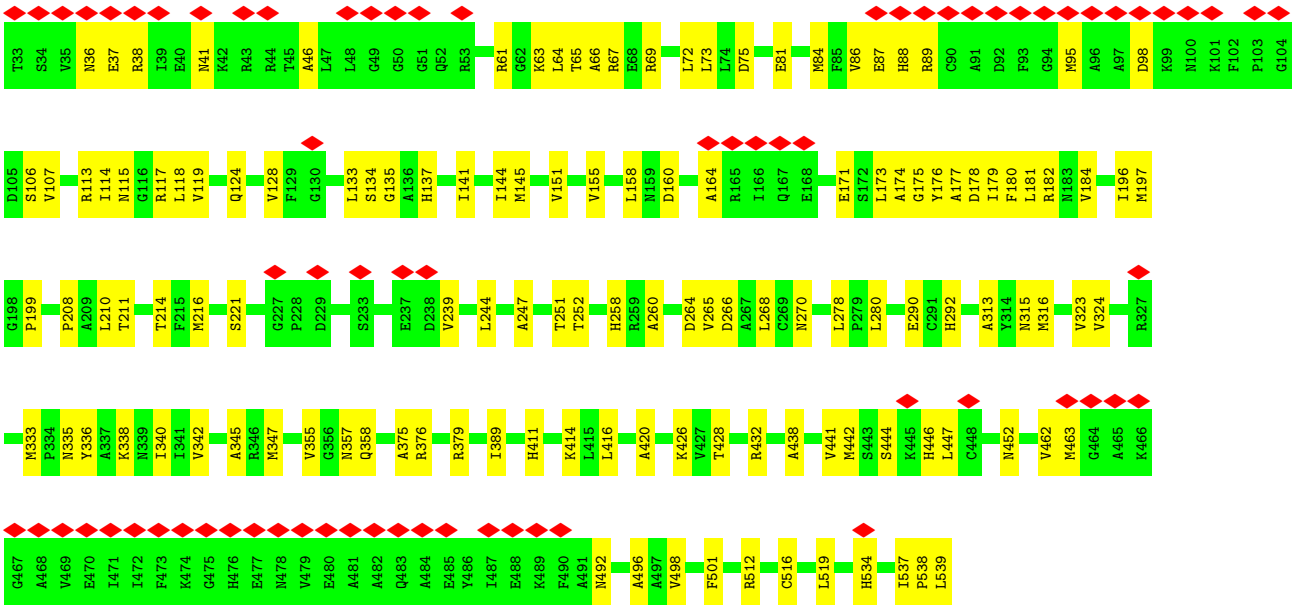




• Molecule 2: Propionyl-CoA carboxylase beta chain, mitochondrial

Chain I:

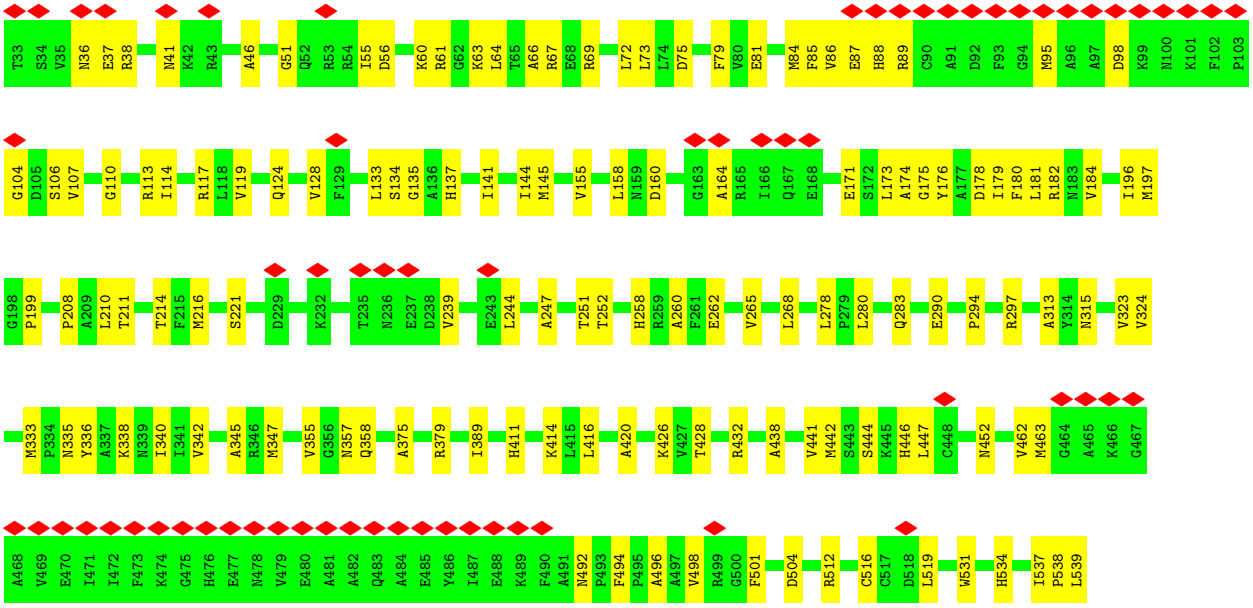




• Molecule 2: Propionyl-CoA carboxylase beta chain, mitochondrial

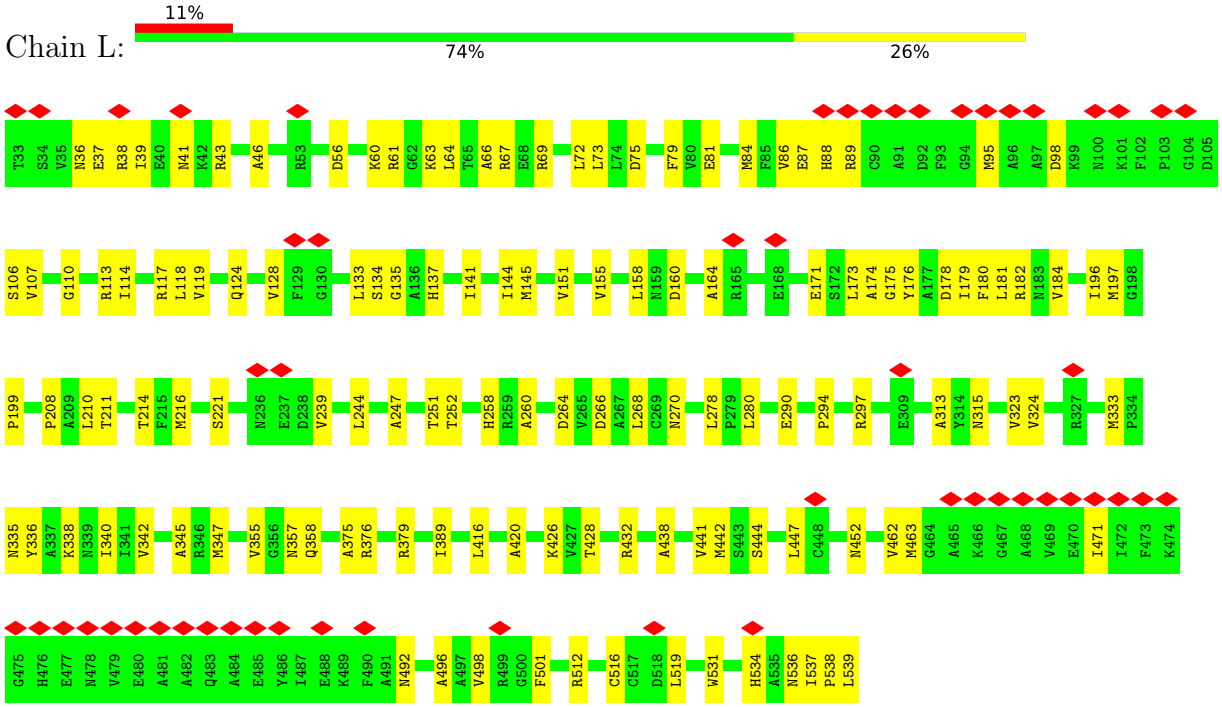
Chain K:





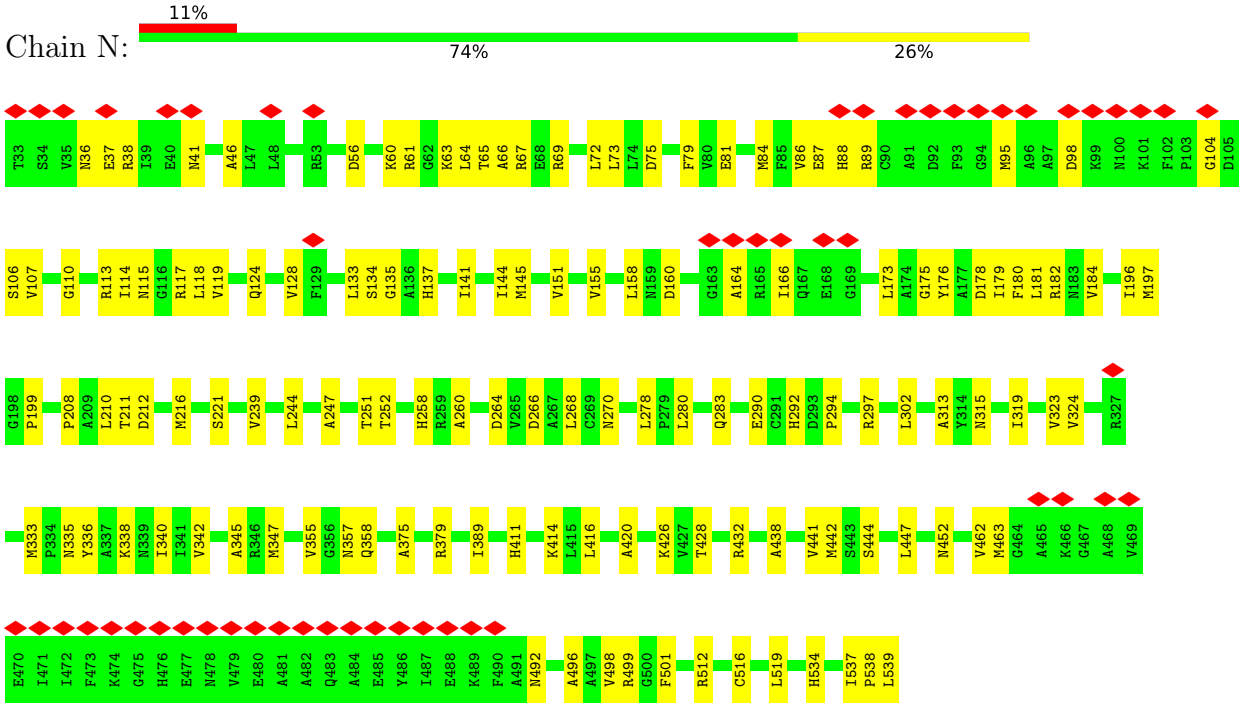
• Molecule 2: Propionyl-CoA carboxylase beta chain, mitochondrial

Chain L:



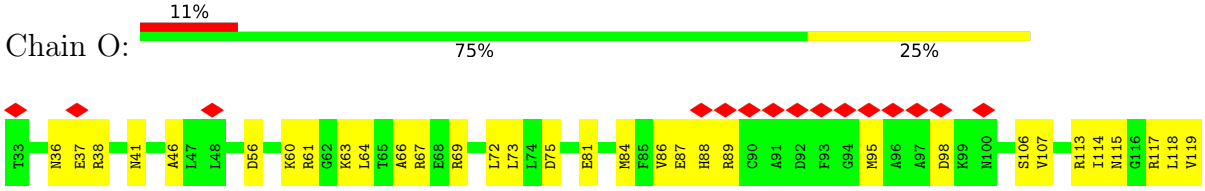
• Molecule 2: Propionyl-CoA carboxylase beta chain, mitochondrial

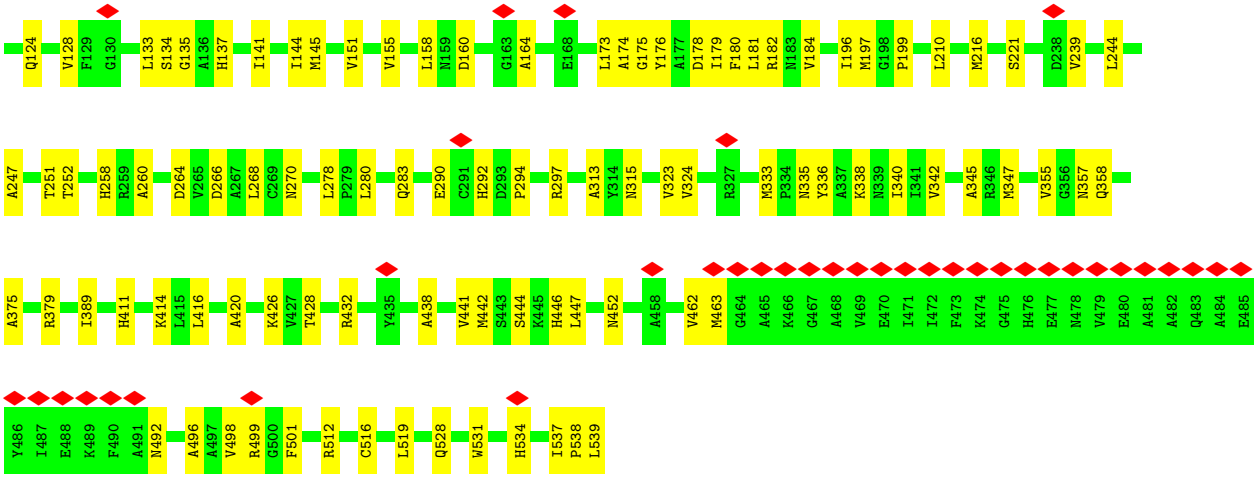
Chain N:



• Molecule 2: Propionyl-CoA carboxylase beta chain, mitochondrial

Chain O:




Q124
V128
F129
G130
L133
S134
G135
A136
H137
I141
I144
M145
V151
V155
L158
N159
D160
G163
A164
E168
L173
A174
G175
Y176
A177
D178
I179
F180
L181
R182
N183
V184
I196
M197
G198
P199
L210
M216
S221
D238
V239
L244
A247
T251
T252
H258
R259
A260
D264
V265
D266
A267
L268
C269
N270
L278
P279
L280
Q283
E290
C291
H292
D293
P294
R297
A313
Y314
N315
V323
V324
R327
M333
P334
N335
Y336
A337
K338
N339
I340
I341
V342
A345
R346
M347
V355
G356
N357
Q358
A375
R379
I389
H411
K414
L415
L416
A420
K426
V427
T428
R432
Y435
A438
V441
M442
S443
S444
K445
H446
L447
N452
A458
V462
M463
G464
A465
K466
G467
A468
V469
E470
I471
I472
F473
K474
G475
H476
E477
N478
V479
E480
A481
A482
Q483
A484
E485
Y486
I487
E488
K489
F490
A491
N492
A496
A497
V498
R499
G500
F501
R512
C516
L519
Q528
W531
H534
I537
P538
L539

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53676	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.021	Depositor
Minimum map value	-1.193	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	347.88, 347.88, 347.88	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8697, 0.8697, 0.8697	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.10	0/5248	0.28	0/7087
1	B	0.10	0/5248	0.28	0/7087
1	D	0.10	0/5248	0.28	0/7087
1	F	0.10	0/5248	0.28	0/7087
1	H	0.10	0/5248	0.28	0/7087
1	J	0.10	0/5248	0.28	0/7087
2	G	0.11	0/3953	0.31	0/5355
2	I	0.11	0/3953	0.31	0/5355
2	K	0.11	0/3953	0.31	0/5355
2	L	0.11	0/3953	0.31	0/5355
2	N	0.11	0/3953	0.31	0/5355
2	O	0.11	0/3953	0.31	0/5355
All	All	0.11	0/55206	0.30	0/74652

There are no bond length outliers.

There are no bond angle outliers.

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	5164	0	5205	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5164	0	5205	112	0
1	D	5164	0	5205	117	0
1	F	5164	0	5205	119	0
1	H	5164	0	5205	111	0
1	J	5164	0	5205	111	0
2	G	3874	0	3852	111	0
2	I	3874	0	3852	112	0
2	K	3874	0	3852	109	0
2	L	3874	0	3852	104	0
2	N	3874	0	3852	112	0
2	O	3874	0	3852	108	0
3	A	15	0	16	0	0
3	B	15	0	16	0	0
3	D	15	0	16	0	0
3	F	15	0	16	0	0
3	H	15	0	16	0	0
3	J	15	0	16	0	0
All	All	54318	0	54438	1201	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 11.

All (1201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:181:LEU:HD21	2:N:447:LEU:HA	1.66	0.76
2:L:179:ILE:HG23	2:L:182:ARG:HH21	1.51	0.75
2:N:179:ILE:HG23	2:N:182:ARG:HH21	1.51	0.75
2:I:179:ILE:HG23	2:I:182:ARG:HH21	1.51	0.75
1:B:401:TYR:HA	1:B:448:MET:HA	1.69	0.74
1:H:290:CYS:HB3	1:H:298:LYS:HD3	1.69	0.74
1:A:290:CYS:HB3	1:A:298:LYS:HD3	1.70	0.74
1:F:290:CYS:HB3	1:F:298:LYS:HD3	1.70	0.74
2:G:179:ILE:HG23	2:G:182:ARG:HH21	1.51	0.74
2:O:179:ILE:HG23	2:O:182:ARG:HH21	1.51	0.74
1:F:401:TYR:HA	1:F:448:MET:HA	1.69	0.74
1:J:401:TYR:HA	1:J:448:MET:HA	1.69	0.74
2:K:179:ILE:HG23	2:K:182:ARG:HH21	1.51	0.74
1:H:401:TYR:HA	1:H:448:MET:HA	1.69	0.74
2:G:498:VAL:HA	2:K:86:VAL:HA	1.67	0.74
1:D:290:CYS:HB3	1:D:298:LYS:HD3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:290:CYS:HB3	1:J:298:LYS:HD3	1.70	0.73
1:B:290:CYS:HB3	1:B:298:LYS:HD3	1.70	0.73
1:F:403:GLU:HB2	1:F:481:ASN:HD22	1.54	0.73
1:A:401:TYR:HA	1:A:448:MET:HA	1.69	0.72
1:D:401:TYR:HA	1:D:448:MET:HA	1.69	0.72
1:A:403:GLU:HB2	1:A:481:ASN:HD22	1.54	0.72
2:G:447:LEU:HA	2:I:181:LEU:HD21	1.70	0.72
1:J:398:CYS:HB3	1:J:485:LEU:HD23	1.72	0.71
1:D:403:GLU:HB2	1:D:481:ASN:HD22	1.54	0.71
1:H:398:CYS:HB3	1:H:485:LEU:HD23	1.72	0.71
1:H:403:GLU:HB2	1:H:481:ASN:HD22	1.54	0.71
2:G:86:VAL:HA	2:L:498:VAL:HA	1.73	0.71
1:B:403:GLU:HB2	1:B:481:ASN:HD22	1.54	0.71
1:D:398:CYS:HB3	1:D:485:LEU:HD23	1.72	0.71
2:K:181:LEU:HD21	2:O:447:LEU:HA	1.70	0.70
1:H:288:ARG:HA	1:H:303:ALA:HA	1.74	0.70
1:A:288:ARG:HA	1:A:303:ALA:HA	1.74	0.70
1:D:419:GLN:HB2	1:D:476:ARG:HB2	1.74	0.70
1:A:398:CYS:HB3	1:A:485:LEU:HD23	1.72	0.70
1:D:288:ARG:HA	1:D:303:ALA:HA	1.74	0.70
1:F:398:CYS:HB3	1:F:485:LEU:HD23	1.72	0.70
1:J:403:GLU:HB2	1:J:481:ASN:HD22	1.54	0.70
1:J:419:GLN:HB2	1:J:476:ARG:HB2	1.74	0.70
1:A:416:ARG:HH11	1:A:418:SER:HA	1.57	0.70
1:B:398:CYS:HB3	1:B:485:LEU:HD23	1.72	0.70
1:D:416:ARG:HH11	1:D:418:SER:HA	1.57	0.70
1:F:288:ARG:HA	1:F:303:ALA:HA	1.74	0.70
1:A:419:GLN:HB2	1:A:476:ARG:HB2	1.74	0.70
1:B:419:GLN:HB2	1:B:476:ARG:HB2	1.74	0.70
1:J:288:ARG:HA	1:J:303:ALA:HA	1.74	0.69
2:G:181:LEU:HD21	2:I:447:LEU:HA	1.73	0.69
1:H:129:GLU:OE1	1:H:132:LYS:NZ	2.25	0.69
2:I:498:VAL:HB	2:N:87:GLU:HG2	1.74	0.69
1:J:416:ARG:HH11	1:J:418:SER:HA	1.57	0.69
1:A:129:GLU:OE1	1:A:132:LYS:NZ	2.25	0.69
1:H:419:GLN:HB2	1:H:476:ARG:HB2	1.74	0.69
1:B:129:GLU:OE1	1:B:132:LYS:NZ	2.25	0.69
1:F:416:ARG:HH11	1:F:418:SER:HA	1.57	0.69
2:L:444:SER:H	2:L:447:LEU:HD12	1.58	0.69
1:B:288:ARG:HA	1:B:303:ALA:HA	1.74	0.69
1:F:129:GLU:OE1	1:F:132:LYS:NZ	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ARG:HH11	1:B:418:SER:HA	1.57	0.69
1:D:129:GLU:OE1	1:D:132:LYS:NZ	2.25	0.69
1:F:419:GLN:HB2	1:F:476:ARG:HB2	1.74	0.69
2:G:66:ALA:HA	2:G:69:ARG:HD2	1.75	0.69
2:N:444:SER:H	2:N:447:LEU:HD12	1.58	0.69
2:O:66:ALA:HA	2:O:69:ARG:HD2	1.74	0.69
1:J:129:GLU:OE1	1:J:132:LYS:NZ	2.25	0.69
2:O:444:SER:H	2:O:447:LEU:HD12	1.58	0.68
1:A:660:SER:HB2	1:A:703:LYS:HG2	1.75	0.68
2:I:444:SER:H	2:I:447:LEU:HD12	1.58	0.68
2:L:66:ALA:HA	2:L:69:ARG:HD2	1.75	0.68
1:D:660:SER:HB2	1:D:703:LYS:HG2	1.75	0.68
1:D:216:VAL:HA	1:D:262:LYS:HA	1.76	0.68
2:K:444:SER:H	2:K:447:LEU:HD12	1.58	0.68
1:A:216:VAL:HA	1:A:262:LYS:HA	1.76	0.68
2:I:87:GLU:HG2	2:O:498:VAL:HB	1.74	0.68
2:G:444:SER:H	2:G:447:LEU:HD12	1.58	0.68
1:H:416:ARG:HH11	1:H:418:SER:HA	1.57	0.68
2:I:66:ALA:HA	2:I:69:ARG:HD2	1.75	0.68
2:N:66:ALA:HA	2:N:69:ARG:HD2	1.75	0.68
2:K:534:HIS:CE1	2:O:379:ARG:HH22	2.12	0.68
2:G:534:HIS:CE1	2:I:379:ARG:HH22	2.12	0.68
2:K:66:ALA:HA	2:K:69:ARG:HD2	1.75	0.68
2:G:462:VAL:HG12	2:G:463:MET:HE2	1.76	0.68
1:F:66:ILE:HG12	1:F:87:ILE:HG21	1.77	0.67
2:L:462:VAL:HG12	2:L:463:MET:HE2	1.76	0.67
2:O:462:VAL:HG12	2:O:463:MET:HE2	1.76	0.67
2:K:447:LEU:HA	2:O:181:LEU:HD21	1.75	0.67
1:H:216:VAL:HA	1:H:262:LYS:HA	1.76	0.67
1:F:660:SER:HB2	1:F:703:LYS:HG2	1.75	0.67
1:H:66:ILE:HG12	1:H:87:ILE:HG21	1.77	0.67
1:J:216:VAL:HA	1:J:262:LYS:HA	1.76	0.67
2:G:416:LEU:HD23	2:I:210:LEU:HD11	1.77	0.67
2:I:462:VAL:HG12	2:I:463:MET:HE2	1.76	0.66
1:A:66:ILE:HG12	1:A:87:ILE:HG21	1.76	0.66
1:B:216:VAL:HA	1:B:262:LYS:HA	1.76	0.66
1:J:660:SER:HB2	1:J:703:LYS:HG2	1.76	0.66
2:N:462:VAL:HG12	2:N:463:MET:HE2	1.76	0.66
1:H:660:SER:HB2	1:H:703:LYS:HG2	1.76	0.66
1:J:66:ILE:HG12	1:J:87:ILE:HG21	1.76	0.66
2:L:538:PRO:HG3	2:N:210:LEU:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:SER:HB2	1:B:703:LYS:HG2	1.75	0.66
1:B:66:ILE:HG12	1:B:87:ILE:HG21	1.77	0.66
1:F:216:VAL:HA	1:F:262:LYS:HA	1.76	0.66
2:K:379:ARG:HH22	2:O:534:HIS:CE1	2.14	0.66
2:K:462:VAL:HG12	2:K:463:MET:HE2	1.77	0.66
1:D:66:ILE:HG12	1:D:87:ILE:HG21	1.76	0.65
1:J:62:THR:HA	1:J:378:LYS:HE3	1.78	0.65
1:B:65:LYS:NZ	1:B:134:THR:O	2.24	0.65
1:F:662:LEU:HB3	1:F:725:VAL:HG12	1.79	0.65
1:H:662:LEU:HB3	1:H:725:VAL:HG12	1.79	0.65
1:D:62:THR:HA	1:D:378:LYS:HE3	1.78	0.64
2:L:379:ARG:HH22	2:N:534:HIS:CE1	2.15	0.64
1:A:662:LEU:HB3	1:A:725:VAL:HG12	1.79	0.64
1:H:62:THR:HA	1:H:378:LYS:HE3	1.78	0.64
1:D:351:ASN:ND2	1:D:355:GLN:OE1	2.31	0.64
1:B:351:ASN:ND2	1:B:355:GLN:OE1	2.31	0.64
1:A:62:THR:HA	1:A:378:LYS:HE3	1.78	0.64
2:G:379:ARG:HH22	2:I:534:HIS:CE1	2.15	0.64
2:K:69:ARG:HD3	2:K:197:MET:SD	2.38	0.64
2:O:69:ARG:HD3	2:O:197:MET:SD	2.38	0.64
1:A:65:LYS:NZ	1:A:134:THR:O	2.24	0.64
1:F:62:THR:HA	1:F:378:LYS:HE3	1.78	0.64
1:H:351:ASN:ND2	1:H:355:GLN:OE1	2.31	0.64
1:B:662:LEU:HB3	1:B:725:VAL:HG12	1.79	0.64
2:G:210:LEU:HD11	2:I:416:LEU:HD23	1.79	0.64
2:L:69:ARG:HD3	2:L:197:MET:SD	2.38	0.64
1:J:662:LEU:HB3	1:J:725:VAL:HG12	1.79	0.63
2:N:69:ARG:HD3	2:N:197:MET:SD	2.38	0.63
1:B:62:THR:HA	1:B:378:LYS:HE3	1.78	0.63
1:D:662:LEU:HB3	1:D:725:VAL:HG12	1.79	0.63
1:F:351:ASN:ND2	1:F:355:GLN:OE1	2.31	0.63
2:G:69:ARG:HD3	2:G:197:MET:SD	2.38	0.63
2:I:335:ASN:HA	2:I:338:LYS:HZ3	1.63	0.63
1:J:351:ASN:ND2	1:J:355:GLN:OE1	2.31	0.63
2:O:416:LEU:HB2	2:O:441:VAL:HG23	1.80	0.63
2:L:416:LEU:HB2	2:L:441:VAL:HG23	1.81	0.63
1:H:646:LEU:HD12	2:K:72:LEU:HG	1.81	0.63
2:L:210:LEU:HA	2:N:538:PRO:HG3	1.79	0.63
2:G:416:LEU:HB2	2:G:441:VAL:HG23	1.80	0.63
1:A:351:ASN:ND2	1:A:355:GLN:OE1	2.31	0.62
2:N:416:LEU:HB2	2:N:441:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LYS:NZ	1:D:134:THR:O	2.24	0.62
1:F:650:MET:HE2	2:N:264:ASP:HB2	1.81	0.62
2:G:335:ASN:HA	2:G:338:LYS:HZ3	1.64	0.62
2:I:69:ARG:HD3	2:I:197:MET:SD	2.38	0.62
2:I:38:ARG:NH1	2:O:492:ASN:OD1	2.32	0.62
2:N:335:ASN:HA	2:N:338:LYS:HZ3	1.63	0.62
2:K:416:LEU:HB2	2:K:441:VAL:HG23	1.80	0.62
2:I:416:LEU:HB2	2:I:441:VAL:HG23	1.80	0.62
2:O:335:ASN:HA	2:O:338:LYS:HZ3	1.64	0.61
2:I:496:ALA:HB1	2:I:501:PHE:HB2	1.83	0.61
1:B:494:PHE:HA	1:B:499:ILE:HD11	1.83	0.61
2:G:210:LEU:HA	2:I:538:PRO:HG3	1.81	0.61
1:D:422:GLU:HG2	1:D:431:VAL:HG11	1.83	0.61
1:F:65:LYS:NZ	1:F:134:THR:O	2.24	0.61
2:K:496:ALA:HB1	2:K:501:PHE:HB2	1.83	0.61
2:L:496:ALA:HB1	2:L:501:PHE:HB2	1.83	0.61
2:N:496:ALA:HB1	2:N:501:PHE:HB2	1.83	0.60
1:F:401:TYR:H	1:F:481:ASN:HD21	1.50	0.60
1:A:422:GLU:HG2	1:A:431:VAL:HG11	1.84	0.60
1:B:422:GLU:HG2	1:B:431:VAL:HG11	1.83	0.60
1:H:401:TYR:H	1:H:481:ASN:HD21	1.50	0.60
2:O:315:ASN:HA	2:O:358:GLN:HE22	1.67	0.60
1:B:272:ILE:HD13	1:B:316:MET:HE1	1.83	0.60
1:F:422:GLU:HG2	1:F:431:VAL:HG11	1.84	0.60
1:B:401:TYR:H	1:B:481:ASN:HD21	1.50	0.60
1:H:494:PHE:HA	1:H:499:ILE:HD11	1.83	0.60
1:H:422:GLU:HG2	1:H:431:VAL:HG11	1.83	0.60
1:J:401:TYR:H	1:J:481:ASN:HD21	1.50	0.60
2:K:315:ASN:HA	2:K:358:GLN:HE22	1.67	0.60
2:L:447:LEU:HA	2:N:181:LEU:HD21	1.83	0.60
1:A:401:TYR:H	1:A:481:ASN:HD21	1.50	0.60
1:D:494:PHE:HA	1:D:499:ILE:HD11	1.83	0.60
1:J:422:GLU:HG2	1:J:431:VAL:HG11	1.83	0.60
2:O:496:ALA:HB1	2:O:501:PHE:HB2	1.83	0.60
1:D:401:TYR:H	1:D:481:ASN:HD21	1.50	0.60
1:H:65:LYS:NZ	1:H:134:THR:O	2.24	0.60
2:L:315:ASN:HA	2:L:358:GLN:HE22	1.67	0.60
2:G:498:VAL:HB	2:K:87:GLU:HG2	1.84	0.59
2:G:496:ALA:HB1	2:G:501:PHE:HB2	1.83	0.59
1:J:494:PHE:HA	1:J:499:ILE:HD11	1.83	0.59
2:I:428:THR:HB	2:I:452:ASN:HD22	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:428:THR:HB	2:O:452:ASN:HD22	1.68	0.59
1:D:272:ILE:HD13	1:D:316:MET:HE1	1.83	0.59
2:G:538:PRO:HG3	2:I:210:LEU:HA	1.82	0.59
1:J:650:MET:HE2	2:O:264:ASP:HB2	1.85	0.59
1:A:272:ILE:HD13	1:A:316:MET:HE1	1.83	0.59
1:A:494:PHE:HA	1:A:499:ILE:HD11	1.83	0.59
1:A:615:GLN:HB2	1:A:628:GLN:HB3	1.84	0.59
1:F:615:GLN:HB2	1:F:628:GLN:HB3	1.84	0.59
1:H:615:GLN:HB2	1:H:628:GLN:HB3	1.84	0.59
1:J:65:LYS:NZ	1:J:134:THR:O	2.24	0.59
1:J:615:GLN:HB2	1:J:628:GLN:HB3	1.84	0.59
2:N:315:ASN:HA	2:N:358:GLN:HE22	1.67	0.59
1:F:272:ILE:HD13	1:F:316:MET:HE1	1.83	0.59
1:H:272:ILE:HD13	1:H:316:MET:HE1	1.83	0.59
1:J:272:ILE:HD13	1:J:316:MET:HE1	1.83	0.59
2:I:315:ASN:HA	2:I:358:GLN:HE22	1.67	0.59
2:L:462:VAL:HA	2:N:173:LEU:HD11	1.85	0.59
2:G:420:ALA:HB3	2:I:184:VAL:HG21	1.85	0.59
1:F:494:PHE:HA	1:F:499:ILE:HD11	1.83	0.59
1:B:421:GLN:HB2	1:B:474:VAL:HB	1.86	0.58
1:A:539:ARG:NH2	2:G:290:GLU:O	2.36	0.58
1:F:421:GLN:HB2	1:F:474:VAL:HB	1.85	0.58
2:G:428:THR:HB	2:G:452:ASN:HD22	1.68	0.58
2:L:534:HIS:CE1	2:N:379:ARG:HH22	2.21	0.58
2:N:158:LEU:HB3	2:N:197:MET:HE2	1.86	0.58
2:N:428:THR:HB	2:N:452:ASN:HD22	1.68	0.58
1:A:646:LEU:HD12	2:G:72:LEU:HG	1.85	0.58
1:D:77:ARG:NH1	1:D:81:THR:OG1	2.37	0.58
1:J:421:GLN:HB2	1:J:474:VAL:HB	1.85	0.58
2:K:462:VAL:HA	2:O:173:LEU:HD11	1.85	0.58
2:G:315:ASN:HA	2:G:358:GLN:HE22	1.67	0.58
2:I:239:VAL:HG21	2:I:244:LEU:HD13	1.86	0.58
2:K:173:LEU:HD11	2:O:462:VAL:HA	1.85	0.58
1:A:421:GLN:HB2	1:A:474:VAL:HB	1.86	0.58
1:D:421:GLN:HB2	1:D:474:VAL:HB	1.85	0.58
2:K:158:LEU:HB3	2:K:197:MET:HE2	1.86	0.58
2:G:87:GLU:HG2	2:L:498:VAL:HB	1.85	0.58
2:L:428:THR:HB	2:L:452:ASN:HD22	1.68	0.58
1:H:77:ARG:NH1	1:H:81:THR:OG1	2.36	0.58
1:J:77:ARG:NH1	1:J:81:THR:OG1	2.37	0.58
2:L:239:VAL:HG21	2:L:244:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:NH1	1:A:81:THR:OG1	2.37	0.58
1:B:77:ARG:NH1	1:B:81:THR:OG1	2.37	0.58
1:H:421:GLN:HB2	1:H:474:VAL:HB	1.85	0.58
2:L:180:PHE:CG	2:N:416:LEU:HD21	2.38	0.58
2:G:158:LEU:HB3	2:G:197:MET:HE2	1.86	0.58
2:K:335:ASN:HA	2:K:338:LYS:HZ3	1.69	0.58
2:L:174:ALA:HB2	2:N:501:PHE:CE1	2.38	0.58
2:L:416:LEU:HD21	2:N:180:PHE:CG	2.39	0.58
1:B:615:GLN:HB2	1:B:628:GLN:HB3	1.84	0.57
2:G:239:VAL:HG21	2:G:244:LEU:HD13	1.86	0.57
1:D:615:GLN:HB2	1:D:628:GLN:HB3	1.84	0.57
1:F:77:ARG:NH1	1:F:81:THR:OG1	2.37	0.57
2:O:239:VAL:HG21	2:O:244:LEU:HD13	1.85	0.57
2:L:158:LEU:HB3	2:L:197:MET:HE2	1.86	0.57
1:A:338:LEU:HD11	1:A:348:LEU:HD12	1.87	0.57
2:K:428:THR:HB	2:K:452:ASN:HD22	1.68	0.57
2:O:158:LEU:HB3	2:O:197:MET:HE2	1.86	0.57
2:K:210:LEU:HD11	2:O:416:LEU:HD23	1.86	0.57
1:D:338:LEU:HD11	1:D:348:LEU:HD12	1.87	0.57
1:D:539:ARG:NH2	2:I:290:GLU:O	2.36	0.57
2:K:239:VAL:HG21	2:K:244:LEU:HD13	1.86	0.57
2:G:75:ASP:OD2	2:G:113:ARG:NH1	2.38	0.57
2:I:158:LEU:HB3	2:I:197:MET:HE2	1.85	0.57
1:F:539:ARG:NH2	2:N:290:GLU:O	2.38	0.56
2:N:239:VAL:HG21	2:N:244:LEU:HD13	1.85	0.56
2:I:75:ASP:OD2	2:I:113:ARG:NH1	2.38	0.56
2:I:208:PRO:O	2:I:211:THR:OG1	2.22	0.56
2:G:64:LEU:O	2:G:69:ARG:NH2	2.38	0.56
1:J:338:LEU:HD11	1:J:348:LEU:HD12	1.87	0.56
1:A:404:ASP:HB3	1:A:411:LEU:HB3	1.87	0.56
1:F:338:LEU:HD11	1:F:348:LEU:HD12	1.87	0.56
1:H:338:LEU:HD11	1:H:348:LEU:HD12	1.87	0.56
1:J:399:ARG:HG2	1:J:451:LYS:HG2	1.88	0.56
1:J:404:ASP:HB3	1:J:411:LEU:HB3	1.87	0.56
2:K:64:LEU:O	2:K:69:ARG:NH2	2.38	0.56
1:B:404:ASP:HB3	1:B:411:LEU:HB3	1.87	0.56
1:B:539:ARG:NH2	2:L:290:GLU:O	2.38	0.56
1:D:549:MET:HE2	2:I:118:LEU:HB2	1.88	0.56
2:N:75:ASP:OD2	2:N:113:ARG:NH1	2.38	0.56
1:D:548:ARG:NH1	2:I:151:VAL:O	2.39	0.56
1:F:399:ARG:HG2	1:F:451:LYS:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:501:PHE:CE1	2:I:174:ALA:HB2	2.40	0.56
2:I:36:ASN:OD1	2:I:37:GLU:N	2.39	0.56
2:L:75:ASP:OD2	2:L:113:ARG:NH1	2.38	0.56
2:N:64:LEU:O	2:N:69:ARG:NH2	2.38	0.56
2:O:36:ASN:OD1	2:O:37:GLU:N	2.39	0.56
2:O:75:ASP:OD2	2:O:113:ARG:NH1	2.38	0.56
2:K:36:ASN:OD1	2:K:37:GLU:N	2.39	0.56
2:L:64:LEU:O	2:L:69:ARG:NH2	2.38	0.56
2:L:179:ILE:HA	2:L:182:ARG:HE	1.71	0.56
2:O:64:LEU:O	2:O:69:ARG:NH2	2.38	0.56
2:K:75:ASP:OD2	2:K:113:ARG:NH1	2.38	0.56
2:L:36:ASN:OD1	2:L:37:GLU:N	2.39	0.56
1:B:338:LEU:HD11	1:B:348:LEU:HD12	1.87	0.56
2:O:179:ILE:HA	2:O:182:ARG:HE	1.71	0.56
1:A:667:PRO:HD3	1:A:720:GLU:HB2	1.88	0.55
1:D:273:GLN:HE21	1:D:288:ARG:HH12	1.55	0.55
1:F:667:PRO:HD3	1:F:720:GLU:HB2	1.88	0.55
1:B:304:PRO:HG2	1:B:394:TRP:HA	1.88	0.55
2:I:64:LEU:O	2:I:69:ARG:NH2	2.38	0.55
1:A:273:GLN:HE21	1:A:288:ARG:HH12	1.54	0.55
2:K:179:ILE:HA	2:K:182:ARG:HE	1.70	0.55
1:B:273:GLN:HE21	1:B:288:ARG:HH12	1.54	0.55
1:F:304:PRO:HG2	1:F:394:TRP:HA	1.88	0.55
2:L:210:LEU:HD11	2:N:416:LEU:HD23	1.88	0.55
1:A:399:ARG:HG2	1:A:451:LYS:HG2	1.88	0.55
1:B:399:ARG:HG2	1:B:451:LYS:HG2	1.88	0.55
1:D:667:PRO:HD3	1:D:720:GLU:HB2	1.88	0.55
1:F:273:GLN:HE21	1:F:288:ARG:HH12	1.55	0.55
2:G:184:VAL:HG21	2:I:420:ALA:HB3	1.87	0.55
1:H:399:ARG:HG2	1:H:451:LYS:HG2	1.88	0.55
2:K:538:PRO:HG3	2:O:210:LEU:HA	1.88	0.55
2:N:36:ASN:OD1	2:N:37:GLU:N	2.39	0.55
1:D:304:PRO:HG2	1:D:394:TRP:HA	1.88	0.55
2:I:179:ILE:HA	2:I:182:ARG:HE	1.71	0.55
1:J:304:PRO:HG2	1:J:394:TRP:HA	1.88	0.55
2:L:335:ASN:HA	2:L:338:LYS:HZ3	1.71	0.55
2:G:36:ASN:OD1	2:G:37:GLU:N	2.39	0.55
2:G:173:LEU:HD11	2:I:462:VAL:HA	1.89	0.55
2:I:124:GLN:HB2	2:I:160:ASP:H	1.72	0.55
1:B:133:LYS:O	1:B:135:ARG:NH1	2.40	0.55
1:B:646:LEU:HD12	2:L:72:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:ASP:HB3	1:D:411:LEU:HB3	1.87	0.55
1:F:404:ASP:HB3	1:F:411:LEU:HB3	1.87	0.55
2:G:124:GLN:HB2	2:G:160:ASP:H	1.72	0.55
1:H:404:ASP:HB3	1:H:411:LEU:HB3	1.87	0.55
2:L:389:ILE:HD11	2:L:519:LEU:HD11	1.89	0.55
2:O:124:GLN:HB2	2:O:160:ASP:H	1.72	0.55
2:G:179:ILE:HA	2:G:182:ARG:HE	1.71	0.55
1:H:273:GLN:HE21	1:H:288:ARG:HH12	1.55	0.55
2:K:114:ILE:HG12	2:K:119:VAL:HG11	1.89	0.55
2:N:124:GLN:HB2	2:N:160:ASP:H	1.72	0.55
1:D:650:MET:HE2	2:I:264:ASP:HB2	1.89	0.55
2:L:184:VAL:HG21	2:N:420:ALA:HB3	1.89	0.55
2:I:389:ILE:HD11	2:I:519:LEU:HD11	1.89	0.54
1:J:133:LYS:O	1:J:135:ARG:NH1	2.40	0.54
2:K:124:GLN:HB2	2:K:160:ASP:H	1.72	0.54
2:L:124:GLN:HB2	2:L:160:ASP:H	1.72	0.54
1:D:133:LYS:O	1:D:135:ARG:NH1	2.40	0.54
1:J:273:GLN:HE21	1:J:288:ARG:HH12	1.55	0.54
1:F:433:SER:HB2	1:F:450:SER:HB2	1.90	0.54
2:K:210:LEU:HA	2:O:538:PRO:HG3	1.88	0.54
2:N:114:ILE:HG12	2:N:119:VAL:HG11	1.89	0.54
2:N:179:ILE:HA	2:N:182:ARG:HE	1.71	0.54
2:O:114:ILE:HG12	2:O:119:VAL:HG11	1.89	0.54
2:O:389:ILE:HD11	2:O:519:LEU:HD11	1.89	0.54
1:B:667:PRO:HD3	1:B:720:GLU:HB2	1.88	0.54
2:L:134:SER:H	2:L:137:HIS:HB3	1.73	0.54
1:B:433:SER:HB2	1:B:450:SER:HB2	1.90	0.54
2:K:134:SER:H	2:K:137:HIS:HB3	1.73	0.54
2:K:416:LEU:HD23	2:O:210:LEU:HD11	1.89	0.54
1:A:433:SER:HB2	1:A:450:SER:HB2	1.90	0.54
1:D:433:SER:HB2	1:D:450:SER:HB2	1.90	0.54
1:F:125:ASP:O	1:F:129:GLU:HG2	2.08	0.54
2:I:134:SER:H	2:I:137:HIS:HB3	1.73	0.54
1:H:433:SER:HB2	1:H:450:SER:HB2	1.90	0.54
1:H:667:PRO:HD3	1:H:720:GLU:HB2	1.88	0.54
2:N:134:SER:H	2:N:137:HIS:HB3	1.73	0.54
1:D:125:ASP:O	1:D:129:GLU:HG2	2.08	0.54
1:F:133:LYS:O	1:F:135:ARG:NH1	2.40	0.54
2:G:134:SER:H	2:G:137:HIS:HB3	1.73	0.54
1:H:304:PRO:HG2	1:H:394:TRP:HA	1.88	0.54
1:A:125:ASP:O	1:A:129:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:O	1:A:135:ARG:NH1	2.40	0.54
2:G:180:PHE:CG	2:I:416:LEU:HD21	2.43	0.54
1:J:667:PRO:HD3	1:J:720:GLU:HB2	1.88	0.54
2:O:134:SER:H	2:O:137:HIS:HB3	1.73	0.54
1:D:399:ARG:HG2	1:D:451:LYS:HG2	1.88	0.54
2:G:499:ARG:NE	2:I:171:GLU:OE2	2.34	0.54
1:H:133:LYS:O	1:H:135:ARG:NH1	2.40	0.54
1:J:433:SER:HB2	1:J:450:SER:HB2	1.90	0.54
1:A:650:MET:HE2	2:G:264:ASP:HB2	1.88	0.53
1:B:125:ASP:O	1:B:129:GLU:HG2	2.08	0.53
1:J:298:LYS:O	1:J:399:ARG:NH2	2.35	0.53
2:K:389:ILE:HD11	2:K:519:LEU:HD11	1.89	0.53
1:F:370:VAL:HA	1:F:373:MET:HE2	1.91	0.53
1:J:125:ASP:O	1:J:129:GLU:HG2	2.08	0.53
2:L:114:ILE:HG12	2:L:119:VAL:HG11	1.89	0.53
1:A:304:PRO:HG2	1:A:394:TRP:HA	1.88	0.53
2:N:389:ILE:HD11	2:N:519:LEU:HD11	1.89	0.53
1:F:206:VAL:HG22	1:F:238:THR:HB	1.91	0.53
2:G:389:ILE:HD11	2:G:519:LEU:HD11	1.89	0.53
1:H:370:VAL:HA	1:H:373:MET:HE2	1.90	0.53
1:J:575:SER:OG	1:J:582:SER:OG	2.26	0.53
2:I:114:ILE:HG12	2:I:119:VAL:HG11	1.89	0.53
1:A:206:VAL:HG22	1:A:238:THR:HB	1.90	0.53
1:H:125:ASP:O	1:H:129:GLU:HG2	2.08	0.53
2:N:498:VAL:HB	2:O:87:GLU:HG2	1.90	0.53
2:O:117:ARG:HB3	2:O:280:LEU:HD21	1.91	0.53
2:G:114:ILE:HG12	2:G:119:VAL:HG11	1.89	0.53
1:H:575:SER:OG	1:H:582:SER:OG	2.25	0.53
2:K:498:VAL:HA	2:L:86:VAL:HA	1.91	0.53
2:N:117:ARG:HB3	2:N:280:LEU:HD21	1.91	0.53
1:D:206:VAL:HG22	1:D:238:THR:HB	1.91	0.53
1:F:646:LEU:HD13	2:N:64:LEU:HD13	1.90	0.53
2:G:376:ARG:NH1	2:I:538:PRO:O	2.42	0.53
1:D:575:SER:OG	1:D:582:SER:OG	2.26	0.52
2:G:538:PRO:O	2:I:376:ARG:NH1	2.42	0.52
2:K:184:VAL:HG21	2:O:420:ALA:HB3	1.90	0.52
1:H:206:VAL:HG22	1:H:238:THR:HB	1.91	0.52
1:H:443:ILE:HD12	1:H:693:MET:HB2	1.92	0.52
2:L:174:ALA:HB2	2:N:501:PHE:HE1	1.74	0.52
1:A:81:THR:O	1:A:85:MET:HG3	2.10	0.52
1:A:303:ALA:HB3	1:A:304:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:HA	1:A:373:MET:HE2	1.91	0.52
2:G:117:ARG:HB3	2:G:280:LEU:HD21	1.91	0.52
1:D:81:THR:O	1:D:85:MET:HG3	2.10	0.52
1:D:400:VAL:HG23	1:D:449:ILE:HB	1.91	0.52
1:D:443:ILE:HD12	1:D:693:MET:HB2	1.92	0.52
1:J:81:THR:O	1:J:85:MET:HG3	2.10	0.52
1:J:646:LEU:HD13	2:O:64:LEU:HD13	1.92	0.52
1:H:81:THR:O	1:H:85:MET:HG3	2.10	0.52
1:D:303:ALA:HB3	1:D:304:PRO:HD3	1.92	0.52
2:G:107:VAL:HG12	2:G:124:GLN:HG2	1.92	0.52
1:H:539:ARG:NH2	2:K:290:GLU:O	2.41	0.52
1:J:443:ILE:HD12	1:J:693:MET:HB2	1.92	0.52
2:L:117:ARG:HB3	2:L:280:LEU:HD21	1.91	0.52
2:L:438:ALA:HA	2:L:441:VAL:HG12	1.92	0.52
1:B:370:VAL:HA	1:B:373:MET:HE2	1.91	0.52
1:B:455:TYR:O	1:B:465:ARG:NH1	2.43	0.52
1:F:81:THR:O	1:F:85:MET:HG3	2.10	0.52
1:F:303:ALA:HB3	1:F:304:PRO:HD3	1.92	0.52
1:F:549:MET:HE2	2:N:118:LEU:HB2	1.90	0.52
2:G:416:LEU:HD21	2:I:180:PHE:CG	2.44	0.52
1:B:575:SER:OG	1:B:582:SER:OG	2.26	0.52
1:F:548:ARG:NH1	2:N:151:VAL:O	2.43	0.52
1:J:400:VAL:HG23	1:J:449:ILE:HB	1.91	0.52
2:O:196:ILE:HB	2:O:216:MET:HB3	1.92	0.52
1:B:81:THR:O	1:B:85:MET:HG3	2.10	0.51
2:I:107:VAL:HG12	2:I:124:GLN:HG2	1.92	0.51
1:B:400:VAL:HG23	1:B:449:ILE:HB	1.91	0.51
1:F:575:SER:OG	1:F:582:SER:OG	2.26	0.51
2:G:196:ILE:HB	2:G:216:MET:HB3	1.92	0.51
2:I:498:VAL:HA	2:N:86:VAL:HA	1.91	0.51
2:K:117:ARG:HB3	2:K:280:LEU:HD21	1.91	0.51
2:O:438:ALA:HA	2:O:441:VAL:HG12	1.92	0.51
1:B:206:VAL:HG22	1:B:238:THR:HB	1.91	0.51
1:B:650:MET:HE2	2:L:264:ASP:HB2	1.91	0.51
1:H:303:ALA:HB3	1:H:304:PRO:HD3	1.92	0.51
1:H:371:GLN:HE22	1:H:375:ARG:HD2	1.76	0.51
1:H:400:VAL:HG23	1:H:449:ILE:HB	1.91	0.51
2:I:86:VAL:HA	2:O:498:VAL:HA	1.93	0.51
1:J:206:VAL:HG22	1:J:238:THR:HB	1.91	0.51
1:B:298:LYS:O	1:B:399:ARG:NH2	2.34	0.51
1:B:303:ALA:HB3	1:B:304:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:GLN:HE22	1:B:375:ARG:HD2	1.76	0.51
2:K:438:ALA:HA	2:K:441:VAL:HG12	1.92	0.51
1:A:79:ILE:HG23	1:A:89:THR:HG21	1.93	0.51
1:A:400:VAL:HG23	1:A:449:ILE:HB	1.91	0.51
1:D:79:ILE:HG23	1:D:89:THR:HG21	1.93	0.51
1:D:370:VAL:HA	1:D:373:MET:HE2	1.91	0.51
1:H:298:LYS:O	1:H:399:ARG:NH2	2.34	0.51
2:I:117:ARG:HB3	2:I:280:LEU:HD21	1.91	0.51
1:A:443:ILE:HD12	1:A:693:MET:HB2	1.92	0.51
1:B:443:ILE:HD12	1:B:693:MET:HB2	1.92	0.51
1:H:455:TYR:O	1:H:465:ARG:NH1	2.43	0.51
2:I:196:ILE:HB	2:I:216:MET:HB3	1.92	0.51
1:J:455:TYR:O	1:J:465:ARG:NH1	2.43	0.51
2:L:208:PRO:O	2:L:211:THR:OG1	2.22	0.51
2:N:134:SER:OG	2:N:135:GLY:N	2.44	0.51
2:K:134:SER:OG	2:K:135:GLY:N	2.44	0.51
2:L:196:ILE:HB	2:L:216:MET:HB3	1.92	0.51
2:N:107:VAL:HG12	2:N:124:GLN:HG2	1.92	0.51
2:N:196:ILE:HB	2:N:216:MET:HB3	1.92	0.51
1:F:362:GLU:HG2	1:F:369:LEU:HD23	1.93	0.51
1:F:443:ILE:HD12	1:F:693:MET:HB2	1.92	0.51
2:I:134:SER:OG	2:I:135:GLY:N	2.44	0.51
2:K:196:ILE:HB	2:K:216:MET:HB3	1.92	0.51
1:A:455:TYR:O	1:A:465:ARG:NH1	2.43	0.51
1:J:303:ALA:HB3	1:J:304:PRO:HD3	1.92	0.51
1:J:370:VAL:HA	1:J:373:MET:HE2	1.91	0.51
2:O:107:VAL:HG12	2:O:124:GLN:HG2	1.92	0.51
1:A:362:GLU:HG2	1:A:369:LEU:HD23	1.93	0.50
1:A:371:GLN:HE22	1:A:375:ARG:HD2	1.76	0.50
1:B:683:GLU:HG2	1:B:703:LYS:HA	1.93	0.50
1:D:455:TYR:O	1:D:465:ARG:NH1	2.43	0.50
1:F:455:TYR:O	1:F:465:ARG:NH1	2.43	0.50
1:H:79:ILE:HG23	1:H:89:THR:HG21	1.93	0.50
2:I:438:ALA:HA	2:I:441:VAL:HG12	1.92	0.50
2:O:134:SER:OG	2:O:135:GLY:N	2.44	0.50
1:F:79:ILE:HG23	1:F:89:THR:HG21	1.93	0.50
2:N:178:ASP:HA	2:N:181:LEU:HD12	1.93	0.50
2:G:134:SER:OG	2:G:135:GLY:N	2.44	0.50
1:J:79:ILE:HG23	1:J:89:THR:HG21	1.93	0.50
1:J:683:GLU:HG2	1:J:703:LYS:HA	1.93	0.50
2:K:107:VAL:HG12	2:K:124:GLN:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:180:PHE:CG	2:O:416:LEU:HD21	2.47	0.50
2:L:251:THR:HG21	2:L:260:ALA:HB2	1.94	0.50
2:O:251:THR:HG21	2:O:260:ALA:HB2	1.94	0.50
1:F:400:VAL:HG23	1:F:449:ILE:HB	1.91	0.50
2:K:420:ALA:HB3	2:O:184:VAL:HG21	1.93	0.50
2:N:251:THR:HG21	2:N:260:ALA:HB2	1.93	0.50
2:N:438:ALA:HA	2:N:441:VAL:HG12	1.92	0.50
1:B:362:GLU:HG2	1:B:369:LEU:HD23	1.93	0.50
1:J:371:GLN:HE22	1:J:375:ARG:HD2	1.76	0.50
2:O:61:ARG:HH11	2:O:63:LYS:HZ2	1.60	0.50
1:D:371:GLN:HE22	1:D:375:ARG:HD2	1.76	0.50
2:K:178:ASP:HA	2:K:181:LEU:HD12	1.93	0.50
2:K:251:THR:HG21	2:K:260:ALA:HB2	1.93	0.50
2:L:107:VAL:HG12	2:L:124:GLN:HG2	1.92	0.50
1:B:76:CYS:HB2	1:B:80:ARG:HH21	1.77	0.50
1:F:76:CYS:HB2	1:F:80:ARG:HH21	1.77	0.50
1:J:240:ASP:OD1	1:J:241:GLY:N	2.45	0.50
2:L:178:ASP:HA	2:L:181:LEU:HD12	1.93	0.50
1:A:76:CYS:HB2	1:A:80:ARG:HH21	1.77	0.50
2:G:438:ALA:HA	2:G:441:VAL:HG12	1.92	0.50
1:H:240:ASP:OD1	1:H:241:GLY:N	2.45	0.50
1:A:240:ASP:OD1	1:A:241:GLY:N	2.45	0.49
1:B:79:ILE:HG23	1:B:89:THR:HG21	1.93	0.49
1:D:362:GLU:HG2	1:D:369:LEU:HD23	1.93	0.49
1:J:625:MET:HB3	1:J:636:VAL:HG23	1.94	0.49
1:B:673:VAL:HG11	1:B:710:VAL:HG11	1.94	0.49
1:D:240:ASP:OD1	1:D:241:GLY:N	2.45	0.49
1:D:683:GLU:HG2	1:D:703:LYS:HA	1.93	0.49
1:F:371:GLN:HE22	1:F:375:ARG:HD2	1.76	0.49
1:F:625:MET:HB3	1:F:636:VAL:HG23	1.95	0.49
1:H:362:GLU:HG2	1:H:369:LEU:HD23	1.93	0.49
1:J:76:CYS:HB2	1:J:80:ARG:HH21	1.77	0.49
2:L:61:ARG:HH11	2:L:63:LYS:HZ2	1.61	0.49
1:A:575:SER:OG	1:A:582:SER:OG	2.26	0.49
1:B:240:ASP:OD1	1:B:241:GLY:N	2.45	0.49
2:G:251:THR:HG21	2:G:260:ALA:HB2	1.93	0.49
1:H:76:CYS:HB2	1:H:80:ARG:HH21	1.77	0.49
2:N:492:ASN:OD1	2:O:38:ARG:NH1	2.45	0.49
1:D:250:ALA:HA	1:D:254:GLY:HA2	1.95	0.49
1:F:249:ALA:O	1:F:254:GLY:N	2.43	0.49
1:F:429:VAL:HG13	1:F:452:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:683:GLU:HG2	1:F:703:LYS:HA	1.93	0.49
2:G:178:ASP:HA	2:G:181:LEU:HD12	1.93	0.49
1:H:250:ALA:HA	1:H:254:GLY:HA2	1.94	0.49
1:H:683:GLU:HG2	1:H:703:LYS:HA	1.93	0.49
2:I:251:THR:HG21	2:I:260:ALA:HB2	1.93	0.49
1:B:625:MET:HB3	1:B:636:VAL:HG23	1.94	0.49
2:K:73:LEU:HB2	2:K:268:LEU:HD22	1.95	0.49
1:D:195:PHE:HE1	1:D:208:ILE:HG12	1.78	0.49
2:O:178:ASP:HA	2:O:181:LEU:HD12	1.93	0.49
1:D:116:PRO:HB2	1:D:119:LYS:HG2	1.95	0.49
1:D:647:ASN:HA	1:D:650:MET:SD	2.53	0.49
1:D:673:VAL:HG11	1:D:710:VAL:HG11	1.94	0.49
1:H:338:LEU:O	1:H:346:TYR:N	2.46	0.49
2:I:73:LEU:HB2	2:I:268:LEU:HD22	1.95	0.49
2:I:178:ASP:HA	2:I:181:LEU:HD12	1.93	0.49
1:A:250:ALA:HA	1:A:254:GLY:HA2	1.94	0.49
1:B:647:ASN:HA	1:B:650:MET:SD	2.53	0.49
1:F:240:ASP:OD1	1:F:241:GLY:N	2.45	0.49
2:G:462:VAL:HA	2:I:173:LEU:HD11	1.95	0.49
1:H:116:PRO:HB2	1:H:119:LYS:HG2	1.95	0.49
1:J:79:ILE:HG21	1:J:105:MET:HG3	1.95	0.49
1:J:116:PRO:HB2	1:J:119:LYS:HG2	1.95	0.49
2:K:492:ASN:OD1	2:L:38:ARG:NH1	2.45	0.49
2:K:537:ILE:HG12	2:K:539:LEU:H	1.78	0.49
1:A:116:PRO:HB2	1:A:119:LYS:HG2	1.95	0.49
1:F:294:ARG:NH2	1:F:403:GLU:OE1	2.40	0.49
1:H:195:PHE:HE1	1:H:208:ILE:HG12	1.78	0.49
1:H:673:VAL:HG11	1:H:710:VAL:HG11	1.94	0.49
1:J:321:VAL:O	1:J:325:ARG:HG2	2.13	0.49
2:K:441:VAL:HG13	2:K:442:MET:SD	2.53	0.49
2:L:88:HIS:CG	2:L:89:ARG:H	2.31	0.49
2:L:441:VAL:HG13	2:L:442:MET:SD	2.53	0.49
2:N:313:ALA:HA	2:N:432:ARG:HH12	1.78	0.49
1:B:321:VAL:O	1:B:325:ARG:HG2	2.13	0.49
1:D:76:CYS:HB2	1:D:80:ARG:HH21	1.77	0.49
2:G:174:ALA:HB2	2:I:501:PHE:CE1	2.48	0.49
1:H:429:VAL:HG13	1:H:452:LEU:HD11	1.94	0.49
1:J:362:GLU:HG2	1:J:369:LEU:HD23	1.93	0.49
1:J:647:ASN:HA	1:J:650:MET:SD	2.53	0.49
2:K:313:ALA:HA	2:K:432:ARG:HH12	1.78	0.49
2:L:537:ILE:HG12	2:L:539:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:441:VAL:HG13	2:O:442:MET:SD	2.53	0.49
1:F:673:VAL:HG11	1:F:710:VAL:HG11	1.94	0.48
2:G:73:LEU:HB2	2:G:268:LEU:HD22	1.95	0.48
2:G:537:ILE:HG12	2:G:539:LEU:H	1.78	0.48
2:L:73:LEU:HB2	2:L:268:LEU:HD22	1.95	0.48
2:N:73:LEU:HB2	2:N:268:LEU:HD22	1.95	0.48
1:F:321:VAL:O	1:F:325:ARG:HG2	2.13	0.48
1:F:408:SER:OG	1:F:409:PHE:N	2.46	0.48
2:G:313:ALA:HA	2:G:432:ARG:HH12	1.78	0.48
1:H:79:ILE:HG21	1:H:105:MET:HG3	1.95	0.48
1:H:408:SER:OG	1:H:409:PHE:N	2.46	0.48
1:H:625:MET:HB3	1:H:636:VAL:HG23	1.94	0.48
1:J:338:LEU:O	1:J:346:TYR:N	2.46	0.48
1:J:549:MET:HE2	2:O:118:LEU:HB2	1.94	0.48
2:K:88:HIS:CG	2:K:89:ARG:H	2.31	0.48
2:L:134:SER:OG	2:L:135:GLY:N	2.44	0.48
2:N:441:VAL:HG13	2:N:442:MET:SD	2.53	0.48
1:A:79:ILE:HG21	1:A:105:MET:HG3	1.95	0.48
1:A:429:VAL:HG13	1:A:452:LEU:HD11	1.94	0.48
1:B:195:PHE:HE1	1:B:208:ILE:HG12	1.78	0.48
1:F:250:ALA:HA	1:F:254:GLY:HA2	1.94	0.48
1:F:646:LEU:HD12	2:N:72:LEU:HG	1.94	0.48
2:G:88:HIS:CG	2:G:89:ARG:H	2.31	0.48
2:K:416:LEU:HD21	2:O:180:PHE:CG	2.48	0.48
2:O:73:LEU:HB2	2:O:268:LEU:HD22	1.95	0.48
1:A:321:VAL:O	1:A:325:ARG:HG2	2.13	0.48
1:A:647:ASN:HA	1:A:650:MET:SD	2.53	0.48
1:B:250:ALA:HA	1:B:254:GLY:HA2	1.95	0.48
1:B:408:SER:OG	1:B:409:PHE:N	2.46	0.48
1:F:647:ASN:HA	1:F:650:MET:SD	2.53	0.48
2:I:537:ILE:HG12	2:I:539:LEU:H	1.78	0.48
1:J:195:PHE:HE1	1:J:208:ILE:HG12	1.78	0.48
1:J:673:VAL:HG11	1:J:710:VAL:HG11	1.94	0.48
2:K:323:VAL:O	2:K:512:ARG:NH1	2.45	0.48
2:L:323:VAL:O	2:L:512:ARG:NH1	2.45	0.48
2:O:313:ALA:HA	2:O:432:ARG:HH12	1.78	0.48
1:A:683:GLU:HG2	1:A:703:LYS:HA	1.93	0.48
1:B:79:ILE:HG21	1:B:105:MET:HG3	1.95	0.48
1:D:321:VAL:O	1:D:325:ARG:HG2	2.13	0.48
1:H:647:ASN:HA	1:H:650:MET:SD	2.53	0.48
1:J:429:VAL:HG13	1:J:452:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:539:ARG:NH2	2:O:290:GLU:O	2.46	0.48
2:K:208:PRO:O	2:K:211:THR:OG1	2.22	0.48
2:L:313:ALA:HA	2:L:432:ARG:HH12	1.78	0.48
1:A:625:MET:HB3	1:A:636:VAL:HG23	1.95	0.48
1:D:429:VAL:HG13	1:D:452:LEU:HD11	1.94	0.48
1:F:114:PRO:O	1:F:120:SER:OG	2.23	0.48
1:F:168:THR:HA	1:F:171:ILE:HD12	1.96	0.48
1:F:256:ASP:OD2	1:F:257:ARG:NH2	2.43	0.48
1:F:338:LEU:O	1:F:346:TYR:N	2.46	0.48
2:O:323:VAL:O	2:O:512:ARG:NH1	2.45	0.48
1:A:673:VAL:HG11	1:A:710:VAL:HG11	1.94	0.48
1:B:429:VAL:HG13	1:B:452:LEU:HD11	1.94	0.48
1:D:79:ILE:HG21	1:D:105:MET:HG3	1.95	0.48
1:D:338:LEU:O	1:D:346:TYR:N	2.46	0.48
1:D:625:MET:HB3	1:D:636:VAL:HG23	1.94	0.48
2:I:313:ALA:HA	2:I:432:ARG:HH12	1.78	0.48
2:I:462:VAL:CG1	2:I:463:MET:HE2	2.44	0.48
1:J:250:ALA:HA	1:J:254:GLY:HA2	1.94	0.48
2:O:88:HIS:CG	2:O:89:ARG:H	2.31	0.48
1:F:195:PHE:HE1	1:F:208:ILE:HG12	1.78	0.48
2:G:375:ALA:O	2:G:379:ARG:HG3	2.14	0.48
2:K:462:VAL:CG1	2:K:463:MET:HE2	2.44	0.48
1:A:195:PHE:HE1	1:A:208:ILE:HG12	1.78	0.48
1:A:269:HIS:NE2	1:A:336:GLU:HG3	2.29	0.48
1:B:74:ILE:HD11	1:B:140:HIS:HE1	1.79	0.48
1:F:74:ILE:HD11	1:F:140:HIS:HE1	1.79	0.48
1:F:298:LYS:O	1:F:399:ARG:NH2	2.35	0.48
1:H:74:ILE:HD11	1:H:140:HIS:HE1	1.79	0.48
2:I:61:ARG:HH11	2:I:63:LYS:HZ2	1.61	0.48
2:I:441:VAL:HG13	2:I:442:MET:SD	2.53	0.48
1:J:74:ILE:HD11	1:J:140:HIS:HE1	1.79	0.48
1:A:168:THR:HA	1:A:171:ILE:HD12	1.96	0.48
1:B:338:LEU:O	1:B:346:TYR:N	2.46	0.48
1:F:116:PRO:HB2	1:F:119:LYS:HG2	1.95	0.48
1:F:269:HIS:NE2	1:F:336:GLU:HG3	2.29	0.48
2:G:441:VAL:HG13	2:G:442:MET:SD	2.53	0.48
2:G:462:VAL:CG1	2:G:463:MET:HE2	2.43	0.48
1:H:269:HIS:NE2	1:H:336:GLU:HG3	2.29	0.48
1:J:269:HIS:NE2	1:J:336:GLU:HG3	2.29	0.48
2:N:88:HIS:CG	2:N:89:ARG:H	2.31	0.48
1:B:116:PRO:HB2	1:B:119:LYS:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:646:LEU:HD12	2:I:72:LEU:HG	1.96	0.47
1:F:79:ILE:HG21	1:F:105:MET:HG3	1.95	0.47
1:H:321:VAL:O	1:H:325:ARG:HG2	2.13	0.47
2:I:375:ALA:O	2:I:379:ARG:HG3	2.14	0.47
2:N:375:ALA:O	2:N:379:ARG:HG3	2.14	0.47
2:N:537:ILE:HG12	2:N:539:LEU:H	1.78	0.47
2:O:375:ALA:O	2:O:379:ARG:HG3	2.14	0.47
1:A:338:LEU:O	1:A:346:TYR:N	2.46	0.47
1:B:269:HIS:NE2	1:B:336:GLU:HG3	2.29	0.47
2:L:375:ALA:O	2:L:379:ARG:HG3	2.14	0.47
1:A:249:ALA:O	1:A:254:GLY:N	2.43	0.47
2:O:537:ILE:HG12	2:O:539:LEU:H	1.78	0.47
1:A:74:ILE:HD11	1:A:140:HIS:HE1	1.79	0.47
1:D:168:THR:HA	1:D:171:ILE:HD12	1.96	0.47
2:I:88:HIS:CG	2:I:89:ARG:H	2.31	0.47
1:A:506:ASP:OD1	1:A:507:VAL:N	2.48	0.47
2:I:258:HIS:CD2	2:I:333:MET:HE3	2.50	0.47
1:J:408:SER:OG	1:J:409:PHE:N	2.46	0.47
1:B:168:THR:HA	1:B:171:ILE:HD12	1.96	0.47
1:D:269:HIS:NE2	1:D:336:GLU:HG3	2.29	0.47
1:D:408:SER:OG	1:D:409:PHE:N	2.46	0.47
2:G:340:ILE:HA	2:G:357:ASN:HA	1.97	0.47
1:H:506:ASP:OD1	1:H:507:VAL:N	2.48	0.47
2:K:375:ALA:O	2:K:379:ARG:HG3	2.14	0.47
1:A:294:ARG:NH2	1:A:403:GLU:OE1	2.40	0.47
1:A:298:LYS:O	1:A:399:ARG:NH2	2.34	0.47
1:B:294:ARG:NH2	1:B:403:GLU:OE1	2.40	0.47
1:D:506:ASP:OD1	1:D:507:VAL:N	2.48	0.47
2:I:46:ALA:O	2:I:67:ARG:NH2	2.48	0.47
2:I:340:ILE:HA	2:I:357:ASN:HA	1.97	0.47
2:K:174:ALA:HB2	2:O:501:PHE:CE1	2.49	0.47
2:O:258:HIS:CD2	2:O:333:MET:HE3	2.50	0.47
1:B:506:ASP:OD1	1:B:507:VAL:N	2.48	0.47
1:F:214:TYR:HB3	1:F:215:PRO:HD3	1.96	0.47
2:G:258:HIS:CD2	2:G:333:MET:HE3	2.50	0.47
2:K:258:HIS:CD2	2:K:333:MET:HE3	2.50	0.47
1:A:677:PRO:HG3	1:A:710:VAL:H	1.80	0.47
1:D:214:TYR:HB3	1:D:215:PRO:HD3	1.96	0.47
1:F:677:PRO:HG3	1:F:710:VAL:H	1.80	0.47
1:H:677:PRO:HG3	1:H:710:VAL:H	1.80	0.47
1:J:506:ASP:OD1	1:J:507:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:61:ARG:HH11	2:K:63:LYS:HZ2	1.62	0.47
2:L:340:ILE:HA	2:L:357:ASN:HA	1.97	0.47
2:N:95:MET:HB2	2:N:98:ASP:O	2.15	0.47
2:N:258:HIS:CD2	2:N:333:MET:HE3	2.50	0.47
2:N:426:LYS:NZ	2:N:447:LEU:O	2.48	0.47
1:H:214:TYR:HB3	1:H:215:PRO:HD3	1.96	0.47
2:I:95:MET:HB2	2:I:98:ASP:O	2.15	0.47
2:K:46:ALA:O	2:K:67:ARG:NH2	2.48	0.47
2:L:258:HIS:CD2	2:L:333:MET:HE3	2.50	0.47
1:D:298:LYS:O	1:D:399:ARG:NH2	2.34	0.46
2:G:216:MET:HE1	2:G:247:ALA:HB2	1.97	0.46
1:J:168:THR:HA	1:J:171:ILE:HD12	1.96	0.46
2:K:216:MET:HE1	2:K:247:ALA:HB2	1.97	0.46
2:O:340:ILE:HA	2:O:357:ASN:HA	1.97	0.46
2:G:46:ALA:O	2:G:67:ARG:NH2	2.48	0.46
1:J:214:TYR:HB3	1:J:215:PRO:HD3	1.96	0.46
2:K:181:LEU:HD11	2:O:446:HIS:HB3	1.97	0.46
2:K:340:ILE:HA	2:K:357:ASN:HA	1.97	0.46
2:N:216:MET:HE1	2:N:247:ALA:HB2	1.97	0.46
2:N:340:ILE:HA	2:N:357:ASN:HA	1.97	0.46
1:D:74:ILE:HD11	1:D:140:HIS:HE1	1.79	0.46
1:F:533:PHE:O	1:F:537:GLN:HG2	2.16	0.46
2:I:133:LEU:HD12	2:I:137:HIS:CG	2.51	0.46
2:O:462:VAL:CG1	2:O:463:MET:HE2	2.43	0.46
1:J:118:SER:HA	1:J:122:LEU:HB2	1.98	0.46
1:J:677:PRO:HG3	1:J:710:VAL:H	1.80	0.46
2:L:46:ALA:O	2:L:67:ARG:NH2	2.48	0.46
2:L:95:MET:HB2	2:L:98:ASP:O	2.15	0.46
1:A:647:ASN:HB2	2:G:265:VAL:HG21	1.98	0.46
1:B:677:PRO:HG3	1:B:710:VAL:H	1.80	0.46
1:D:677:PRO:HG3	1:D:710:VAL:H	1.80	0.46
1:F:70:ASN:HD22	1:F:143:TYR:H	1.63	0.46
1:F:506:ASP:OD1	1:F:507:VAL:N	2.48	0.46
2:I:216:MET:HE1	2:I:247:ALA:HB2	1.97	0.46
2:L:133:LEU:HD12	2:L:137:HIS:CG	2.51	0.46
2:N:323:VAL:O	2:N:512:ARG:NH1	2.45	0.46
2:N:462:VAL:CG1	2:N:463:MET:HE2	2.44	0.46
1:A:533:PHE:O	1:A:537:GLN:HG2	2.16	0.46
1:B:214:TYR:HB3	1:B:215:PRO:HD3	1.96	0.46
1:F:118:SER:HA	1:F:122:LEU:HB2	1.98	0.46
2:G:426:LYS:NZ	2:G:447:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:SER:HA	1:H:122:LEU:HB2	1.98	0.46
2:L:426:LYS:NZ	2:L:447:LEU:O	2.48	0.46
2:L:536:ASN:ND2	2:N:212:ASP:OD1	2.49	0.46
2:N:46:ALA:O	2:N:67:ARG:NH2	2.48	0.46
1:D:249:ALA:O	1:D:254:GLY:N	2.42	0.46
1:H:168:THR:HA	1:H:171:ILE:HD12	1.96	0.46
2:K:95:MET:HB2	2:K:98:ASP:O	2.16	0.46
2:K:494:PHE:HZ	2:L:39:ILE:HA	1.81	0.46
2:L:216:MET:HE1	2:L:247:ALA:HB2	1.97	0.46
1:A:70:ASN:HD22	1:A:143:TYR:H	1.63	0.46
1:A:408:SER:OG	1:A:409:PHE:N	2.46	0.46
1:B:533:PHE:O	1:B:537:GLN:HG2	2.16	0.46
2:G:38:ARG:NH1	2:L:492:ASN:OD1	2.48	0.46
2:G:133:LEU:HD12	2:G:137:HIS:CG	2.51	0.46
1:J:249:ALA:O	1:J:254:GLY:N	2.43	0.46
1:J:563:VAL:HG12	1:J:638:ILE:HG13	1.98	0.46
2:O:46:ALA:O	2:O:67:ARG:NH2	2.48	0.46
1:D:599:ALA:H	2:I:292:HIS:HE2	1.63	0.46
2:G:446:HIS:HB3	2:I:181:LEU:HD11	1.96	0.46
1:H:114:PRO:O	1:H:120:SER:OG	2.23	0.46
1:H:457:SER:N	1:H:461:GLU:OE2	2.43	0.46
1:H:563:VAL:HG12	1:H:638:ILE:HG13	1.98	0.46
2:I:426:LYS:NZ	2:I:447:LEU:O	2.48	0.46
2:N:208:PRO:O	2:N:211:THR:OG1	2.22	0.46
1:A:114:PRO:O	1:A:120:SER:OG	2.23	0.46
1:A:214:TYR:HB3	1:A:215:PRO:HD3	1.96	0.46
1:B:118:SER:HA	1:B:122:LEU:HB2	1.98	0.46
1:B:218:ILE:HG12	1:B:260:ILE:HD12	1.98	0.46
1:H:533:PHE:O	1:H:537:GLN:HG2	2.16	0.46
2:L:462:VAL:CG1	2:L:463:MET:HE2	2.44	0.46
2:O:133:LEU:HD12	2:O:137:HIS:CG	2.51	0.46
1:F:710:VAL:HA	1:F:725:VAL:HG23	1.98	0.45
2:I:347:MET:HE1	2:I:516:CYS:HA	1.98	0.45
2:L:471:ILE:HG22	2:N:166:ILE:HG21	1.97	0.45
2:N:133:LEU:HD12	2:N:137:HIS:CG	2.51	0.45
1:A:118:SER:HA	1:A:122:LEU:HB2	1.98	0.45
1:B:563:VAL:HG12	1:B:638:ILE:HG13	1.98	0.45
1:F:218:ILE:HG12	1:F:260:ILE:HD12	1.98	0.45
1:F:563:VAL:HG12	1:F:638:ILE:HG13	1.98	0.45
2:G:181:LEU:HD11	2:I:446:HIS:HB3	1.97	0.45
1:J:218:ILE:HG12	1:J:260:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:216:MET:HE1	2:O:247:ALA:HB2	1.97	0.45
2:O:347:MET:HE1	2:O:516:CYS:HA	1.98	0.45
2:O:426:LYS:NZ	2:O:447:LEU:O	2.48	0.45
1:A:710:VAL:HA	1:A:725:VAL:HG23	1.99	0.45
1:B:249:ALA:O	1:B:254:GLY:N	2.42	0.45
1:D:70:ASN:HD22	1:D:143:TYR:H	1.63	0.45
1:J:533:PHE:O	1:J:537:GLN:HG2	2.16	0.45
2:K:252:THR:HG22	2:K:335:ASN:HB3	1.99	0.45
2:K:426:LYS:NZ	2:K:447:LEU:O	2.48	0.45
2:N:61:ARG:HH11	2:N:63:LYS:HZ2	1.63	0.45
1:B:457:SER:N	1:B:461:GLU:OE2	2.42	0.45
1:D:533:PHE:O	1:D:537:GLN:HG2	2.16	0.45
1:F:199:VAL:HG12	1:F:204:GLU:HG2	1.98	0.45
2:G:61:ARG:HH11	2:G:63:LYS:HZ2	1.63	0.45
2:G:208:PRO:O	2:G:211:THR:OG1	2.22	0.45
2:L:531:TRP:HZ3	2:N:283:GLN:HG3	1.81	0.45
1:D:118:SER:HA	1:D:122:LEU:HB2	1.98	0.45
2:G:252:THR:HG22	2:G:335:ASN:HB3	1.99	0.45
1:H:199:VAL:HG12	1:H:204:GLU:HG2	1.98	0.45
1:J:70:ASN:HD22	1:J:143:TYR:H	1.63	0.45
2:K:347:MET:HE1	2:K:516:CYS:HA	1.98	0.45
1:D:710:VAL:HA	1:D:725:VAL:HG23	1.99	0.45
2:G:95:MET:HB2	2:G:98:ASP:O	2.16	0.45
2:G:347:MET:HE1	2:G:516:CYS:HA	1.98	0.45
1:H:70:ASN:HD22	1:H:143:TYR:H	1.63	0.45
2:L:252:THR:HG22	2:L:335:ASN:HB3	1.99	0.45
2:N:252:THR:HG22	2:N:335:ASN:HB3	1.99	0.45
2:O:95:MET:HB2	2:O:98:ASP:O	2.15	0.45
2:N:266:ASP:O	2:N:270:ASN:ND2	2.32	0.45
2:O:252:THR:HG22	2:O:335:ASN:HB3	1.99	0.45
2:K:133:LEU:HD12	2:K:137:HIS:CG	2.51	0.45
2:O:145:MET:HG2	2:O:155:VAL:HG21	1.99	0.45
1:D:294:ARG:NH2	1:D:403:GLU:OE1	2.40	0.45
2:G:175:GLY:O	2:G:179:ILE:HG12	2.17	0.45
1:H:650:MET:SD	2:K:265:VAL:HG23	2.57	0.45
2:I:252:THR:HG22	2:I:335:ASN:HB3	1.99	0.45
2:K:342:VAL:HG12	2:K:355:VAL:HG22	1.99	0.45
2:G:145:MET:HG2	2:G:155:VAL:HG21	1.99	0.45
1:H:710:VAL:HA	1:H:725:VAL:HG23	1.99	0.45
2:N:342:VAL:HG12	2:N:355:VAL:HG22	1.99	0.45
1:A:199:VAL:HG12	1:A:204:GLU:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:SER:N	1:A:461:GLU:OE2	2.43	0.44
1:D:563:VAL:HG12	1:D:638:ILE:HG13	1.98	0.44
1:J:548:ARG:NH1	2:O:151:VAL:O	2.50	0.44
2:L:347:MET:HE1	2:L:516:CYS:HA	1.98	0.44
2:N:175:GLY:O	2:N:179:ILE:HG12	2.17	0.44
1:A:563:VAL:HG12	1:A:638:ILE:HG13	1.98	0.44
1:B:199:VAL:HG12	1:B:204:GLU:HG2	1.98	0.44
1:F:493:ARG:HA	1:F:496:LYS:HG2	1.99	0.44
1:J:493:ARG:HA	1:J:496:LYS:HG2	1.99	0.44
2:K:171:GLU:OE2	2:O:499:ARG:NE	2.40	0.44
2:N:347:MET:HE1	2:N:516:CYS:HA	1.98	0.44
2:O:342:VAL:HG12	2:O:355:VAL:HG22	1.99	0.44
1:A:192:ILE:HD13	1:A:346:TYR:HB3	2.00	0.44
1:A:218:ILE:HG12	1:A:260:ILE:HD12	1.99	0.44
2:G:342:VAL:HG12	2:G:355:VAL:HG22	1.99	0.44
1:H:493:ARG:HA	1:H:496:LYS:HG2	2.00	0.44
2:I:342:VAL:HG12	2:I:355:VAL:HG22	1.99	0.44
2:K:446:HIS:HB3	2:O:181:LEU:HD11	2.00	0.44
2:L:342:VAL:HG12	2:L:355:VAL:HG22	1.99	0.44
1:A:400:VAL:O	1:A:449:ILE:N	2.50	0.44
1:B:200:LYS:HA	1:B:200:LYS:HD3	1.75	0.44
1:B:710:VAL:HA	1:B:725:VAL:HG23	1.99	0.44
1:D:218:ILE:HG12	1:D:260:ILE:HD12	1.98	0.44
1:F:262:LYS:HE2	1:F:262:LYS:HB2	1.86	0.44
2:G:492:ASN:OD1	2:K:38:ARG:NH1	2.50	0.44
1:H:218:ILE:HG12	1:H:260:ILE:HD12	1.98	0.44
2:I:145:MET:HG2	2:I:155:VAL:HG21	1.99	0.44
1:B:70:ASN:HD22	1:B:143:TYR:H	1.63	0.44
1:B:707:VAL:HA	1:B:727:LEU:HD23	1.99	0.44
1:F:192:ILE:HD13	1:F:346:TYR:HB3	2.00	0.44
2:G:501:PHE:HE1	2:I:174:ALA:HB2	1.79	0.44
1:J:199:VAL:HG12	1:J:204:GLU:HG2	1.98	0.44
1:J:646:LEU:HD12	2:O:72:LEU:HG	1.98	0.44
2:L:145:MET:HG2	2:L:155:VAL:HG21	1.99	0.44
1:B:493:ARG:HA	1:B:496:LYS:HG2	1.99	0.44
2:G:323:VAL:O	2:G:512:ARG:NH1	2.45	0.44
2:G:446:HIS:HD2	2:I:177:ALA:HB3	1.83	0.44
2:I:175:GLY:O	2:I:179:ILE:HG12	2.17	0.44
1:J:146:LEU:HD22	1:J:149:ASN:HD22	1.83	0.44
1:J:707:VAL:HA	1:J:727:LEU:HD23	1.99	0.44
1:J:710:VAL:HA	1:J:725:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:145:MET:HG2	2:N:155:VAL:HG21	1.99	0.44
1:A:356:VAL:HG21	1:A:399:ARG:NH1	2.33	0.44
1:A:493:ARG:HA	1:A:496:LYS:HG2	1.99	0.44
1:B:192:ILE:HD13	1:B:346:TYR:HB3	2.00	0.44
1:B:664:SER:HB3	1:B:722:ASP:HB2	1.99	0.44
1:D:356:VAL:HG21	1:D:399:ARG:NH1	2.33	0.44
1:F:200:LYS:HD3	1:F:200:LYS:HA	1.75	0.44
1:J:192:ILE:HD13	1:J:346:TYR:HB3	2.00	0.44
2:G:61:ARG:HH22	2:G:199:PRO:HD3	1.83	0.44
1:J:664:SER:HB3	1:J:722:ASP:HB2	1.99	0.44
2:K:145:MET:HG2	2:K:155:VAL:HG21	1.99	0.44
2:K:175:GLY:O	2:K:179:ILE:HG12	2.17	0.44
1:D:707:VAL:HA	1:D:727:LEU:HD23	1.99	0.44
2:L:175:GLY:O	2:L:179:ILE:HG12	2.17	0.44
1:B:400:VAL:O	1:B:449:ILE:N	2.50	0.43
1:D:400:VAL:O	1:D:449:ILE:N	2.50	0.43
1:F:664:SER:HB3	1:F:722:ASP:HB2	1.99	0.43
1:H:146:LEU:HD22	1:H:149:ASN:HD22	1.83	0.43
1:J:262:LYS:HE3	1:J:346:TYR:CZ	2.53	0.43
1:A:397:GLU:OE2	1:A:453:ILE:HG13	2.18	0.43
1:A:707:VAL:HA	1:A:727:LEU:HD23	1.99	0.43
1:D:199:VAL:HG12	1:D:204:GLU:HG2	1.98	0.43
1:H:262:LYS:HE3	1:H:346:TYR:CZ	2.53	0.43
1:H:664:SER:HB3	1:H:722:ASP:HB2	1.99	0.43
1:J:457:SER:N	1:J:461:GLU:OE2	2.43	0.43
2:L:173:LEU:HD11	2:N:462:VAL:HA	2.00	0.43
1:B:146:LEU:HD22	1:B:149:ASN:HD22	1.83	0.43
1:B:356:VAL:HG21	1:B:399:ARG:NH1	2.33	0.43
1:D:664:SER:HB3	1:D:722:ASP:HB2	1.99	0.43
1:J:397:GLU:OE2	1:J:453:ILE:HG13	2.18	0.43
1:J:540:ALA:C	2:O:115:ASN:HD21	2.27	0.43
2:L:197:MET:C	2:L:221:SER:HB3	2.44	0.43
2:N:498:VAL:HA	2:O:86:VAL:HA	1.99	0.43
2:O:61:ARG:HH22	2:O:199:PRO:HD3	1.83	0.43
2:O:106:SER:HB3	2:O:128:VAL:HG13	2.00	0.43
1:A:664:SER:HB3	1:A:722:ASP:HB2	1.99	0.43
1:D:397:GLU:OE2	1:D:453:ILE:HG13	2.18	0.43
1:F:183:LEU:HD13	1:F:327:VAL:HG12	2.00	0.43
1:F:356:VAL:HG21	1:F:399:ARG:NH1	2.33	0.43
1:F:599:ALA:H	2:N:292:HIS:HE2	1.65	0.43
1:H:233:TRP:HZ2	1:H:265:ASP:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:370:VAL:O	1:H:374:ILE:HG12	2.19	0.43
1:H:397:GLU:OE2	1:H:453:ILE:HG13	2.18	0.43
2:L:416:LEU:HD23	2:N:210:LEU:HD11	2.00	0.43
2:N:141:ILE:HA	2:N:144:ILE:HG22	2.01	0.43
1:B:169:HIS:HA	1:B:172:GLN:NE2	2.34	0.43
1:D:493:ARG:HA	1:D:496:LYS:HG2	1.99	0.43
2:K:141:ILE:HA	2:K:144:ILE:HG22	2.01	0.43
2:K:283:GLN:HG3	2:O:531:TRP:CZ3	2.54	0.43
2:O:175:GLY:O	2:O:179:ILE:HG12	2.17	0.43
2:O:266:ASP:O	2:O:270:ASN:ND2	2.32	0.43
1:B:397:GLU:OE2	1:B:453:ILE:HG13	2.18	0.43
1:F:650:MET:CE	2:N:264:ASP:HB2	2.49	0.43
1:H:169:HIS:HA	1:H:172:GLN:NE2	2.34	0.43
1:H:356:VAL:HG21	1:H:399:ARG:NH1	2.33	0.43
2:I:214:THR:H	2:I:258:HIS:HD1	1.67	0.43
1:J:356:VAL:HG21	1:J:399:ARG:NH1	2.33	0.43
2:O:197:MET:C	2:O:221:SER:HB3	2.44	0.43
1:A:233:TRP:HZ2	1:A:265:ASP:HB2	1.84	0.43
1:B:262:LYS:HE3	1:B:346:TYR:CZ	2.54	0.43
1:D:183:LEU:HD13	1:D:327:VAL:HG12	2.00	0.43
1:F:233:TRP:HZ2	1:F:265:ASP:HB2	1.83	0.43
1:F:275:LEU:HD11	1:F:369:LEU:HD11	2.01	0.43
1:H:707:VAL:HA	1:H:727:LEU:HD23	1.99	0.43
2:K:37:GLU:HG3	2:K:41:ASN:HD21	1.84	0.43
2:K:61:ARG:HH22	2:K:199:PRO:HD3	1.83	0.43
2:L:61:ARG:HH22	2:L:199:PRO:HD3	1.83	0.43
2:N:197:MET:C	2:N:221:SER:HB3	2.44	0.43
1:A:370:VAL:O	1:A:374:ILE:HG12	2.19	0.43
1:B:183:LEU:HD13	1:B:327:VAL:HG12	2.00	0.43
1:D:370:VAL:O	1:D:374:ILE:HG12	2.19	0.43
1:F:397:GLU:OE2	1:F:453:ILE:HG13	2.19	0.43
2:G:141:ILE:HA	2:G:144:ILE:HG22	2.00	0.43
2:G:197:MET:C	2:G:221:SER:HB3	2.44	0.43
1:H:183:LEU:HD13	1:H:327:VAL:HG12	2.00	0.43
1:H:192:ILE:HD13	1:H:346:TYR:HB3	2.00	0.43
2:I:37:GLU:HG3	2:I:41:ASN:HD21	1.84	0.43
2:I:61:ARG:HH22	2:I:199:PRO:HD3	1.83	0.43
2:L:37:GLU:HG3	2:L:41:ASN:HD21	1.84	0.43
1:D:146:LEU:HD22	1:D:149:ASN:HD22	1.83	0.43
1:D:233:TRP:HZ2	1:D:265:ASP:HB2	1.83	0.43
1:D:262:LYS:HE3	1:D:346:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:646:LEU:HD13	2:I:64:LEU:HD13	2.00	0.43
2:G:37:GLU:HG3	2:G:41:ASN:HD21	1.84	0.43
2:G:534:HIS:HE1	2:I:379:ARG:HH22	1.63	0.43
1:H:166:PRO:HG3	1:H:352:THR:HB	2.01	0.43
2:I:197:MET:C	2:I:221:SER:HB3	2.44	0.43
1:J:370:VAL:O	1:J:374:ILE:HG12	2.19	0.43
2:K:214:THR:H	2:K:258:HIS:HD1	1.67	0.43
2:L:214:THR:H	2:L:258:HIS:HD1	1.67	0.43
2:O:37:GLU:HG3	2:O:41:ASN:HD21	1.84	0.43
2:O:141:ILE:HA	2:O:144:ILE:HG22	2.01	0.43
1:A:146:LEU:HD22	1:A:149:ASN:HD22	1.83	0.43
1:A:169:HIS:HA	1:A:172:GLN:NE2	2.34	0.43
1:A:262:LYS:HE3	1:A:346:TYR:CZ	2.53	0.43
1:B:662:LEU:HD11	1:B:699:MET:HB3	2.01	0.43
1:D:275:LEU:HD11	1:D:369:LEU:HD11	2.01	0.43
1:D:540:ALA:C	2:I:115:ASN:HD21	2.27	0.43
1:J:169:HIS:HA	1:J:172:GLN:NE2	2.34	0.43
1:J:662:LEU:HD11	1:J:699:MET:HB3	2.01	0.43
2:K:106:SER:HB3	2:K:128:VAL:HG13	2.01	0.43
2:K:197:MET:C	2:K:221:SER:HB3	2.44	0.43
2:L:266:ASP:O	2:L:270:ASN:ND2	2.32	0.43
2:N:37:GLU:HG3	2:N:41:ASN:HD21	1.84	0.43
2:N:106:SER:HB3	2:N:128:VAL:HG13	2.00	0.43
2:O:438:ALA:O	2:O:441:VAL:HG12	2.19	0.43
1:F:169:HIS:HA	1:F:172:GLN:NE2	2.34	0.42
1:F:404:ASP:H	1:F:411:LEU:H	1.67	0.42
2:G:214:THR:H	2:G:258:HIS:HD1	1.67	0.42
1:H:249:ALA:O	1:H:254:GLY:N	2.42	0.42
1:H:662:LEU:HD11	1:H:699:MET:HB3	2.01	0.42
2:I:87:GLU:CG	2:O:498:VAL:HB	2.47	0.42
2:I:251:THR:O	2:I:336:TYR:HB2	2.19	0.42
2:N:438:ALA:O	2:N:441:VAL:HG12	2.19	0.42
1:A:599:ALA:H	2:G:292:HIS:HE2	1.66	0.42
1:F:166:PRO:HG3	1:F:352:THR:HB	2.01	0.42
1:F:262:LYS:HE3	1:F:346:TYR:CZ	2.54	0.42
1:F:370:VAL:O	1:F:374:ILE:HG12	2.19	0.42
1:F:707:VAL:HA	1:F:727:LEU:HD23	1.99	0.42
2:I:141:ILE:HA	2:I:144:ILE:HG22	2.01	0.42
1:J:233:TRP:HZ2	1:J:265:ASP:HB2	1.83	0.42
1:J:537:GLN:O	1:J:541:GLN:HG3	2.19	0.42
1:A:183:LEU:HD13	1:A:327:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:TRP:HZ2	1:B:265:ASP:HB2	1.83	0.42
1:D:132:LYS:HE2	1:D:133:LYS:HE3	2.02	0.42
1:F:132:LYS:HE2	1:F:133:LYS:HE3	2.02	0.42
1:F:540:ALA:C	2:N:115:ASN:HD21	2.28	0.42
2:G:251:THR:O	2:G:336:TYR:HB2	2.19	0.42
2:O:81:GLU:HG2	2:O:84:MET:HB3	2.02	0.42
1:D:192:ILE:HD13	1:D:346:TYR:HB3	2.00	0.42
1:F:537:GLN:O	1:F:541:GLN:HG3	2.19	0.42
2:I:438:ALA:O	2:I:441:VAL:HG12	2.19	0.42
2:L:81:GLU:HG2	2:L:84:MET:HB3	2.02	0.42
2:L:141:ILE:HA	2:L:144:ILE:HG22	2.01	0.42
2:N:79:PHE:HE1	2:N:110:GLY:HA3	1.85	0.42
2:N:81:GLU:HG2	2:N:84:MET:HB3	2.02	0.42
1:A:227:LYS:HE3	1:A:253:PHE:CE2	2.55	0.42
1:A:404:ASP:H	1:A:411:LEU:H	1.67	0.42
1:B:256:ASP:OD2	1:B:257:ARG:NH2	2.43	0.42
1:B:537:GLN:O	1:B:541:GLN:HG3	2.20	0.42
1:F:146:LEU:HD22	1:F:149:ASN:HD22	1.83	0.42
1:J:183:LEU:HD13	1:J:327:VAL:HG12	2.00	0.42
1:J:599:ALA:H	2:O:292:HIS:HE2	1.67	0.42
2:K:81:GLU:HG2	2:K:84:MET:HB3	2.02	0.42
2:K:531:TRP:CZ3	2:O:283:GLN:HG3	2.53	0.42
1:A:132:LYS:HE2	1:A:133:LYS:HE3	2.02	0.42
1:D:168:THR:O	1:D:171:ILE:HB	2.20	0.42
1:D:169:HIS:HA	1:D:172:GLN:NE2	2.34	0.42
1:D:650:MET:HE1	2:I:265:VAL:HG23	2.02	0.42
2:G:81:GLU:HG2	2:G:84:MET:HB3	2.01	0.42
2:G:117:ARG:NH2	2:G:278:LEU:O	2.53	0.42
1:H:404:ASP:H	1:H:411:LEU:H	1.67	0.42
2:I:87:GLU:HG3	2:I:88:HIS:O	2.20	0.42
2:I:324:VAL:HG11	2:I:345:ALA:HB1	2.02	0.42
1:A:168:THR:O	1:A:171:ILE:HB	2.20	0.42
1:D:227:LYS:HE3	1:D:253:PHE:CE2	2.55	0.42
2:G:106:SER:HB3	2:G:128:VAL:HG13	2.01	0.42
2:G:266:ASP:O	2:G:270:ASN:ND2	2.32	0.42
2:L:251:THR:O	2:L:336:TYR:HB2	2.19	0.42
2:N:117:ARG:NH2	2:N:278:LEU:O	2.53	0.42
2:O:117:ARG:NH2	2:O:278:LEU:O	2.53	0.42
1:A:200:LYS:HD3	1:A:200:LYS:HA	1.75	0.42
1:B:168:THR:O	1:B:171:ILE:HB	2.20	0.42
1:D:662:LEU:HD11	1:D:699:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:THR:O	1:F:171:ILE:HB	2.20	0.42
1:H:132:LYS:HE2	1:H:133:LYS:HE3	2.01	0.42
2:K:251:THR:O	2:K:336:TYR:HB2	2.19	0.42
2:K:534:HIS:HE1	2:O:379:ARG:HH22	1.64	0.42
2:L:106:SER:HB3	2:L:128:VAL:HG13	2.00	0.42
2:L:438:ALA:O	2:L:441:VAL:HG12	2.19	0.42
2:N:61:ARG:HH22	2:N:199:PRO:HD3	1.83	0.42
1:B:166:PRO:HG3	1:B:352:THR:HB	2.01	0.42
1:B:370:VAL:O	1:B:374:ILE:HG12	2.19	0.42
1:D:599:ALA:N	2:I:292:HIS:HE2	2.18	0.42
1:F:662:LEU:HD11	1:F:699:MET:HB3	2.01	0.42
2:G:438:ALA:O	2:G:441:VAL:HG12	2.19	0.42
1:H:275:LEU:HD11	1:H:369:LEU:HD11	2.01	0.42
2:I:81:GLU:HG2	2:I:84:MET:HB3	2.01	0.42
2:L:164:ALA:HB2	2:L:176:TYR:HE2	1.85	0.42
2:L:171:GLU:OE2	2:N:499:ARG:NE	2.39	0.42
1:A:275:LEU:HD11	1:A:369:LEU:HD11	2.01	0.42
1:A:486:ARG:HH12	1:A:630:LEU:HD13	1.85	0.42
1:B:629:PHE:CE2	1:B:630:LEU:HD23	2.55	0.42
1:D:486:ARG:HH12	1:D:630:LEU:HD13	1.85	0.42
1:F:227:LYS:HE3	1:F:253:PHE:CE2	2.55	0.42
2:G:324:VAL:HG11	2:G:345:ALA:HB1	2.02	0.42
2:G:426:LYS:HB2	2:G:426:LYS:HE3	1.90	0.42
1:H:85:MET:HE2	1:H:85:MET:HB2	1.98	0.42
1:H:537:GLN:O	1:H:541:GLN:HG3	2.19	0.42
2:I:323:VAL:O	2:I:512:ARG:NH1	2.45	0.42
2:I:426:LYS:HB2	2:I:426:LYS:HE3	1.90	0.42
1:J:227:LYS:HE3	1:J:253:PHE:CE2	2.55	0.42
1:B:132:LYS:HE2	1:B:133:LYS:HE3	2.02	0.41
2:G:501:PHE:CZ	2:I:174:ALA:HB2	2.55	0.41
1:H:227:LYS:HE3	1:H:253:PHE:CE2	2.55	0.41
1:H:629:PHE:CE2	1:H:630:LEU:HD23	2.55	0.41
2:I:106:SER:HB3	2:I:128:VAL:HG13	2.00	0.41
2:I:117:ARG:NH2	2:I:278:LEU:O	2.53	0.41
2:I:164:ALA:HB2	2:I:176:TYR:HE2	1.85	0.41
2:I:411:HIS:HA	2:I:414:LYS:HD3	2.02	0.41
2:N:178:ASP:O	2:N:181:LEU:HB2	2.20	0.41
1:A:537:GLN:O	1:A:541:GLN:HG3	2.19	0.41
1:A:662:LEU:HD11	1:A:699:MET:HB3	2.01	0.41
1:D:537:GLN:O	1:D:541:GLN:HG3	2.19	0.41
1:H:650:MET:HE3	2:K:64:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:178:ASP:O	2:I:181:LEU:HB2	2.21	0.41
1:J:132:LYS:HE2	1:J:133:LYS:HE3	2.02	0.41
1:J:166:PRO:HG3	1:J:352:THR:HB	2.01	0.41
2:L:178:ASP:O	2:L:181:LEU:HB2	2.20	0.41
2:L:294:PRO:HD2	2:L:297:ARG:HD2	2.02	0.41
2:L:324:VAL:HG11	2:L:345:ALA:HB1	2.02	0.41
2:N:251:THR:O	2:N:336:TYR:HB2	2.19	0.41
1:B:262:LYS:HE2	1:B:262:LYS:HB2	1.86	0.41
1:B:275:LEU:HD11	1:B:369:LEU:HD11	2.01	0.41
1:B:378:LYS:HG2	1:B:379:GLY:H	1.86	0.41
1:D:74:ILE:HB	1:D:143:TYR:CE2	2.56	0.41
1:D:278:LYS:HB2	1:D:278:LYS:HE3	1.87	0.41
1:D:458:ASP:OD2	1:D:460:THR:OG1	2.36	0.41
1:F:74:ILE:HB	1:F:143:TYR:CE2	2.56	0.41
2:G:164:ALA:HB2	2:G:176:TYR:HE2	1.85	0.41
1:H:168:THR:O	1:H:171:ILE:HB	2.20	0.41
2:I:492:ASN:OD1	2:N:38:ARG:NH1	2.53	0.41
1:J:629:PHE:CE2	1:J:630:LEU:HD23	2.55	0.41
2:L:87:GLU:HG3	2:L:88:HIS:O	2.20	0.41
2:L:117:ARG:NH2	2:L:278:LEU:O	2.53	0.41
1:B:74:ILE:HB	1:B:143:TYR:CE2	2.56	0.41
1:B:404:ASP:H	1:B:411:LEU:H	1.67	0.41
1:D:166:PRO:HG3	1:D:352:THR:HB	2.01	0.41
1:F:402:ALA:HB2	1:F:449:ILE:HG13	2.02	0.41
2:G:178:ASP:O	2:G:181:LEU:HB2	2.20	0.41
2:K:79:PHE:HE1	2:K:110:GLY:HA3	1.85	0.41
2:K:117:ARG:NH2	2:K:278:LEU:O	2.53	0.41
2:L:133:LEU:HA	2:L:137:HIS:ND1	2.35	0.41
1:B:227:LYS:HE3	1:B:253:PHE:CE2	2.55	0.41
1:D:629:PHE:CE2	1:D:630:LEU:HD23	2.55	0.41
1:F:378:LYS:HG2	1:F:379:GLY:H	1.86	0.41
2:G:79:PHE:HE1	2:G:110:GLY:HA3	1.85	0.41
2:G:87:GLU:HG3	2:G:88:HIS:O	2.20	0.41
1:H:304:PRO:HB2	1:H:394:TRP:CE3	2.56	0.41
1:H:486:ARG:HH12	1:H:630:LEU:HD13	1.85	0.41
1:J:378:LYS:HG2	1:J:379:GLY:H	1.86	0.41
1:J:486:ARG:HH12	1:J:630:LEU:HD13	1.85	0.41
2:L:531:TRP:CZ3	2:N:283:GLN:HG3	2.55	0.41
2:O:178:ASP:O	2:O:181:LEU:HB2	2.20	0.41
1:B:358:HIS:N	1:B:359:PRO:HD2	2.35	0.41
1:D:262:LYS:HB2	1:D:262:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:HIS:N	1:F:359:PRO:HD2	2.36	0.41
2:K:178:ASP:O	2:K:181:LEU:HB2	2.20	0.41
2:K:438:ALA:O	2:K:441:VAL:HG12	2.19	0.41
2:K:501:PHE:CE1	2:O:174:ALA:HB2	2.56	0.41
2:L:420:ALA:HB3	2:N:184:VAL:HG21	2.02	0.41
2:N:411:HIS:HA	2:N:414:LYS:HD3	2.02	0.41
2:O:87:GLU:HG3	2:O:88:HIS:O	2.20	0.41
1:B:548:ARG:NH1	2:L:151:VAL:O	2.53	0.41
1:D:402:ALA:HB2	1:D:449:ILE:HG13	2.02	0.41
2:G:133:LEU:HA	2:G:137:HIS:ND1	2.35	0.41
2:G:411:HIS:HA	2:G:414:LYS:HD3	2.02	0.41
1:H:400:VAL:O	1:H:449:ILE:N	2.50	0.41
2:I:145:MET:HB3	2:I:182:ARG:NH1	2.36	0.41
1:J:358:HIS:N	1:J:359:PRO:HD2	2.36	0.41
1:J:402:ALA:HB2	1:J:449:ILE:HG13	2.02	0.41
2:K:133:LEU:HA	2:K:137:HIS:ND1	2.35	0.41
2:N:164:ALA:HB2	2:N:176:TYR:HE2	1.85	0.41
1:A:74:ILE:HB	1:A:143:TYR:CE2	2.56	0.41
1:D:404:ASP:H	1:D:411:LEU:H	1.67	0.41
1:F:304:PRO:HB2	1:F:394:TRP:CE3	2.56	0.41
2:G:145:MET:HB3	2:G:182:ARG:NH1	2.36	0.41
1:H:74:ILE:HB	1:H:143:TYR:CE2	2.56	0.41
1:H:650:MET:HE1	2:K:265:VAL:HG23	2.03	0.41
2:I:133:LEU:HA	2:I:137:HIS:ND1	2.35	0.41
1:J:74:ILE:HB	1:J:143:TYR:CE2	2.56	0.41
1:J:400:VAL:O	1:J:449:ILE:N	2.50	0.41
1:J:404:ASP:H	1:J:411:LEU:H	1.67	0.41
2:K:283:GLN:HG3	2:O:531:TRP:HZ3	1.86	0.41
2:L:145:MET:HB3	2:L:182:ARG:NH1	2.36	0.41
1:A:378:LYS:HG2	1:A:379:GLY:H	1.86	0.41
1:A:629:PHE:CE2	1:A:630:LEU:HD23	2.55	0.41
1:D:278:LYS:HD3	1:D:379:GLY:HA2	2.03	0.41
1:F:446:ASP:HA	1:F:447:PRO:HD3	1.93	0.41
1:F:629:PHE:CE2	1:F:630:LEU:HD23	2.56	0.41
2:G:294:PRO:HD2	2:G:297:ARG:HD2	2.02	0.41
2:I:266:ASP:O	2:I:270:ASN:ND2	2.32	0.41
1:J:168:THR:O	1:J:171:ILE:HB	2.20	0.41
1:J:275:LEU:HD11	1:J:369:LEU:HD11	2.01	0.41
1:J:304:PRO:HB2	1:J:394:TRP:CE3	2.56	0.41
2:K:164:ALA:HB2	2:K:176:TYR:HE2	1.85	0.41
2:K:411:HIS:HA	2:K:414:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:504:ASP:OD1	2:L:43:ARG:NH2	2.54	0.41
2:N:145:MET:HB3	2:N:182:ARG:NH1	2.36	0.41
2:N:294:PRO:HD2	2:N:297:ARG:HD2	2.02	0.41
2:N:324:VAL:HG11	2:N:345:ALA:HB1	2.02	0.41
2:O:133:LEU:HA	2:O:137:HIS:ND1	2.36	0.41
2:O:251:THR:O	2:O:336:TYR:HB2	2.19	0.41
1:A:166:PRO:HG3	1:A:352:THR:HB	2.01	0.41
1:A:262:LYS:HE2	1:A:262:LYS:HB2	1.86	0.41
1:A:358:HIS:N	1:A:359:PRO:HD2	2.36	0.41
1:A:402:ALA:HB2	1:A:449:ILE:HG13	2.02	0.41
1:B:304:PRO:HB2	1:B:394:TRP:CE3	2.55	0.41
1:D:171:ILE:O	1:D:174:MET:HG3	2.21	0.41
1:D:256:ASP:OD2	1:D:257:ARG:NH2	2.43	0.41
1:D:358:HIS:N	1:D:359:PRO:HD2	2.36	0.41
1:F:486:ARG:HH12	1:F:630:LEU:HD13	1.85	0.41
2:G:65:THR:O	2:G:69:ARG:HG3	2.21	0.41
1:H:358:HIS:N	1:H:359:PRO:HD2	2.35	0.41
1:J:278:LYS:HD3	1:J:379:GLY:HA2	2.03	0.41
2:K:56:ASP:O	2:K:60:LYS:HG2	2.21	0.41
2:K:87:GLU:HG3	2:K:88:HIS:O	2.20	0.41
2:K:324:VAL:HG11	2:K:345:ALA:HB1	2.02	0.41
2:L:79:PHE:HE1	2:L:110:GLY:HA3	1.85	0.41
2:N:86:VAL:O	2:N:104:GLY:HA2	2.21	0.41
2:O:56:ASP:O	2:O:60:LYS:HG2	2.21	0.41
1:A:304:PRO:HB2	1:A:394:TRP:CE3	2.55	0.40
1:B:486:ARG:HH12	1:B:630:LEU:HD13	1.85	0.40
1:B:549:MET:HE2	2:L:118:LEU:HB2	2.03	0.40
1:H:171:ILE:O	1:H:174:MET:HG3	2.21	0.40
1:H:402:ALA:HB2	1:H:449:ILE:HG13	2.02	0.40
2:I:65:THR:O	2:I:69:ARG:HG3	2.21	0.40
2:K:294:PRO:HD2	2:K:297:ARG:HD2	2.02	0.40
2:K:531:TRP:HZ3	2:O:283:GLN:HG3	1.85	0.40
2:N:133:LEU:HA	2:N:137:HIS:ND1	2.35	0.40
2:O:145:MET:HB3	2:O:182:ARG:NH1	2.36	0.40
2:O:179:ILE:HG23	2:O:182:ARG:NH2	2.28	0.40
1:A:195:PHE:CE1	1:A:208:ILE:HG12	2.56	0.40
1:B:278:LYS:HD3	1:B:379:GLY:HA2	2.03	0.40
1:D:195:PHE:CE1	1:D:208:ILE:HG12	2.56	0.40
1:F:195:PHE:CE1	1:F:208:ILE:HG12	2.56	0.40
2:G:56:ASP:O	2:G:60:LYS:HG2	2.21	0.40
2:G:528:GLN:HG2	2:O:528:GLN:NE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:GLU:O	1:J:182:LEU:HG	2.22	0.40
2:L:56:ASP:O	2:L:60:LYS:HG2	2.21	0.40
2:N:87:GLU:HG3	2:N:88:HIS:O	2.20	0.40
2:O:294:PRO:HD2	2:O:297:ARG:HD2	2.02	0.40
2:O:324:VAL:HG11	2:O:345:ALA:HB1	2.02	0.40
2:O:411:HIS:HA	2:O:414:LYS:HD3	2.02	0.40
1:A:171:ILE:O	1:A:174:MET:HG3	2.21	0.40
1:B:402:ALA:HB2	1:B:449:ILE:HG13	2.02	0.40
1:B:724:LEU:HD23	1:B:724:LEU:HA	1.96	0.40
1:F:554:PRO:HB3	2:N:113:ARG:CZ	2.51	0.40
1:H:465:ARG:HA	1:H:468:ASP:OD2	2.22	0.40
1:H:654:VAL:HG11	2:K:262:GLU:HG2	2.04	0.40
2:I:316:MET:O	2:I:316:MET:HG3	2.21	0.40
2:K:51:GLY:O	2:K:55:ILE:HG12	2.22	0.40
2:K:145:MET:HB3	2:K:182:ARG:NH1	2.36	0.40
2:L:376:ARG:NH1	2:N:538:PRO:O	2.54	0.40
2:N:56:ASP:O	2:N:60:LYS:HG2	2.22	0.40
2:N:65:THR:O	2:N:69:ARG:HG3	2.21	0.40
2:N:426:LYS:HB2	2:N:426:LYS:HE3	1.90	0.40
1:A:278:LYS:HD3	1:A:379:GLY:HA2	2.03	0.40
1:B:195:PHE:CE1	1:B:208:ILE:HG12	2.56	0.40
1:D:304:PRO:HB2	1:D:394:TRP:CE3	2.55	0.40
1:F:579:SER:O	1:F:579:SER:OG	2.37	0.40
2:G:321:HIS:CE1	2:G:329:PHE:HB3	2.57	0.40
2:G:498:VAL:HG12	2:K:85:PHE:O	2.21	0.40
1:H:278:LYS:HD3	1:H:379:GLY:HA2	2.03	0.40
1:J:195:PHE:CE1	1:J:208:ILE:HG12	2.56	0.40
2:K:86:VAL:O	2:K:104:GLY:HA2	2.21	0.40
2:N:179:ILE:HG23	2:N:182:ARG:NH2	2.28	0.40
1:D:465:ARG:HA	1:D:468:ASP:OD2	2.22	0.40
1:F:171:ILE:O	1:F:174:MET:HG3	2.21	0.40
1:F:179:GLU:O	1:F:182:LEU:HG	2.22	0.40
1:F:532:LEU:HD12	1:F:532:LEU:HA	1.93	0.40
1:H:458:ASP:OD2	1:H:460:THR:OG1	2.35	0.40
2:L:144:ILE:HD12	2:L:144:ILE:HA	1.95	0.40
2:N:302:LEU:HD22	2:N:319:ILE:HG13	2.04	0.40
2:O:164:ALA:HB2	2:O:176:TYR:HE2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	668/670 (100%)	653 (98%)	15 (2%)	0	100	100
1	B	668/670 (100%)	653 (98%)	15 (2%)	0	100	100
1	D	668/670 (100%)	653 (98%)	15 (2%)	0	100	100
1	F	668/670 (100%)	653 (98%)	15 (2%)	0	100	100
1	H	668/670 (100%)	653 (98%)	15 (2%)	0	100	100
1	J	668/670 (100%)	653 (98%)	15 (2%)	0	100	100
2	G	505/507 (100%)	486 (96%)	19 (4%)	0	100	100
2	I	505/507 (100%)	486 (96%)	19 (4%)	0	100	100
2	K	505/507 (100%)	486 (96%)	19 (4%)	0	100	100
2	L	505/507 (100%)	486 (96%)	19 (4%)	0	100	100
2	N	505/507 (100%)	487 (96%)	18 (4%)	0	100	100
2	O	505/507 (100%)	485 (96%)	20 (4%)	0	100	100
All	All	7038/7062 (100%)	6834 (97%)	204 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/563 (100%)	563 (100%)	0	100	100
1	B	563/563 (100%)	563 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	563/563 (100%)	563 (100%)	0	100	100
1	F	563/563 (100%)	563 (100%)	0	100	100
1	H	563/563 (100%)	563 (100%)	0	100	100
1	J	563/563 (100%)	563 (100%)	0	100	100
2	G	413/413 (100%)	413 (100%)	0	100	100
2	I	413/413 (100%)	413 (100%)	0	100	100
2	K	413/413 (100%)	413 (100%)	0	100	100
2	L	413/413 (100%)	413 (100%)	0	100	100
2	N	413/413 (100%)	413 (100%)	0	100	100
2	O	413/413 (100%)	413 (100%)	0	100	100
All	All	5856/5856 (100%)	5856 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	149	ASN
1	A	273	GLN
1	A	296	ASN
1	A	371	GLN
1	A	481	ASN
1	A	546	ASN
1	A	558	ASN
1	A	628	GLN
1	B	93	HIS
1	B	149	ASN
1	B	273	GLN
1	B	296	ASN
1	B	371	GLN
1	B	481	ASN
1	B	546	ASN
1	B	558	ASN
1	B	628	GLN
1	D	93	HIS
1	D	149	ASN
1	D	273	GLN

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Mol	Chain	Res	Type
1	D	296	ASN
1	D	371	GLN
1	D	481	ASN
1	D	546	ASN
1	D	558	ASN
1	D	628	GLN
1	F	93	HIS
1	F	149	ASN
1	F	273	GLN
1	F	296	ASN
1	F	371	GLN
1	F	392	ASN
1	F	481	ASN
1	F	546	ASN
1	F	558	ASN
1	F	628	GLN
2	G	41	ASN
2	G	52	GLN
2	G	115	ASN
2	G	167	GLN
2	G	236	ASN
2	G	276	ASN
2	G	321	HIS
2	G	335	ASN
2	G	358	GLN
2	G	369	ASN
2	G	452	ASN
2	G	476	HIS
2	G	534	HIS
1	H	93	HIS
1	H	149	ASN
1	H	273	GLN
1	H	296	ASN
1	H	371	GLN
1	H	384	HIS
1	H	481	ASN
1	H	546	ASN
1	H	558	ASN
1	H	628	GLN
2	I	41	ASN
2	I	52	GLN
2	I	88	HIS

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Mol	Chain	Res	Type
2	I	115	ASN
2	I	167	GLN
2	I	276	ASN
2	I	321	HIS
2	I	335	ASN
2	I	358	GLN
2	I	452	ASN
2	I	476	HIS
2	I	534	HIS
1	J	93	HIS
1	J	149	ASN
1	J	273	GLN
1	J	296	ASN
1	J	371	GLN
1	J	384	HIS
1	J	481	ASN
1	J	546	ASN
1	J	558	ASN
1	J	628	GLN
2	K	41	ASN
2	K	52	GLN
2	K	167	GLN
2	K	236	ASN
2	K	276	ASN
2	K	321	HIS
2	K	335	ASN
2	K	358	GLN
2	K	369	ASN
2	K	452	ASN
2	K	476	HIS
2	K	534	HIS
2	L	41	ASN
2	L	52	GLN
2	L	115	ASN
2	L	147	GLN
2	L	167	GLN
2	L	236	ASN
2	L	276	ASN
2	L	321	HIS
2	L	335	ASN
2	L	358	GLN
2	L	369	ASN

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Mol	Chain	Res	Type
2	L	403	GLN
2	L	452	ASN
2	L	476	HIS
2	L	534	HIS
2	N	41	ASN
2	N	52	GLN
2	N	115	ASN
2	N	167	GLN
2	N	236	ASN
2	N	276	ASN
2	N	321	HIS
2	N	335	ASN
2	N	358	GLN
2	N	369	ASN
2	N	452	ASN
2	N	476	HIS
2	N	528	GLN
2	N	534	HIS
2	O	41	ASN
2	O	52	GLN
2	O	115	ASN
2	O	167	GLN
2	O	236	ASN
2	O	276	ASN
2	O	321	HIS
2	O	335	ASN
2	O	358	GLN
2	O	369	ASN
2	O	403	GLN
2	O	452	ASN
2	O	476	HIS
2	O	534	HIS

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)

6 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	BTI	A	801	-	16,16,16	1.14	1 (6%)	21,21,21	1.59	5 (23%)
3	BTI	H	801	-	16,16,16	1.15	1 (6%)	21,21,21	1.59	5 (23%)
3	BTI	J	801	-	16,16,16	1.16	1 (6%)	21,21,21	1.58	4 (19%)
3	BTI	B	801	-	16,16,16	1.14	1 (6%)	21,21,21	1.59	4 (19%)
3	BTI	F	801	-	16,16,16	1.16	1 (6%)	21,21,21	1.58	4 (19%)
3	BTI	D	801	-	16,16,16	1.15	1 (6%)	21,21,21	1.59	4 (19%)

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	BTI	A	801	-	-	0/5/27/27	0/2/2/2
3	BTI	H	801	-	-	0/5/27/27	0/2/2/2
3	BTI	J	801	-	-	0/5/27/27	0/2/2/2
3	BTI	B	801	-	-	0/5/27/27	0/2/2/2
3	BTI	F	801	-	-	0/5/27/27	0/2/2/2
3	BTI	D	801	-	-	0/5/27/27	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	BTI	C2-S1	-3.62	1.76	1.82
3	F	801	BTI	C2-S1	-3.61	1.76	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	801	BTI	C2-S1	-3.59	1.76	1.82
3	H	801	BTI	C2-S1	-3.58	1.76	1.82
3	A	801	BTI	C2-S1	-3.56	1.76	1.82
3	B	801	BTI	C2-S1	-3.56	1.76	1.82

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	BTI	C4-C2-S1	3.20	108.25	105.20
3	D	801	BTI	C4-C2-S1	3.17	108.22	105.20
3	J	801	BTI	C4-C2-S1	3.17	108.22	105.20
3	F	801	BTI	C4-C2-S1	3.12	108.18	105.20
3	B	801	BTI	C4-C2-S1	3.12	108.17	105.20
3	H	801	BTI	C4-C2-S1	3.12	108.17	105.20
3	D	801	BTI	C6-C5-C4	2.72	111.02	108.66
3	B	801	BTI	C6-C5-C4	2.71	111.01	108.66
3	J	801	BTI	C6-C5-C4	2.70	111.00	108.66
3	F	801	BTI	C6-C5-C4	2.68	110.99	108.66
3	F	801	BTI	C6-S1-C2	2.66	95.35	89.89
3	B	801	BTI	C6-S1-C2	2.66	95.35	89.89
3	A	801	BTI	C6-C5-C4	2.66	110.97	108.66
3	H	801	BTI	C6-S1-C2	2.65	95.34	89.89
3	J	801	BTI	C6-S1-C2	2.65	95.34	89.89
3	D	801	BTI	C6-S1-C2	2.64	95.32	89.89
3	H	801	BTI	C6-C5-C4	2.64	110.95	108.66
3	A	801	BTI	C6-S1-C2	2.63	95.28	89.89
3	B	801	BTI	C2-C4-N2	-2.33	111.04	113.13
3	D	801	BTI	C2-C4-N2	-2.32	111.05	113.13
3	H	801	BTI	C2-C4-N2	-2.31	111.05	113.13
3	A	801	BTI	C2-C4-N2	-2.29	111.07	113.13
3	F	801	BTI	C2-C4-N2	-2.29	111.07	113.13
3	J	801	BTI	C2-C4-N2	-2.27	111.09	113.13
3	A	801	BTI	C5-C6-S1	2.03	108.05	106.31
3	H	801	BTI	C5-C6-S1	2.03	108.04	106.31

There are no chirality outliers.

There are no torsion outliers.

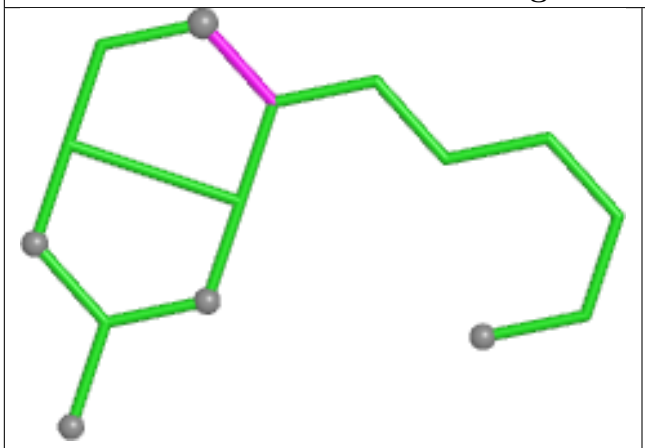
There are no ring outliers.

No monomer is involved in short contacts.

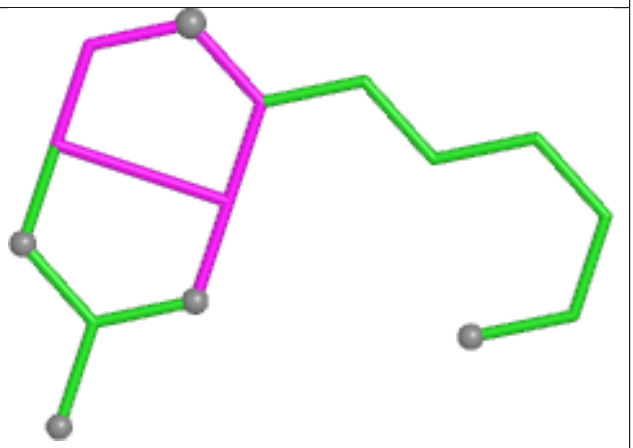
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

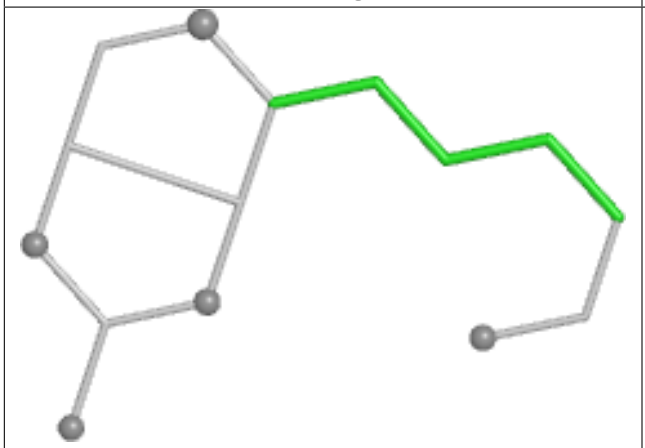
Ligand BTI A 801



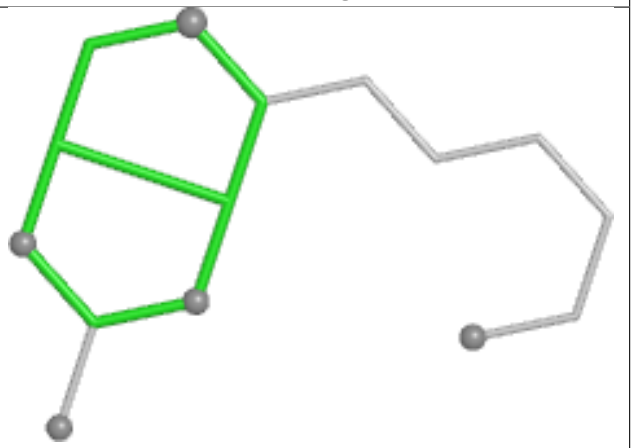
Bond lengths



Bond angles

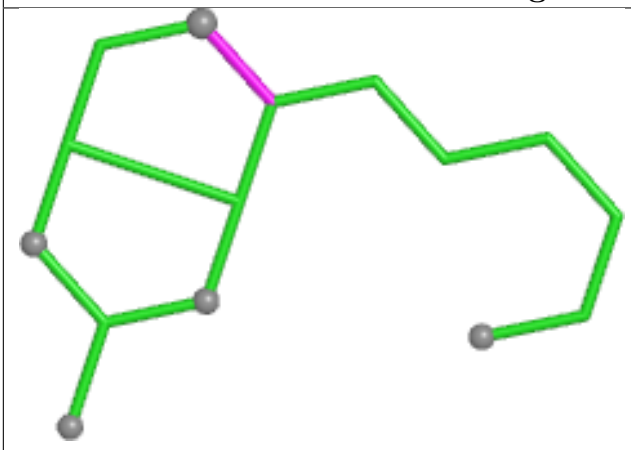


Torsions

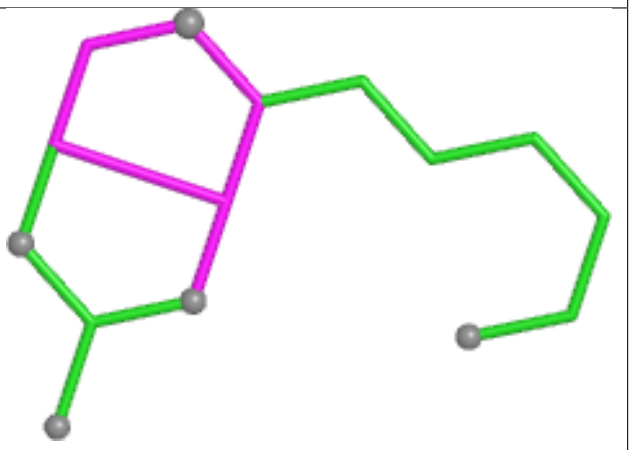


Rings

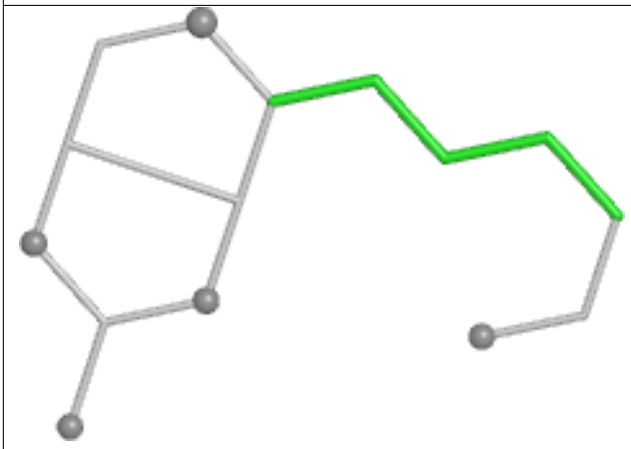
Ligand BTI H 801



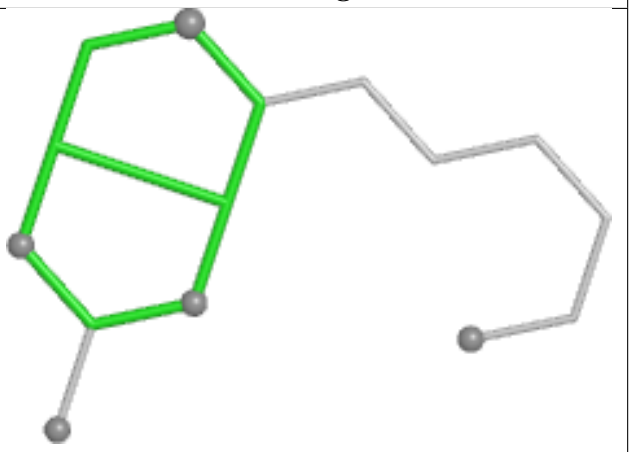
Bond lengths



Bond angles

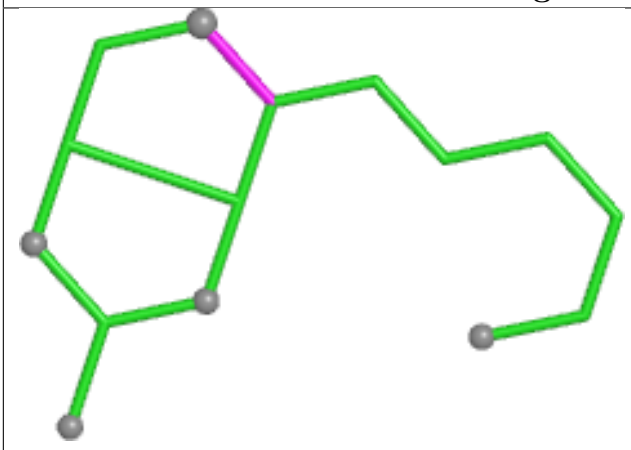


Torsions

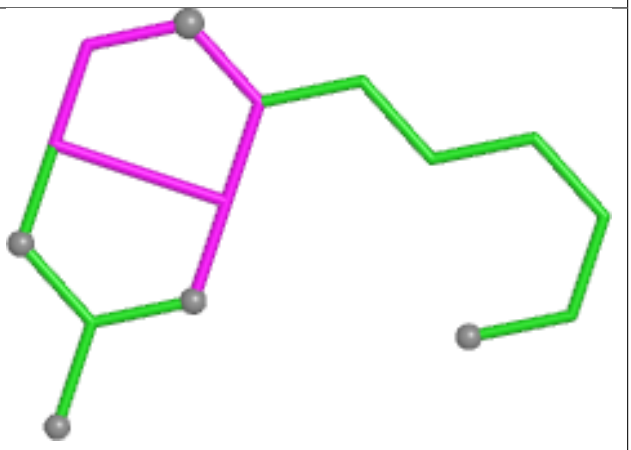


Rings

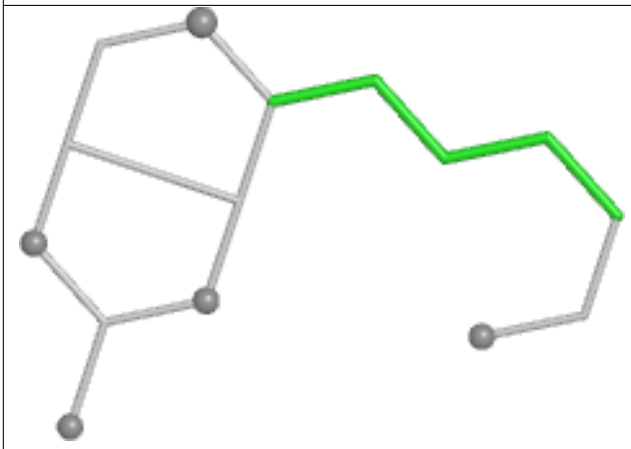
Ligand BTI J 801



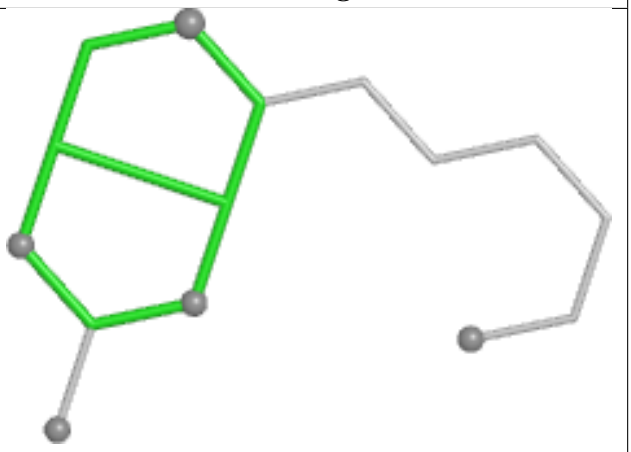
Bond lengths



Bond angles

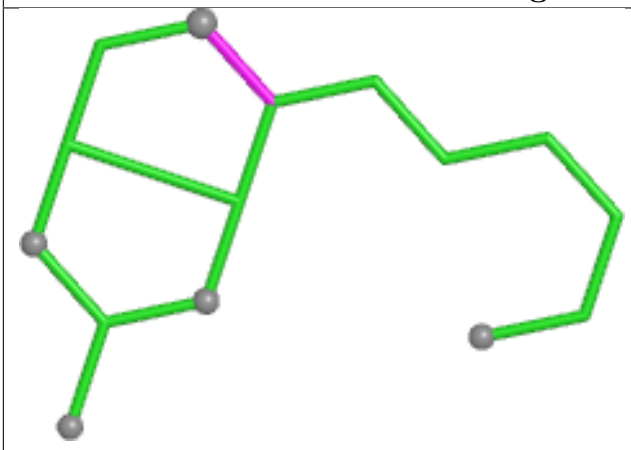


Torsions

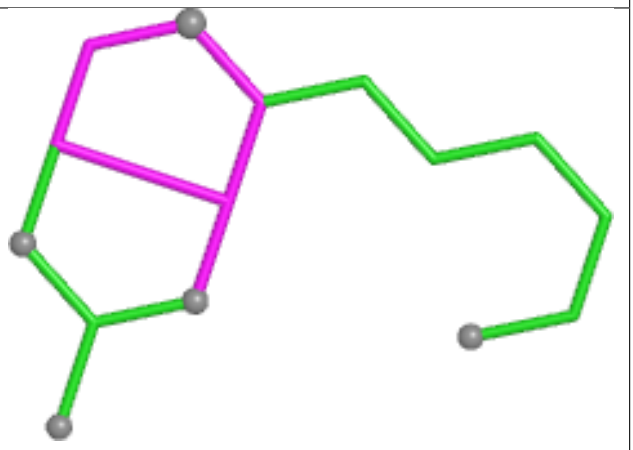


Rings

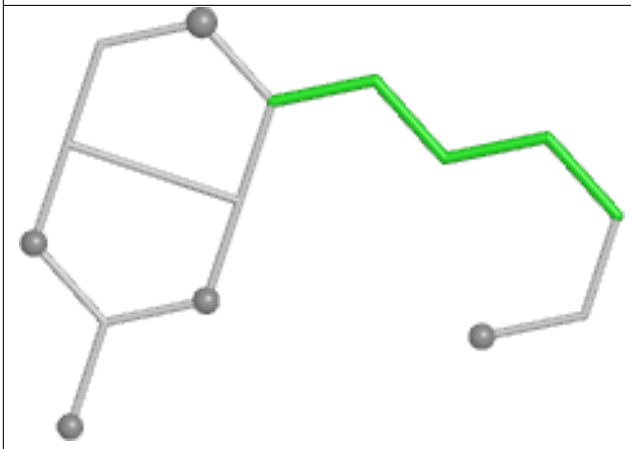
Ligand BTI B 801



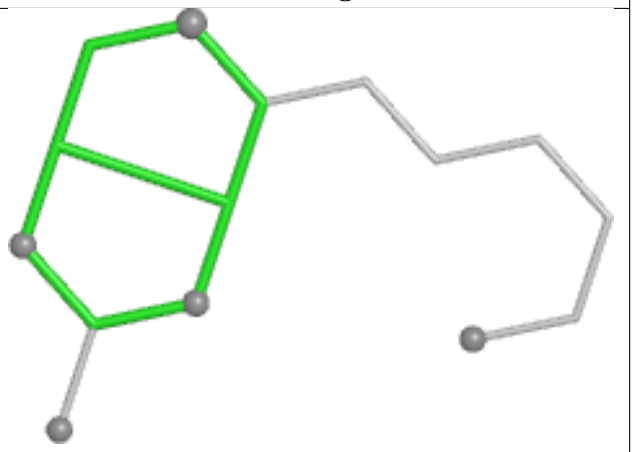
Bond lengths



Bond angles

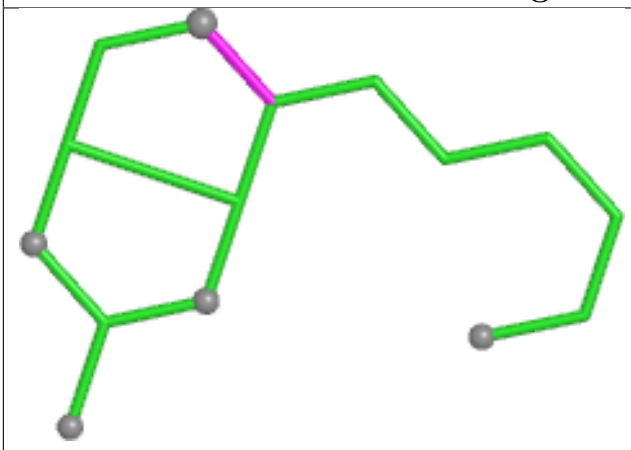


Torsions

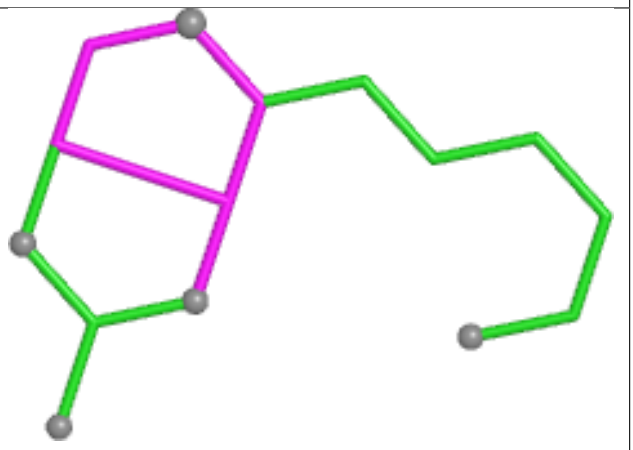


Rings

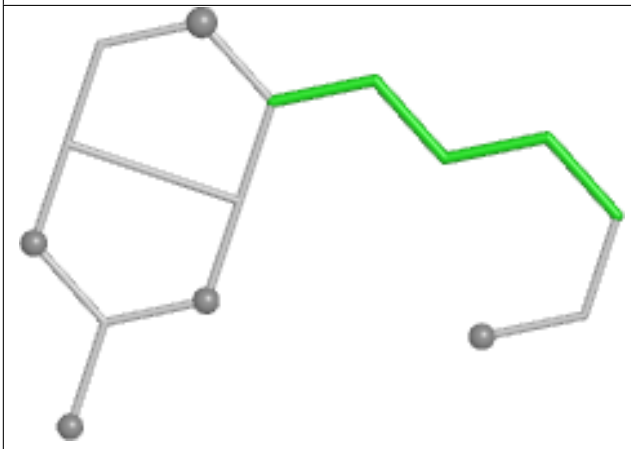
Ligand BTI F 801



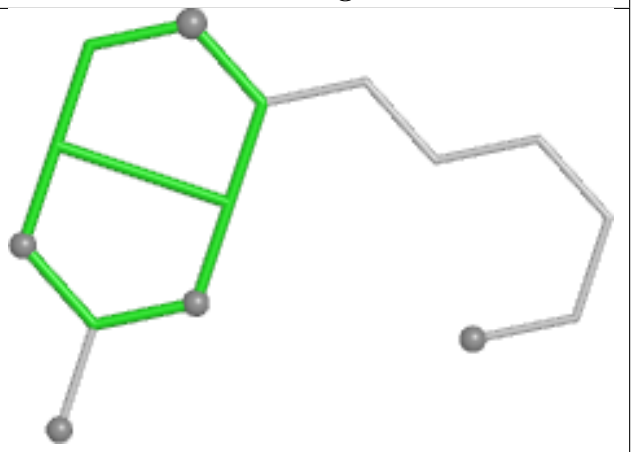
Bond lengths



Bond angles

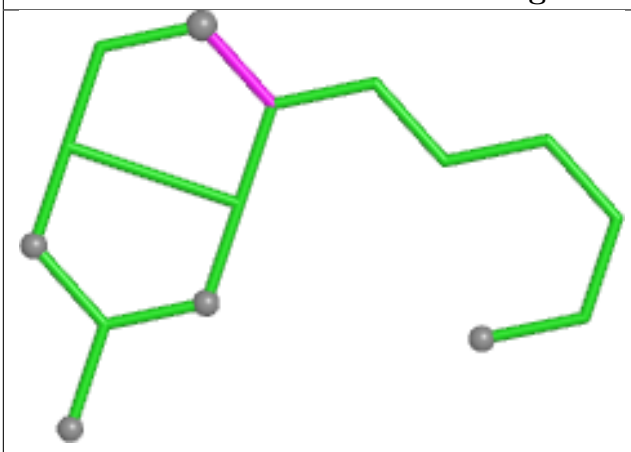


Torsions

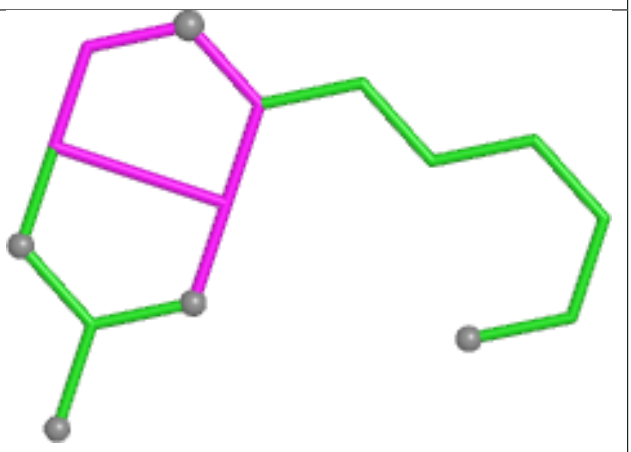


Rings

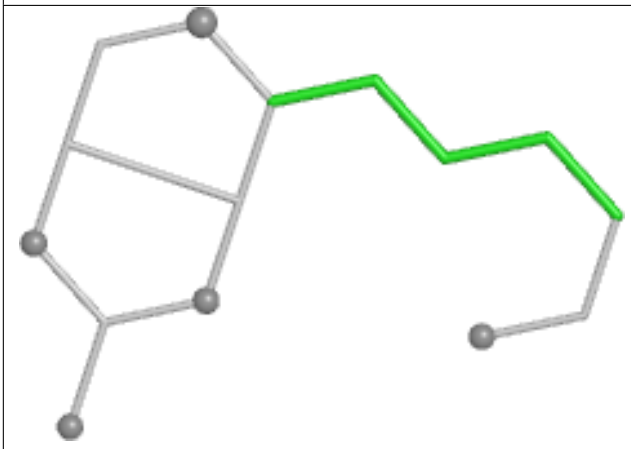
Ligand BTI D 801



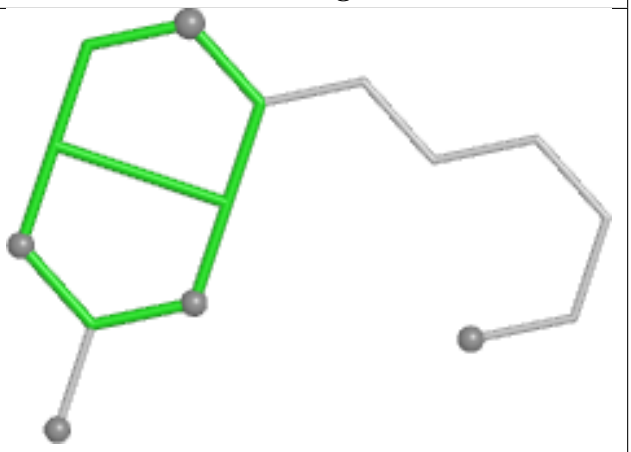
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

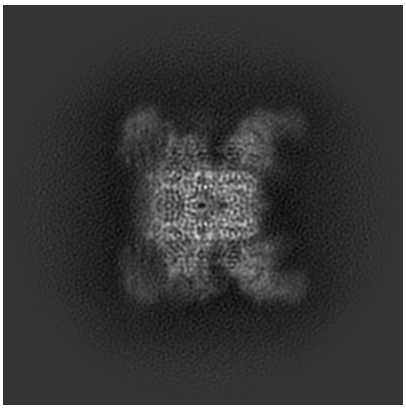
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66037. These allow visual inspection of the internal detail of the map and identification of artifacts.

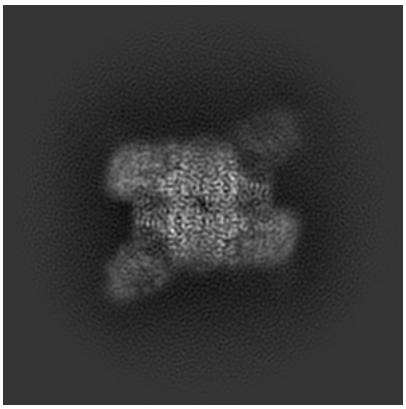
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

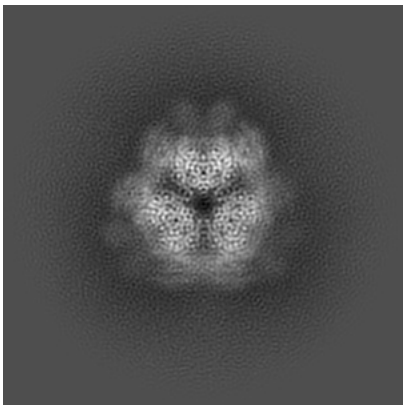
6.1.1 Primary map



X

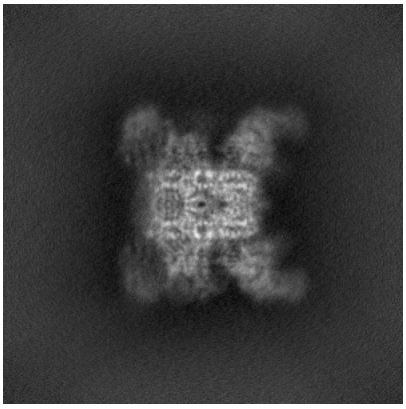


Y

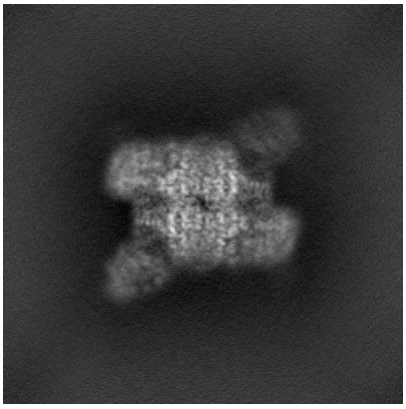


Z

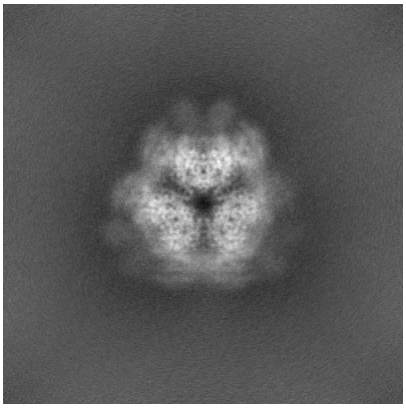
6.1.2 Raw map



X



Y

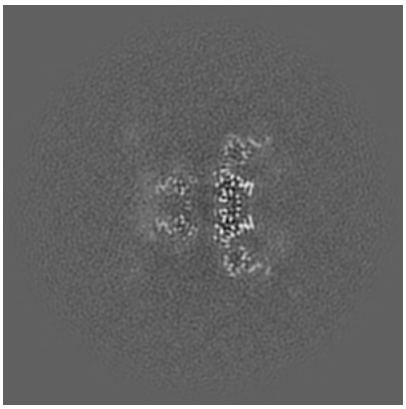


Z

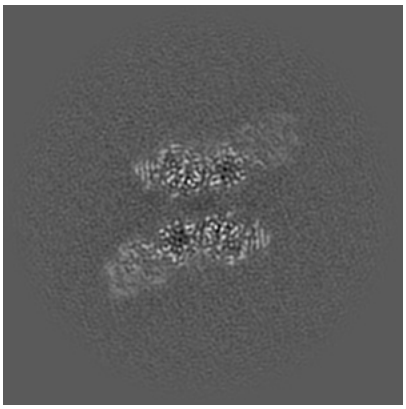
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

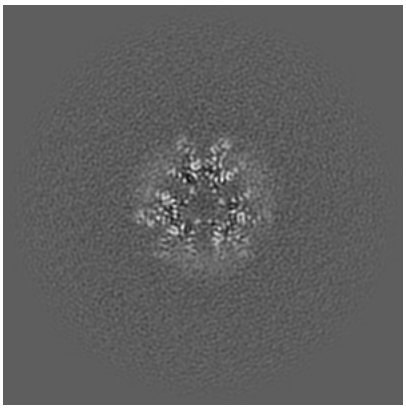
6.2.1 Primary map



X Index: 200

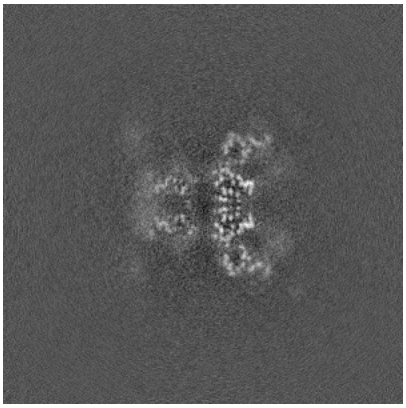


Y Index: 200

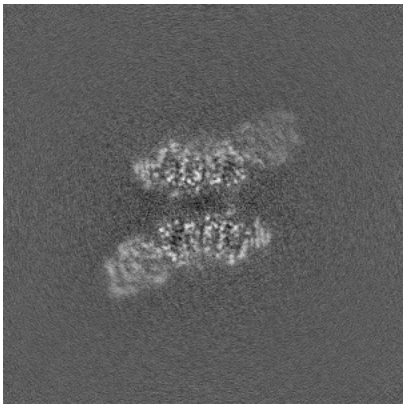


Z Index: 200

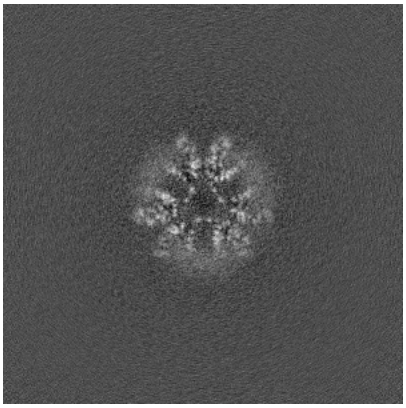
6.2.2 Raw map



X Index: 200



Y Index: 200

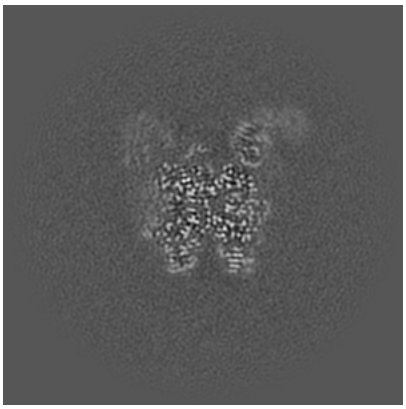


Z Index: 200

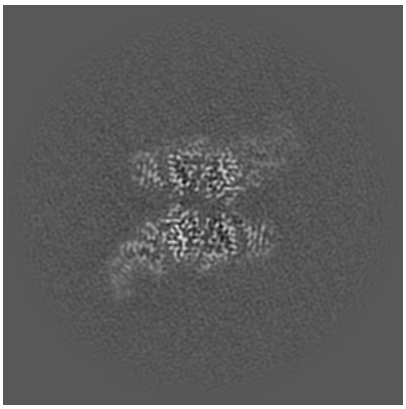
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

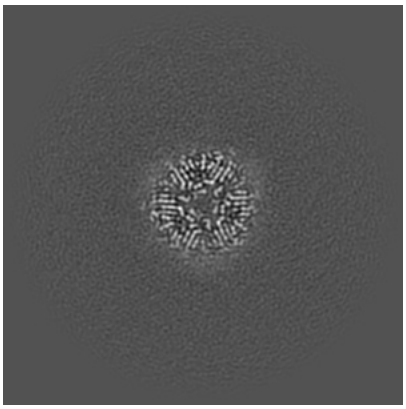
6.3.1 Primary map



X Index: 182

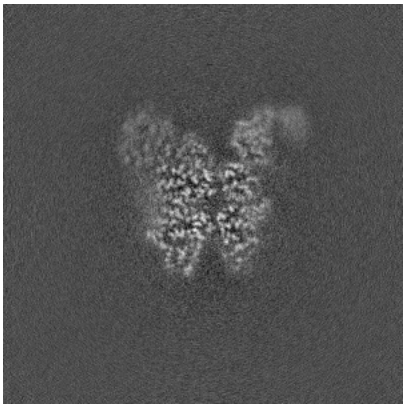


Y Index: 192

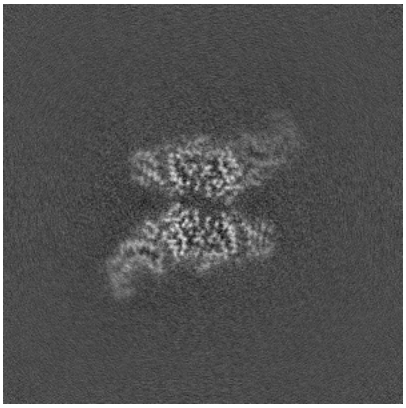


Z Index: 179

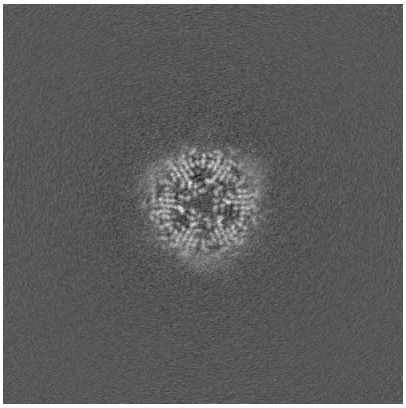
6.3.2 Raw map



X Index: 178



Y Index: 192

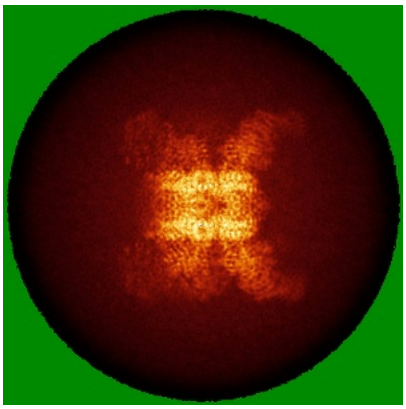


Z Index: 180

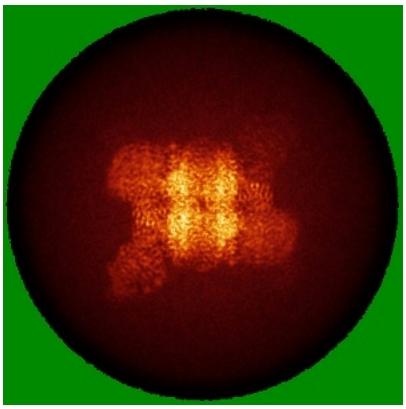
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

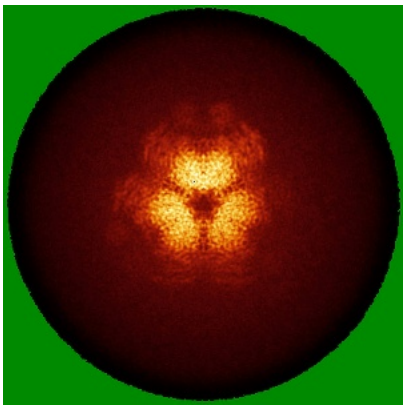
6.4.1 Primary map



X

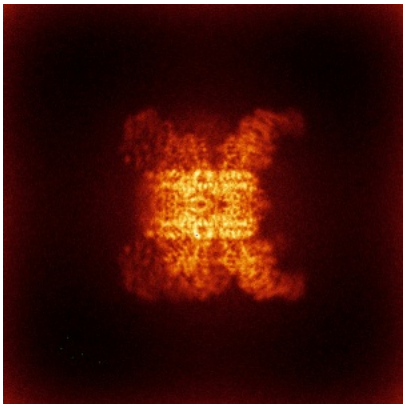


Y

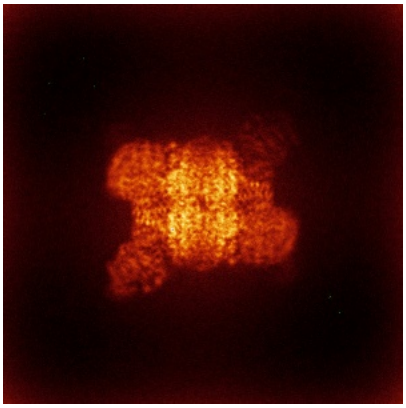


Z

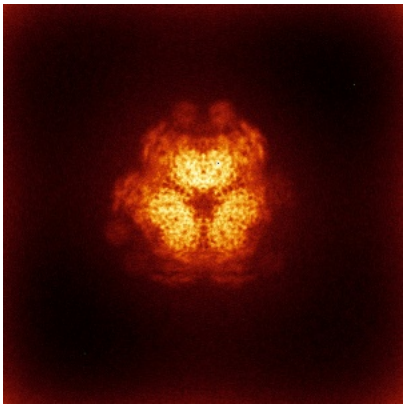
6.4.2 Raw map



X



Y

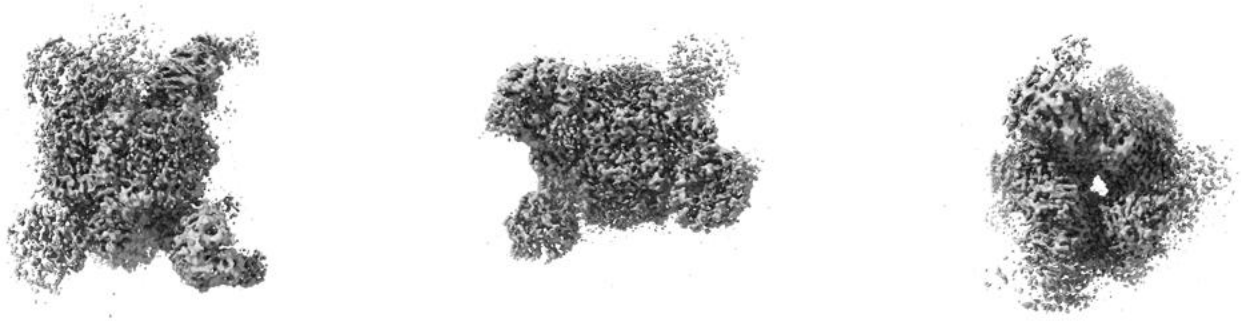


Z

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

6.5 Orthogonal surface views (i)

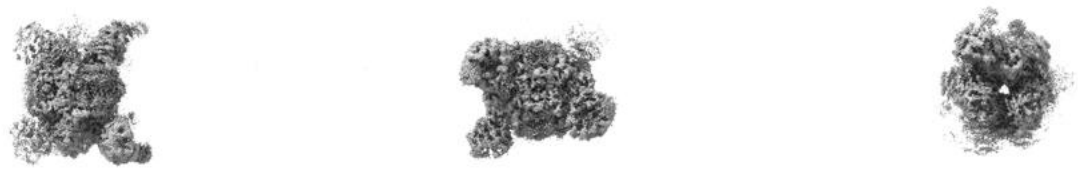
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

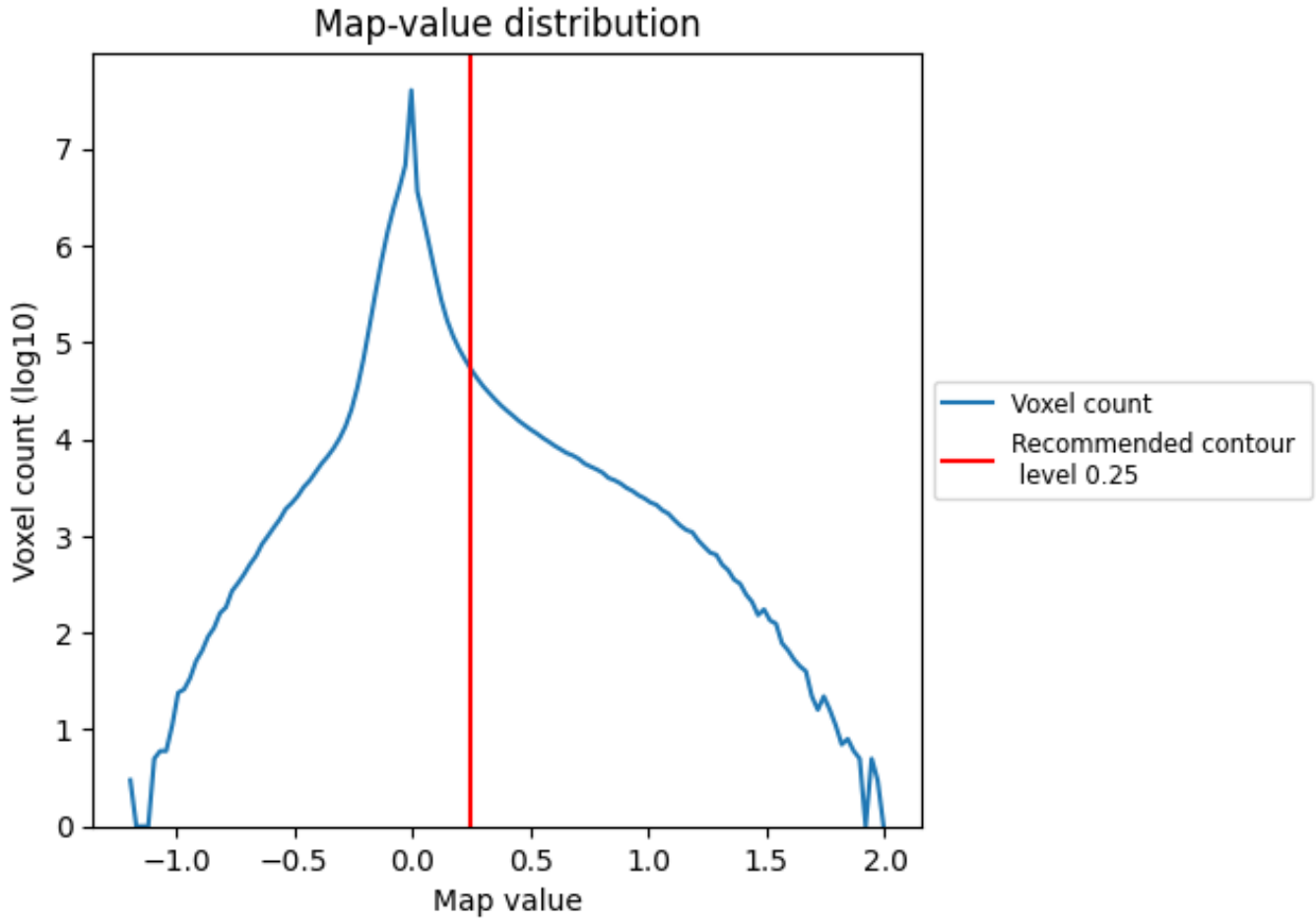
6.6 Mask visualisation (i)

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

7 Map analysis

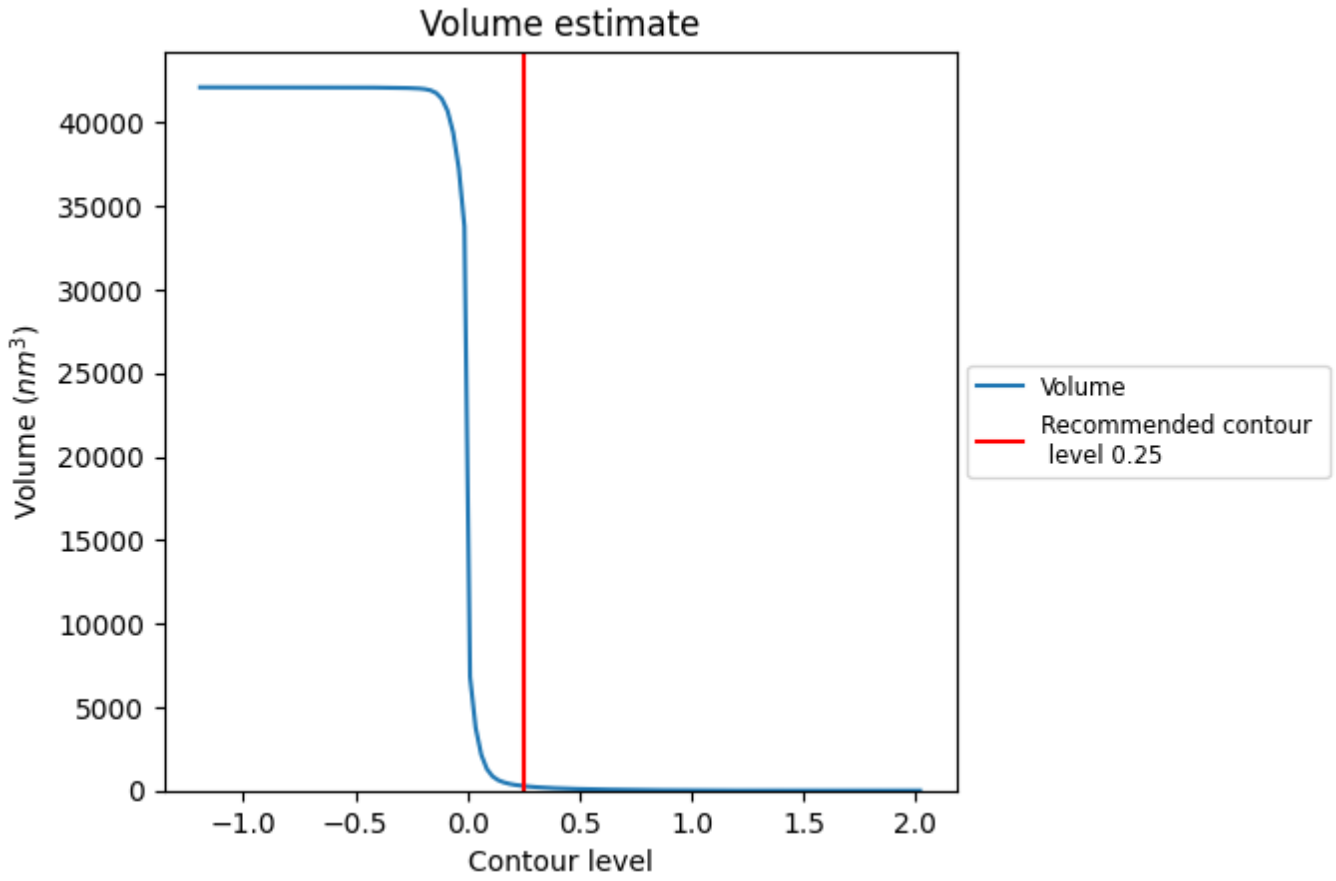
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

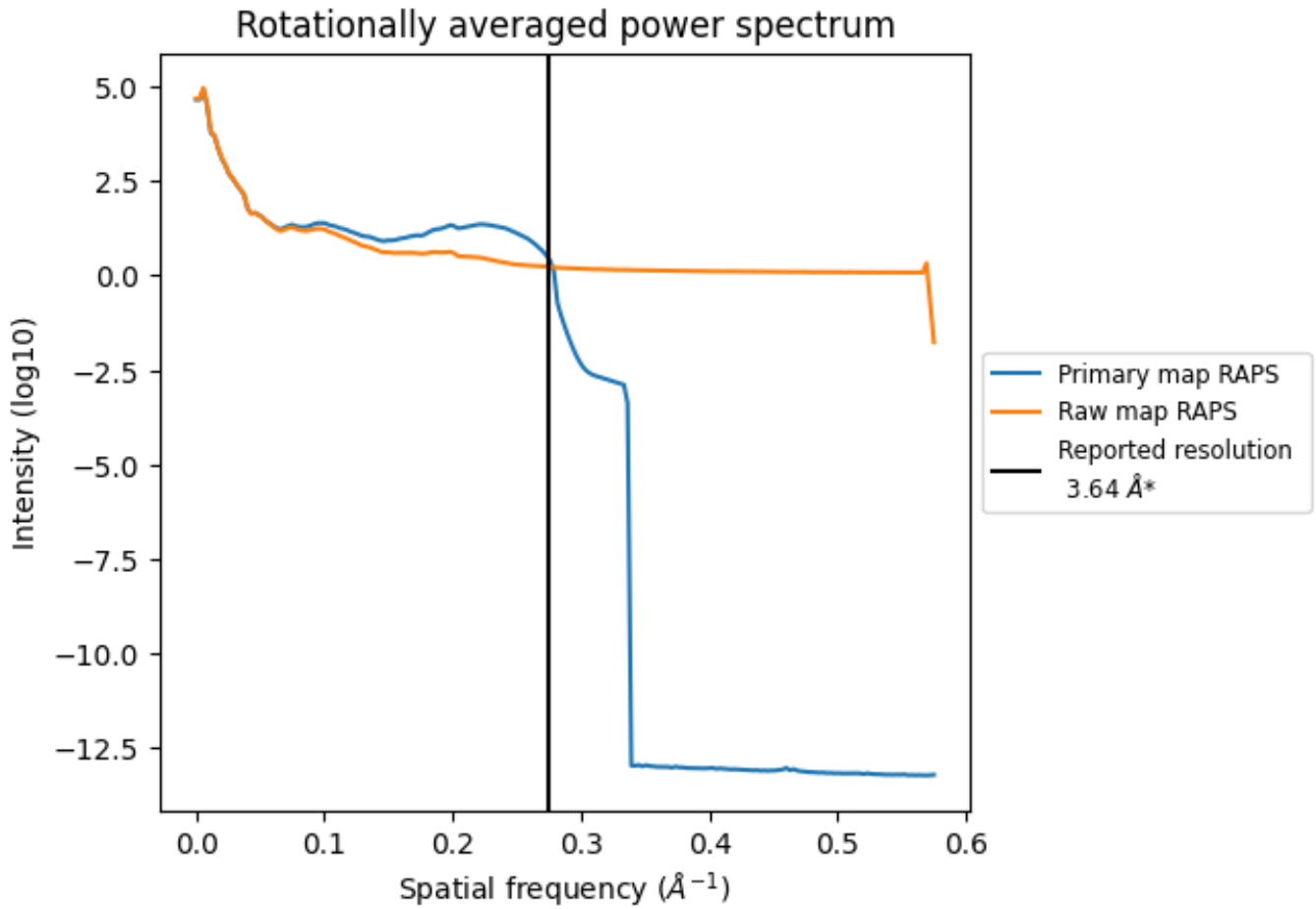
7.2 Volume estimate



The volume at the recommended contour level is 273 nm^3; this corresponds to an approximate mass of 247 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)

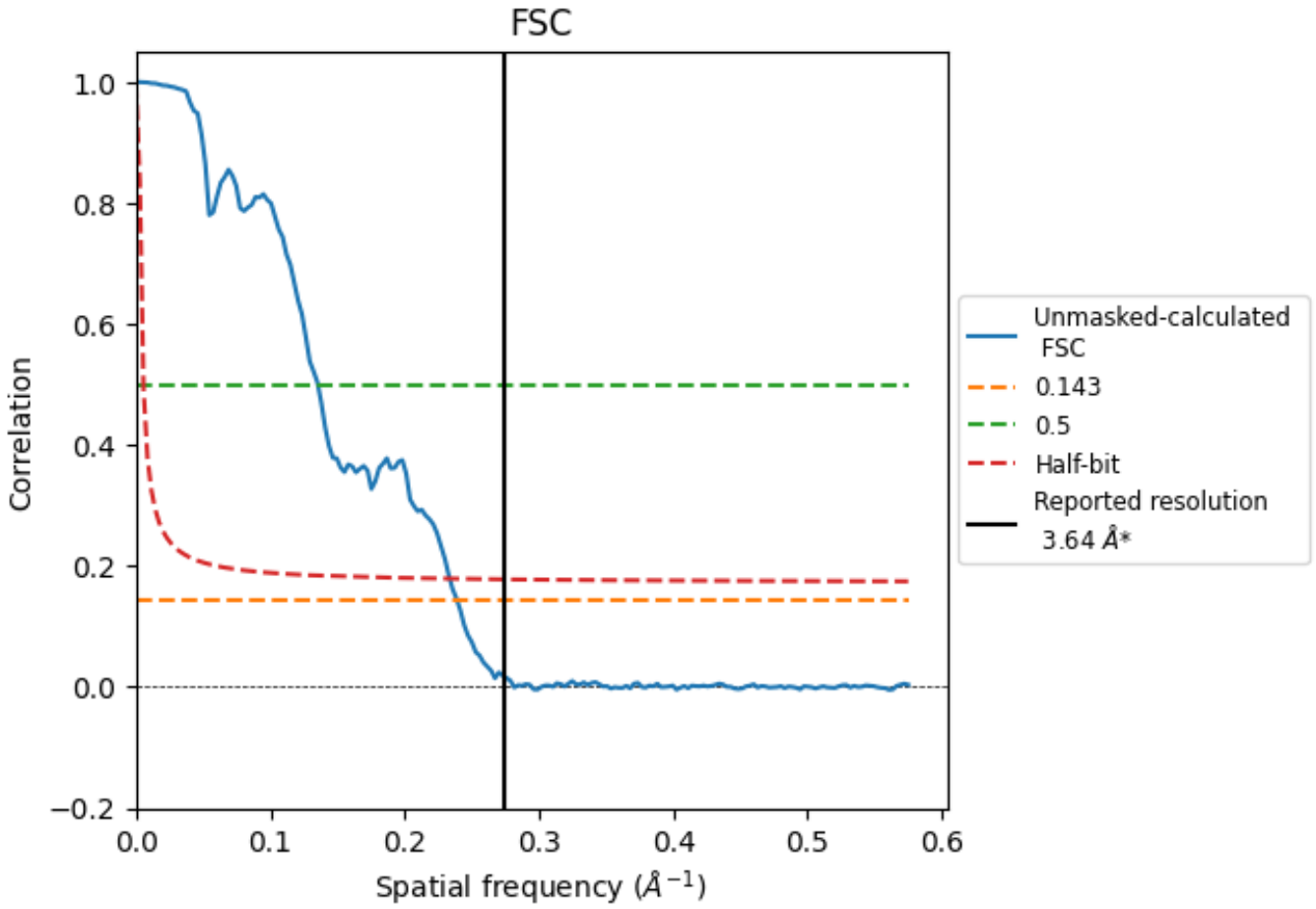


*Reported resolution corresponds to spatial frequency of 0.275 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8.2 Resolution estimates (i)

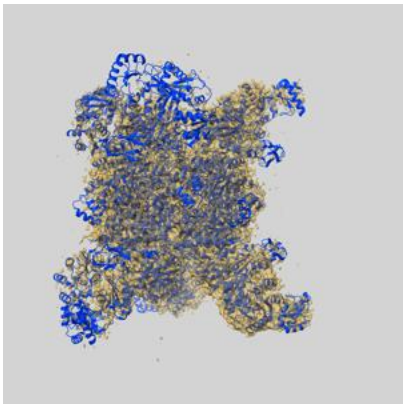
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	7.39	4.28

*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 4.18 differs from the reported value 3.64 by more than 10 %

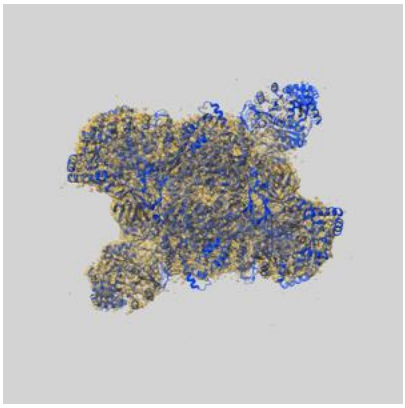
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66037 and PDB model 9WKR. Per-residue inclusion information can be found in section 3 on page 6.

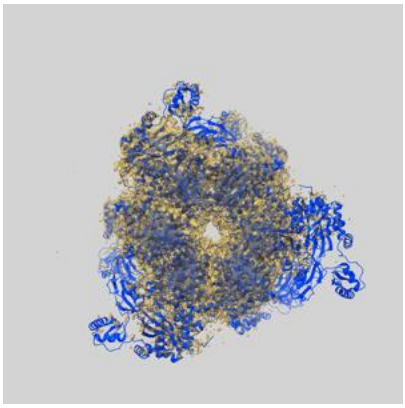
9.1 Map-model overlay



X



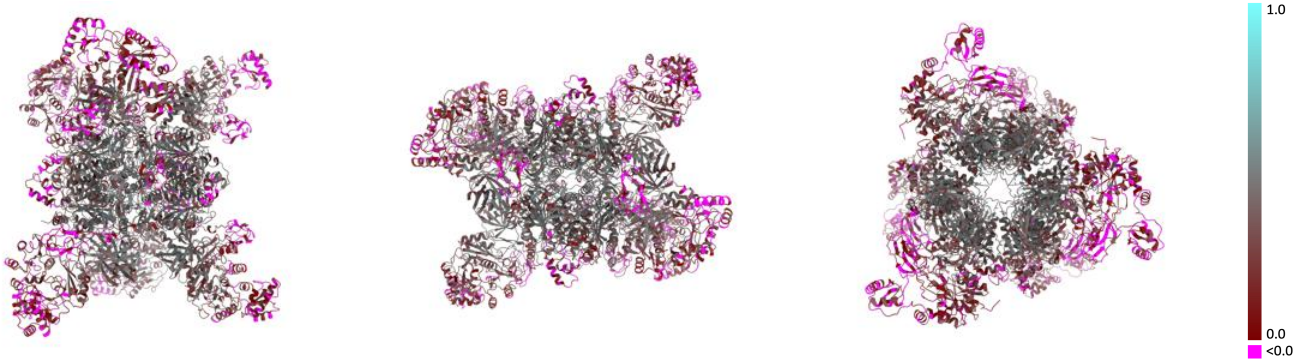
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

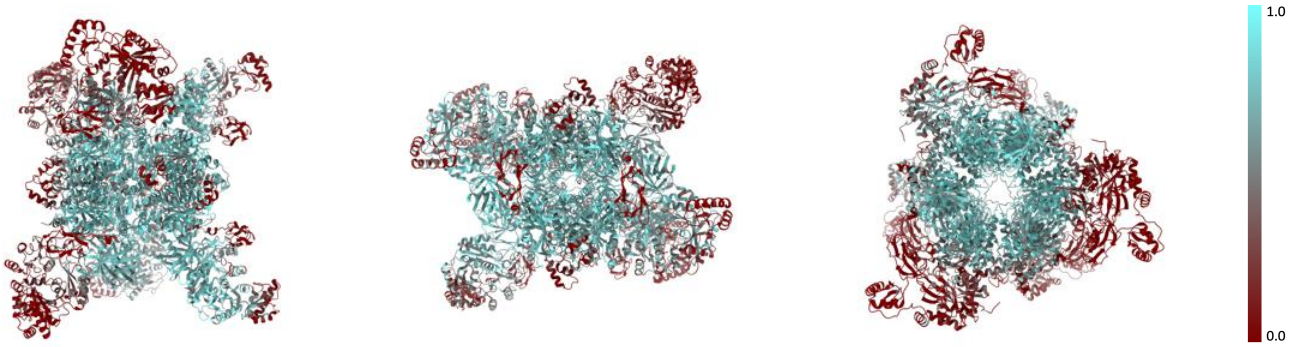
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

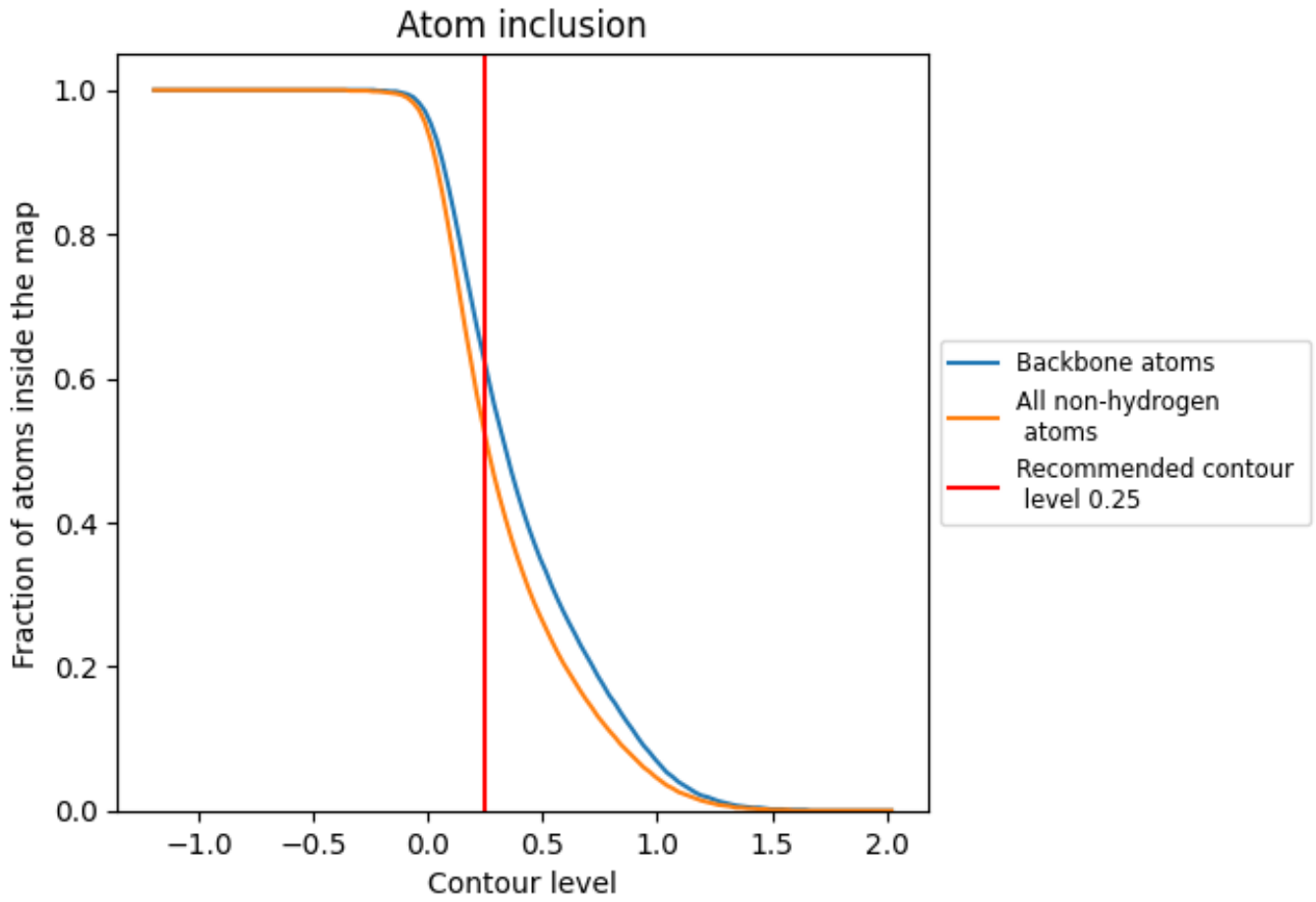
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 52% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5190	0.2960
A	0.2860	0.2070
B	0.5840	0.2760
D	0.1820	0.1820
F	0.4770	0.2410
G	0.6940	0.3810
H	0.4890	0.2620
I	0.6770	0.3740
J	0.2650	0.2130
K	0.7040	0.3810
L	0.7220	0.3900
N	0.7290	0.3940
O	0.7040	0.3890

