Full wwPDB EM Validation Report

May 8, 2023 – 10:48 PM EDT

PDB ID	:	8SGX
EMDB ID	:	EMD-40472
Title	:	Leishmania tarentolae propionyl-CoA carboxylase (alpha-4-beta-6)
Authors	:	Lee, J.K.J.; Liu, Y.T.; Hu, J.J.; Aphasizheva, I.; Aphasizhev, R.; Zhou, Z.H.
Deposited on	:	2023-04-13
Resolution	:	10.30 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:

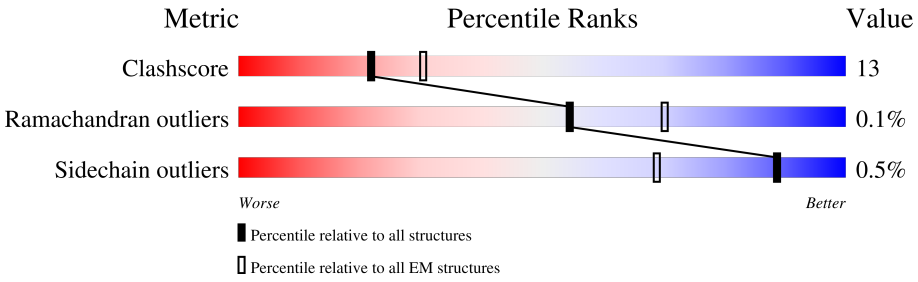
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 10.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	C	489	50% 83% 17%
1	D	489	69% 84% 16%
1	E	489	48% 83% 17%
1	F	489	54% 83% 17%
1	G	489	57% 83% 17%
1	H	489	53% 83% 17%
2	S	657	92% 67% 32%
2	V	657	75% 67% 32%

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Mol	Chain	Length	Quality of chain
2	X	657	82% 66% 33%
2	Z	657	86% 67% 32%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BTI	F	801	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 43182 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.

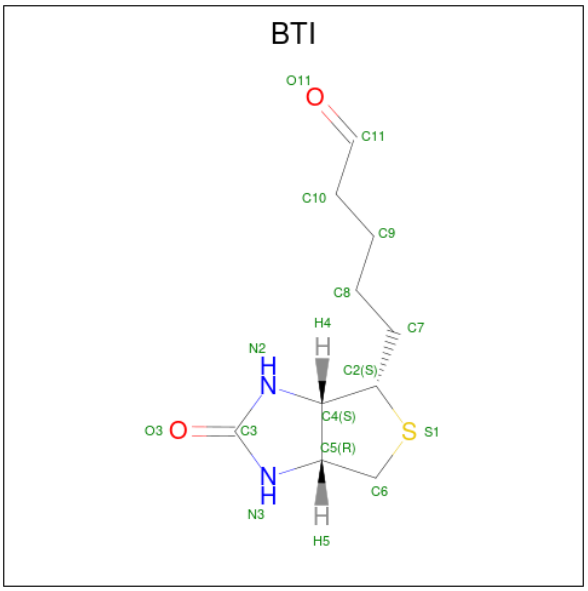
- Molecule 1 is a protein called Propionyl-coa carboxylase beta chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	489	Total	C	N	O	S	0	0
			3766	2395	658	693	20		
1	D	489	Total	C	N	O	S	0	0
			3766	2395	658	693	20		
1	E	489	Total	C	N	O	S	0	0
			3766	2395	658	693	20		
1	F	489	Total	C	N	O	S	0	0
			3766	2395	658	693	20		
1	G	489	Total	C	N	O	S	0	0
			3766	2395	658	693	20		
1	H	489	Total	C	N	O	S	0	0
			3766	2395	658	693	20		

- Molecule 2 is a protein called propionyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	657	Total	C	N	O	S	0	0
			5124	3209	897	980	38		
2	V	657	Total	C	N	O	S	0	0
			5124	3209	897	980	38		
2	X	657	Total	C	N	O	S	0	0
			5124	3209	897	980	38		
2	Z	657	Total	C	N	O	S	0	0
			5124	3209	897	980	38		

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



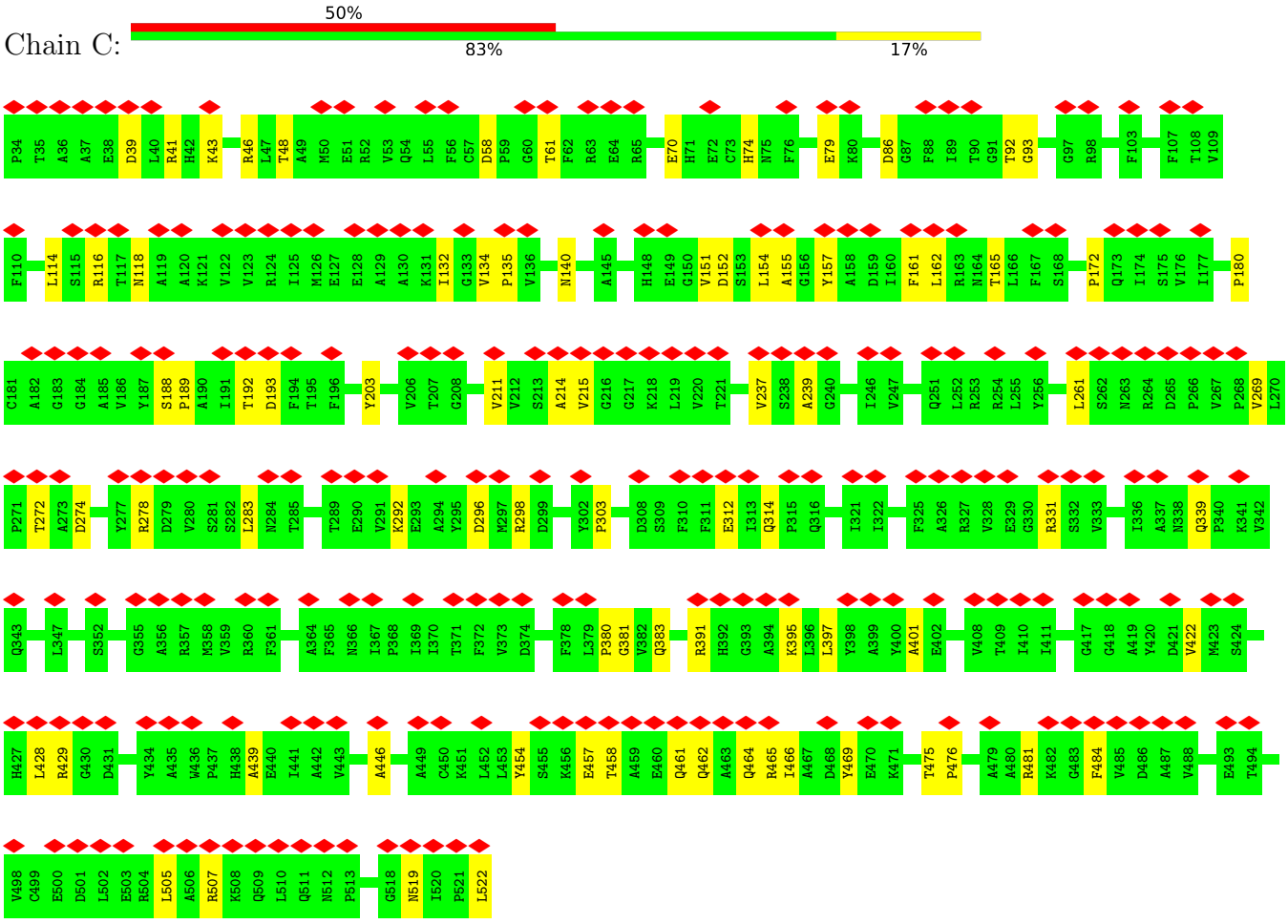
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	E	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	F	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	G	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	H	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	V	1	Total	C	N	O	S	0
			15	10	2	2	1	

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.

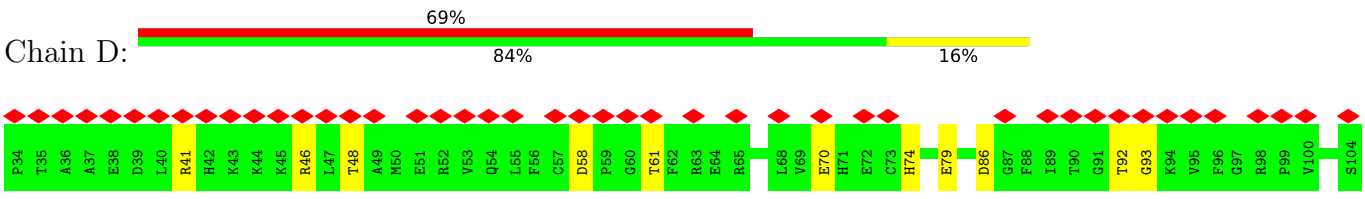
• Molecule 1: Propionyl-coa carboxylase beta chain, putative

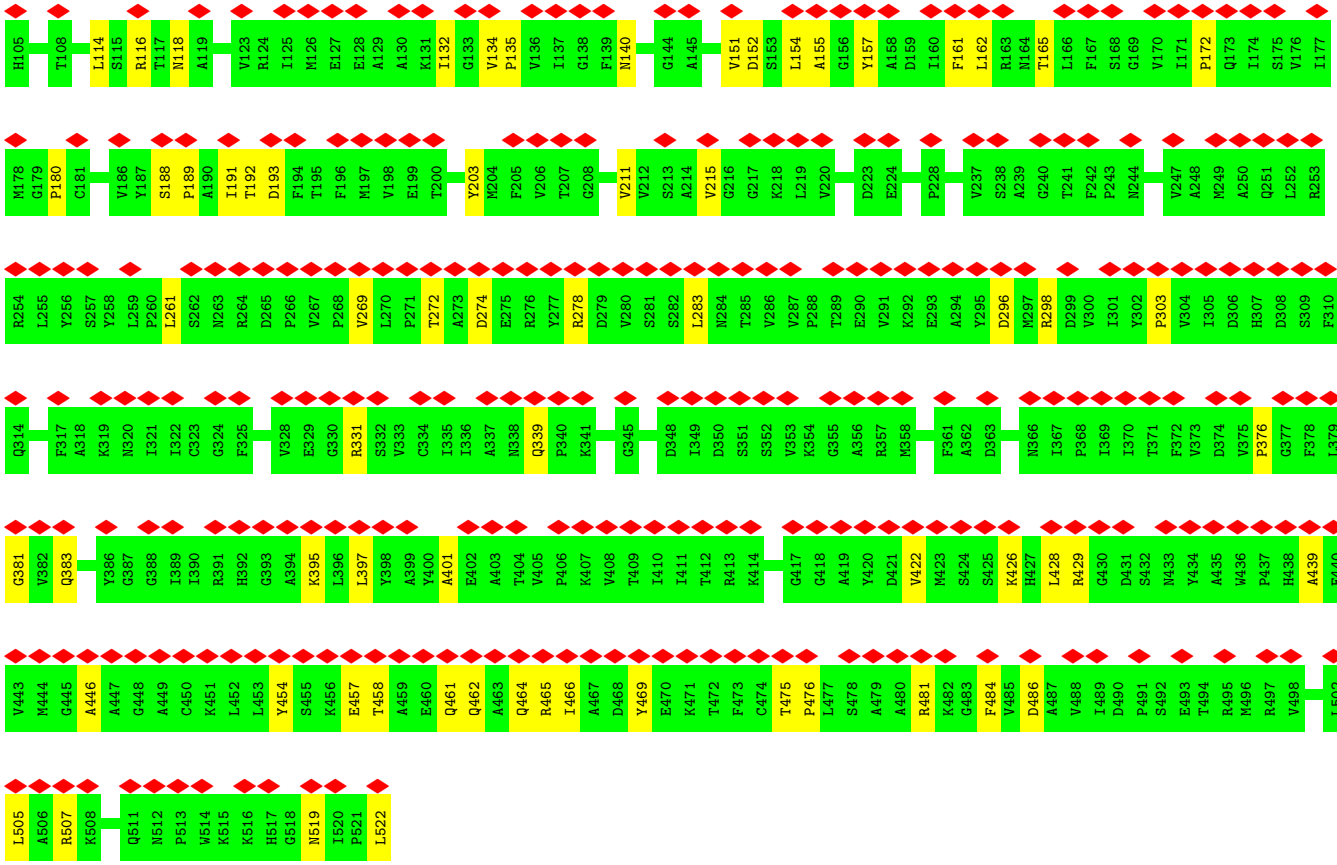
Chain C:



• Molecule 1: Propionyl-coa carboxylase beta chain, putative

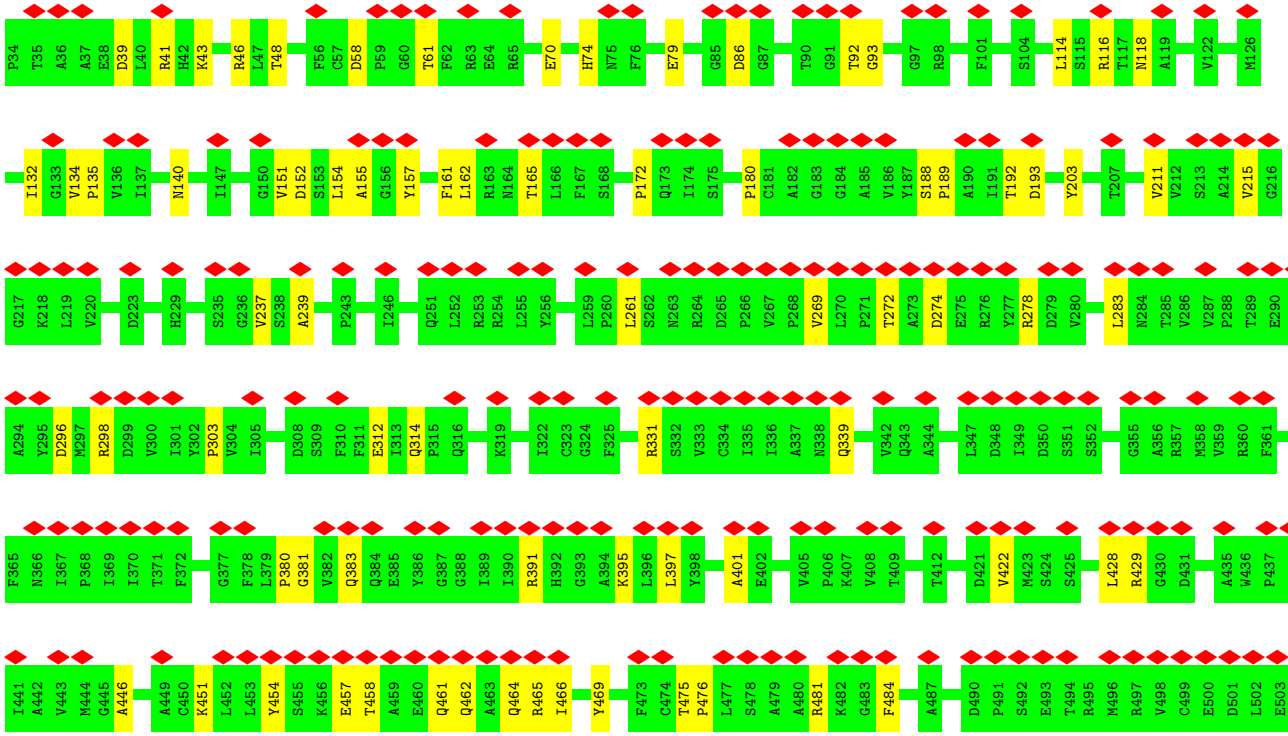
Chain D:

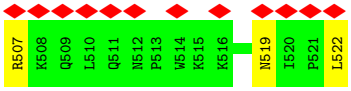




• Molecule 1: Propionyl-coa carboxylase beta chain, putative

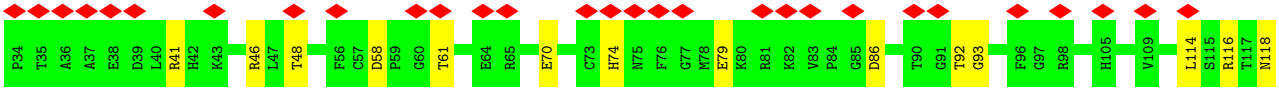
Chain E:

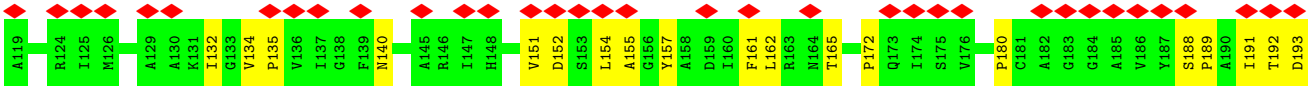


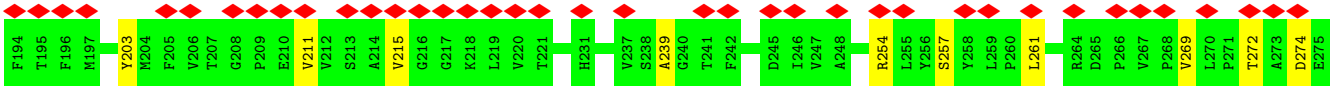


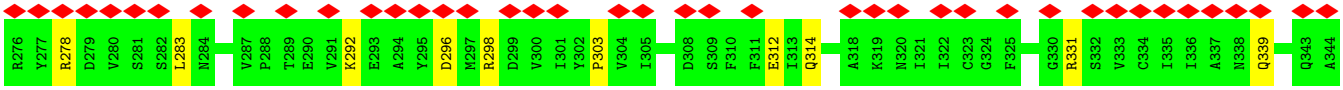
• Molecule 1: Propionyl-coa carboxylase beta chain, putative

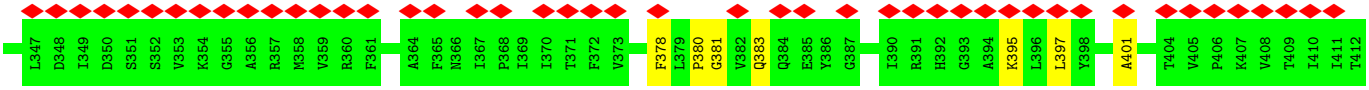
Chain F:

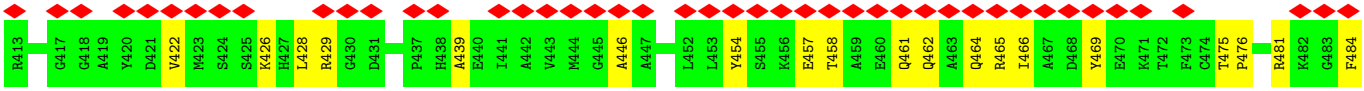


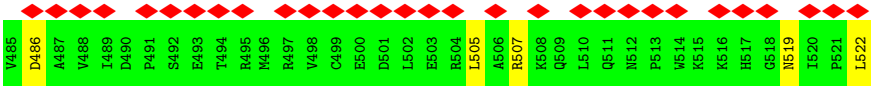






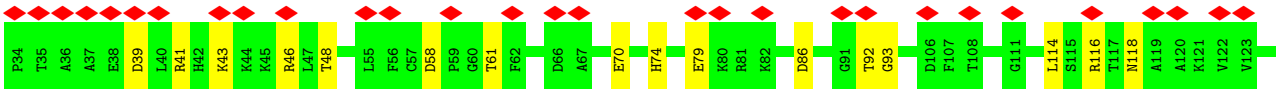


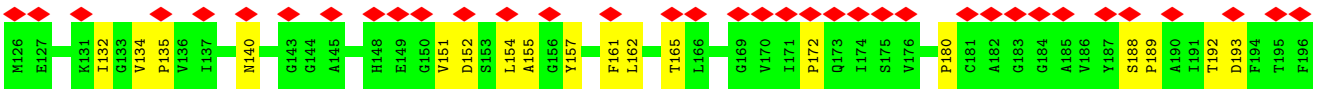


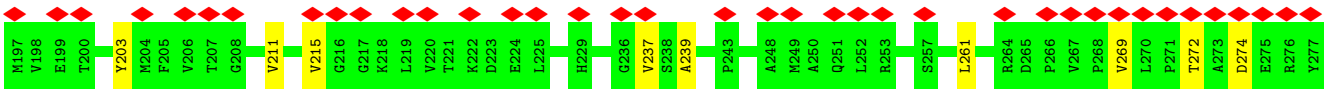


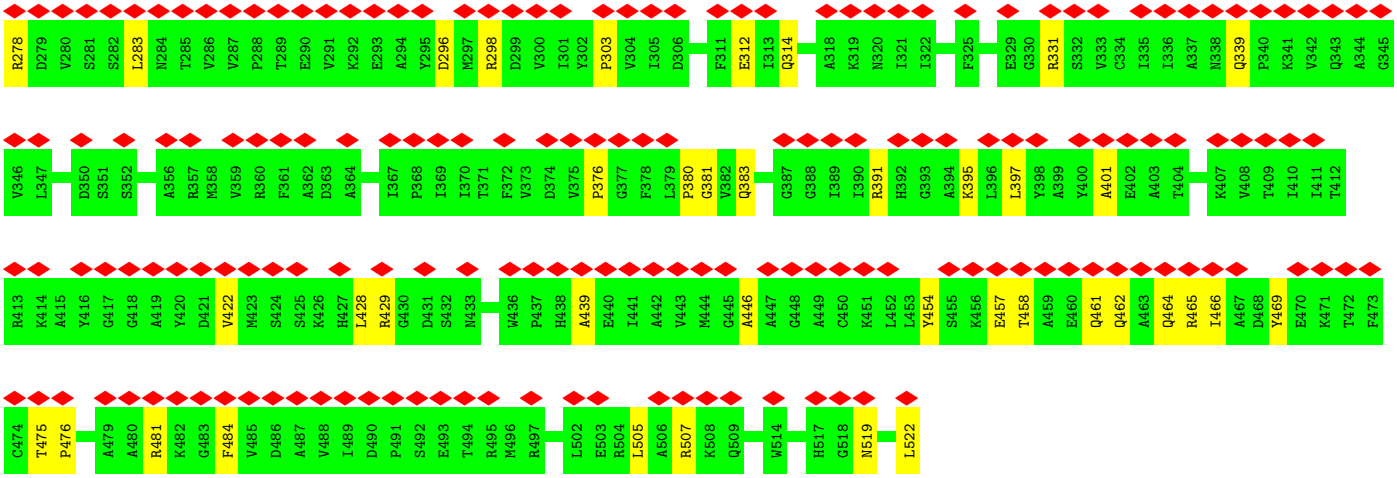
• Molecule 1: Propionyl-coa carboxylase beta chain, putative

Chain G:



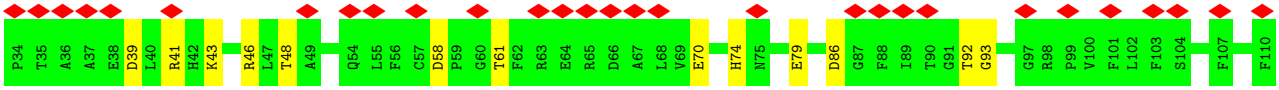






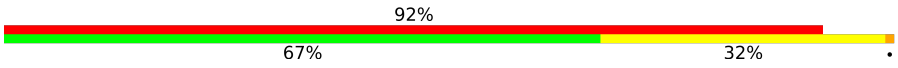
• Molecule 1: Propionyl-coa carboxylase beta chain, putative

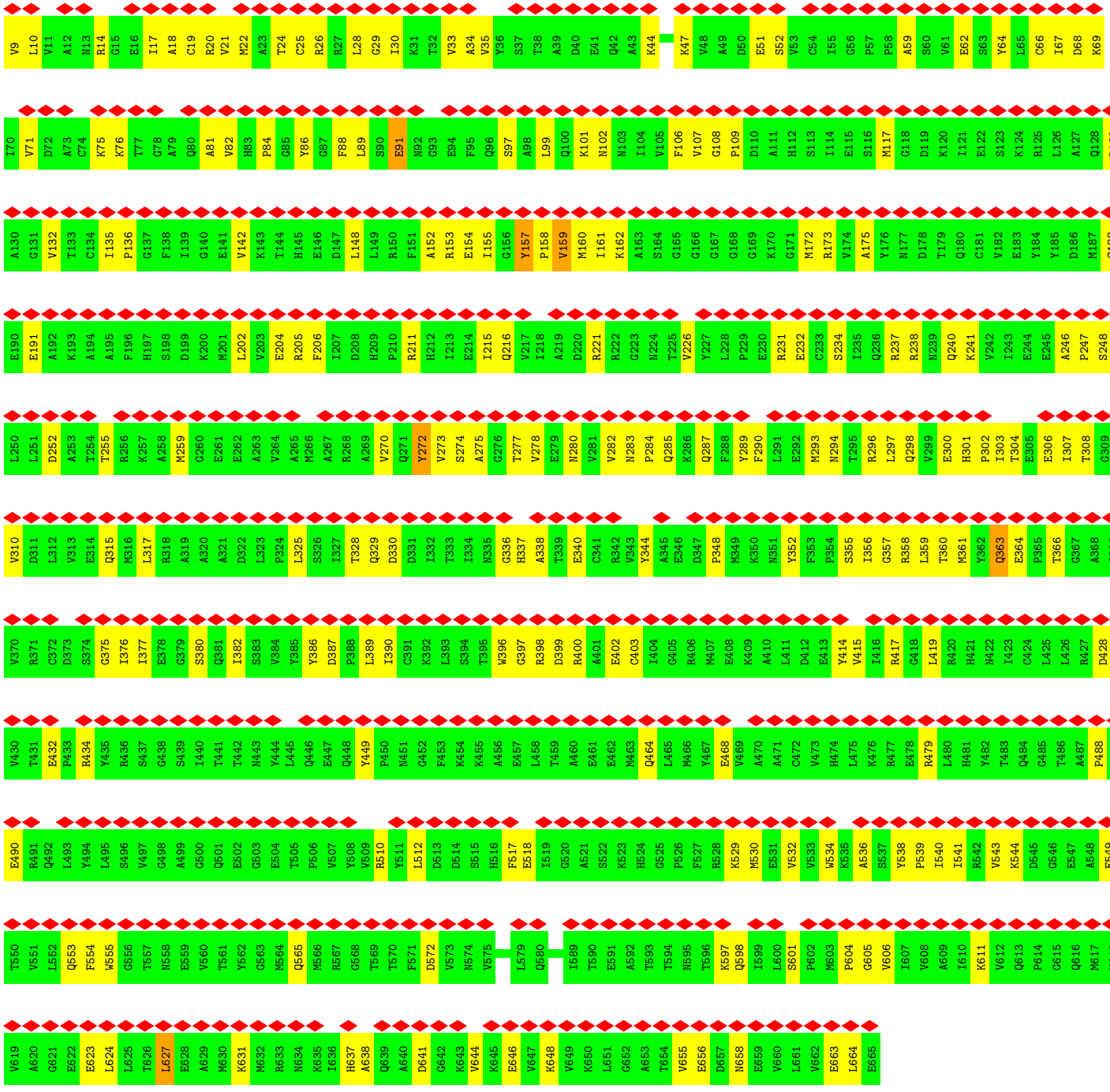
Chain H:



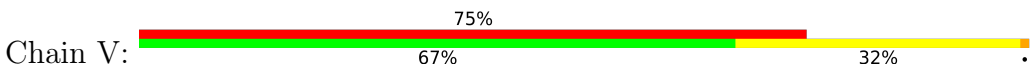
• Molecule 2: propionyl-CoA carboxylase

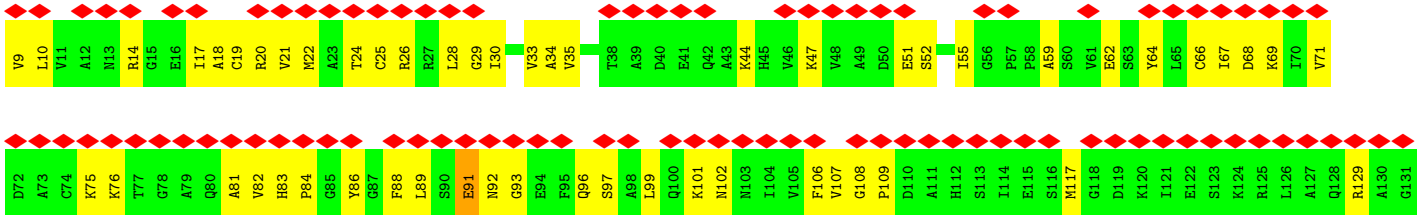
Chain S:

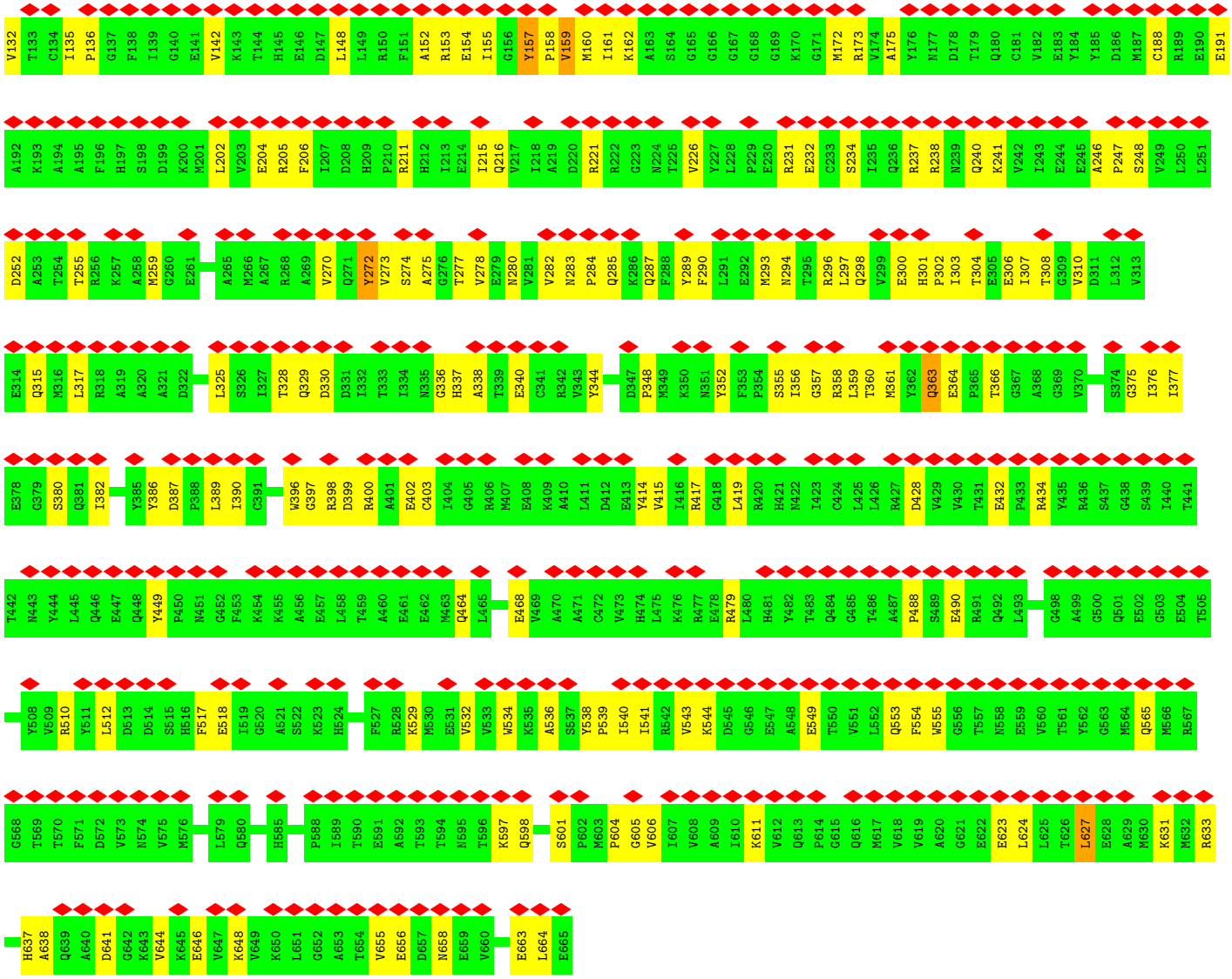




• Molecule 2: propionyl-CoA carboxylase

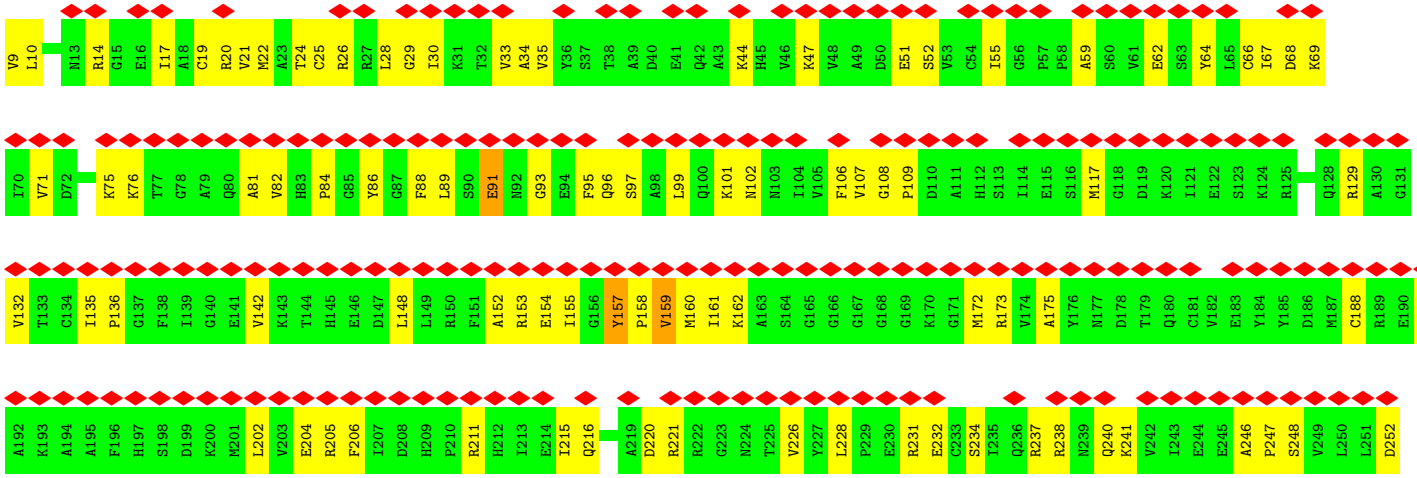


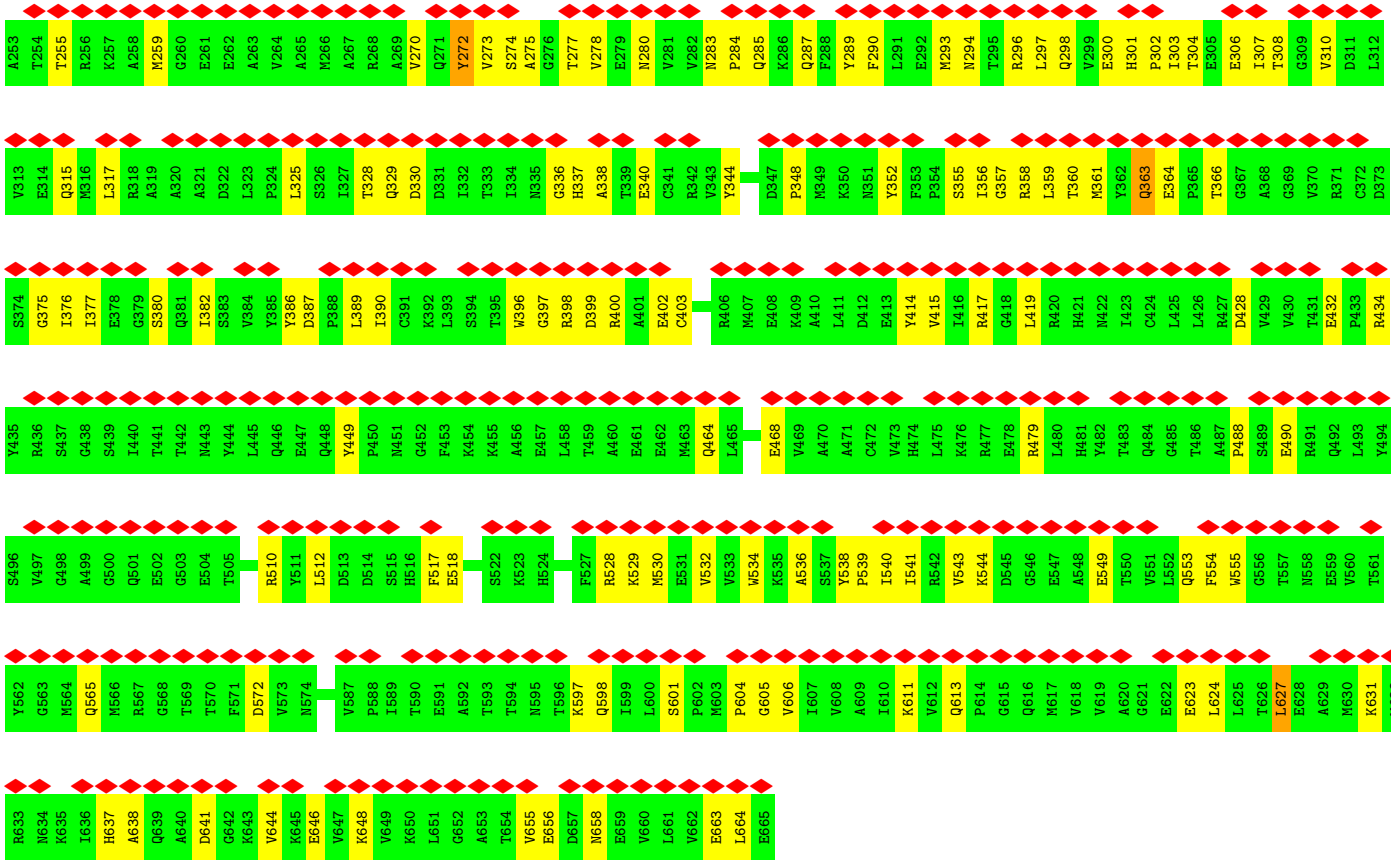




• Molecule 2: propionyl-CoA carboxylase

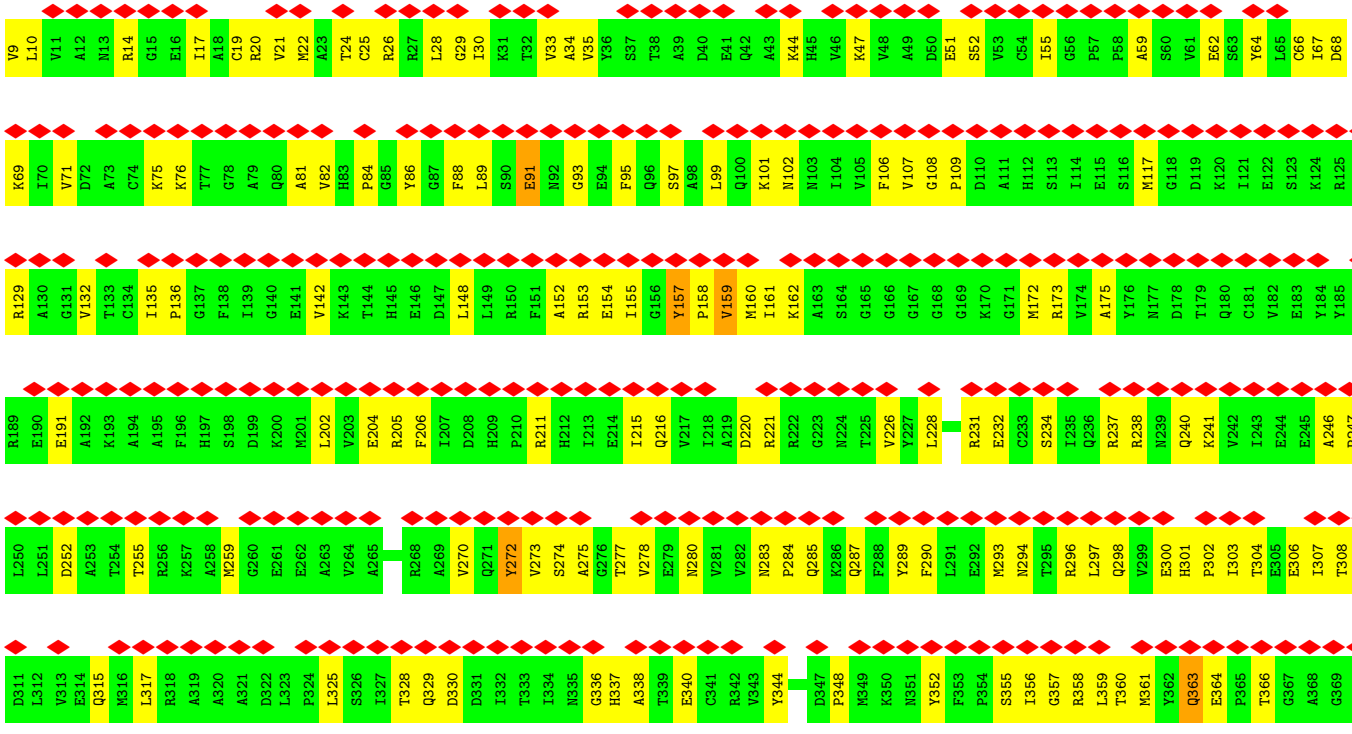
Chain X:

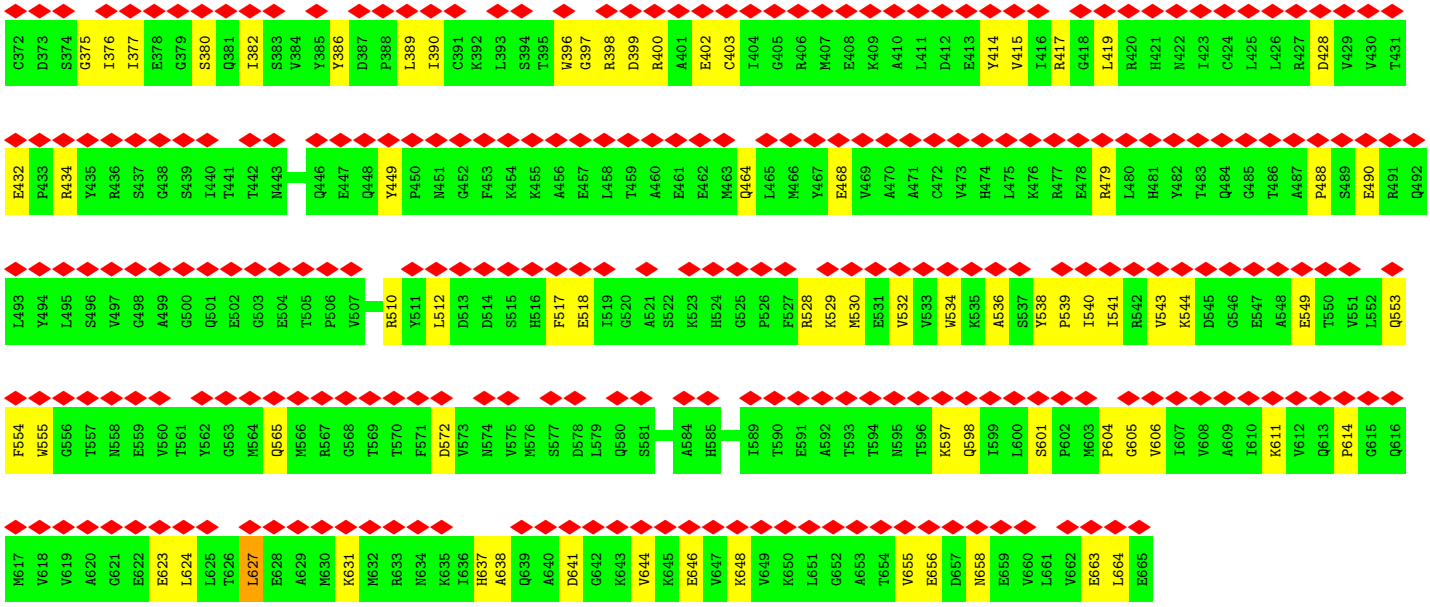




• Molecule 2: propionyl-CoA carboxylase

Chain Z:




C372 D373 S374 G375 I376 I377 E378 G379 S380 Q381 I382 S383 V384 Y385 Y386 D387 P388 L389 I390 C391 K392 L393 S394 T395 W396 G397 R398 D399 R400 A401 E402 C403 I404 G405 R406 M407 E408 K409 A410 L411 D412 E413 Y414 V415 I416 R417 G418 L419 R420 H421 N422 I423 C424 L425 L426 R427 D428 V429 V430 T431
E432 P433 R434 Y435 R436 S437 G438 S439 I440 T441 T442 N443 Q446 E447 Q448 Y449 P450 N451 G452 F453 K454 K455 A456 E457 L458 T459 A460 E461 E462 M463 Q464 L465 M466 Y467 E468 V469 A470 A471 C472 V473 H474 L475 K476 R477 E478 R479 L480 H481 Y482 T483 Q484 G485 T486 A487 P488 S489 E490 R491 Q492
L493 Y494 L495 S496 V497 G498 A499 G500 Q501 E502 G503 E504 T505 P506 V507 R510 Y511 L512 D513 D514 S515 H516 F517 E518 I519 G520 A521 S522 K523 H524 G525 P526 F527 R528 K529 M530 E531 V532 V533 W534 K535 A536 S537 Y538 P539 I540 I541 R542 V543 K544 D545 G546 E547 A548 E549 T550 V551 L552 Q553
F554 W555 G556 T557 N558 E559 V560 T561 Y562 G563 M564 Q565 M566 R567 G568 T569 T570 F571 D572 V573 N574 V575 M576 S577 D578 L579 Q580 S581 A584 H585 I589 T590 E591 A592 T593 T594 N595 T596 K597 Q598 I599 L600 S601 P602 M603 P604 G605 V606 I607 V608 A609 I610 K611 V612 Q613 P614 G615 Q616
M617 V618 V619 A620 G621 E622 E623 L624 L625 T626 L627 E628 A629 M630 K631 M632 R633 N634 K635 I636 H637 A638 Q639 A640 D641 G642 K643 V644 K645 E646 V647 K648 V649 K650 L651 G652 A653 T654 V655 E656 D657 N658 E659 V660 L661 V662 E663 L664 E665

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5933	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0121	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	C	0.30	0/3851	0.50	0/5217
1	D	0.29	0/3851	0.50	0/5217
1	E	0.29	0/3851	0.50	0/5217
1	F	0.30	0/3851	0.50	0/5217
1	G	0.30	0/3851	0.50	0/5217
1	H	0.30	0/3851	0.50	0/5217
2	S	0.27	0/5213	0.51	0/7048
2	V	0.27	0/5213	0.51	0/7048
2	X	0.27	0/5213	0.51	0/7048
2	Z	0.27	0/5213	0.51	0/7048
All	All	0.28	0/43958	0.50	0/59494

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	C	3766	0	3762	71	0
1	D	3766	0	3762	68	0
1	E	3766	0	3762	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3766	0	3762	76	0
1	G	3766	0	3762	67	0
1	H	3766	0	3762	70	0
2	S	5124	0	5108	193	0
2	V	5124	0	5108	196	0
2	X	5124	0	5108	195	0
2	Z	5124	0	5108	194	0
3	D	15	0	16	5	0
3	E	15	0	16	1	0
3	F	15	0	16	8	0
3	G	15	0	16	3	0
3	H	15	0	16	6	0
3	V	15	0	16	2	0
All	All	43182	0	43100	1112	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 13.

All (1112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:PRO:HD3	3:F:801:BTI:H63	1.28	1.05
1:H:380:PRO:HD3	3:H:801:BTI:H63	1.50	0.92
2:S:158:PRO:HB2	2:S:206:PHE:HB3	1.57	0.86
2:Z:158:PRO:HB2	2:Z:206:PHE:HB3	1.57	0.86
1:C:507:ARG:HH22	1:E:261:LEU:HD13	1.40	0.85
2:X:158:PRO:HB2	2:X:206:PHE:HB3	1.57	0.85
2:V:158:PRO:HB2	2:V:206:PHE:HB3	1.57	0.85
1:C:261:LEU:HD13	1:D:507:ARG:HH22	1.41	0.85
1:G:507:ARG:HH22	1:H:261:LEU:HD13	1.40	0.85
1:F:261:LEU:HD13	1:H:507:ARG:HH22	1.41	0.84
1:D:261:LEU:HD13	1:E:507:ARG:HH22	1.40	0.84
1:F:507:ARG:HH22	1:G:261:LEU:HD13	1.42	0.83
2:V:109:PRO:HG3	2:V:274:SER:HB3	1.60	0.83
2:S:364:GLU:HG3	2:S:415:VAL:HB	1.63	0.81
2:S:109:PRO:HG3	2:S:274:SER:HB3	1.61	0.81
2:V:364:GLU:HG3	2:V:415:VAL:HB	1.63	0.80
2:Z:109:PRO:HG3	2:Z:274:SER:HB3	1.61	0.80
2:X:109:PRO:HG3	2:X:274:SER:HB3	1.61	0.79
1:C:462:GLN:HG2	1:C:466:ILE:HD12	1.64	0.79
2:X:364:GLU:HG3	2:X:415:VAL:HB	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:364:GLU:HG3	2:Z:415:VAL:HB	1.63	0.79
1:F:462:GLN:HG2	1:F:466:ILE:HD12	1.64	0.79
1:G:462:GLN:HG2	1:G:466:ILE:HD12	1.65	0.79
1:D:462:GLN:HG2	1:D:466:ILE:HD12	1.65	0.79
1:E:462:GLN:HG2	1:E:466:ILE:HD12	1.64	0.79
2:S:646:GLU:OE2	2:S:648:LYS:NZ	2.15	0.79
1:H:462:GLN:HG2	1:H:466:ILE:HD12	1.65	0.79
2:V:117:MET:SD	2:V:270:VAL:HG21	2.24	0.78
2:X:117:MET:SD	2:X:270:VAL:HG21	2.24	0.78
2:X:646:GLU:OE2	2:X:648:LYS:NZ	2.15	0.78
2:Z:117:MET:SD	2:Z:270:VAL:HG21	2.24	0.78
2:Z:646:GLU:OE2	2:Z:648:LYS:NZ	2.15	0.77
2:V:646:GLU:OE2	2:V:648:LYS:NZ	2.15	0.77
2:S:117:MET:SD	2:S:270:VAL:HG21	2.24	0.77
1:D:376:PRO:HB2	3:D:801:BTI:H4	1.68	0.76
1:F:380:PRO:HD3	3:F:801:BTI:C6	2.11	0.75
1:F:378:PHE:O	3:F:801:BTI:C5	2.34	0.75
2:S:157:TYR:HB3	2:S:205:ARG:HG2	1.68	0.75
2:Z:157:TYR:HB3	2:Z:205:ARG:HG2	1.68	0.75
2:X:157:TYR:HB3	2:X:205:ARG:HG2	1.68	0.74
2:V:157:TYR:HB3	2:V:205:ARG:HG2	1.68	0.74
2:Z:159:VAL:HG13	2:Z:161:ILE:HG13	1.70	0.74
2:X:159:VAL:HG13	2:X:161:ILE:HG13	1.70	0.74
1:D:395:LYS:HD3	1:F:522:LEU:HD12	1.69	0.73
2:S:231:ARG:HA	2:S:246:ALA:HA	1.71	0.73
2:V:231:ARG:HA	2:V:246:ALA:HA	1.71	0.73
2:S:159:VAL:HG13	2:S:161:ILE:HG13	1.70	0.73
2:X:528:ARG:HH12	2:X:530:MET:HE3	1.52	0.73
1:C:41:ARG:HE	1:C:46:ARG:HE	1.37	0.73
1:G:41:ARG:HE	1:G:46:ARG:HE	1.37	0.72
2:X:231:ARG:HA	2:X:246:ALA:HA	1.71	0.72
2:X:272:TYR:CE2	2:X:275:ALA:HA	2.24	0.72
2:Z:231:ARG:HA	2:Z:246:ALA:HA	1.71	0.72
2:Z:272:TYR:CE2	2:Z:275:ALA:HA	2.24	0.72
2:Z:336:GLY:HA3	2:Z:398:ARG:HA	1.71	0.72
1:C:395:LYS:HD3	1:H:522:LEU:HD12	1.70	0.72
1:F:41:ARG:HE	1:F:46:ARG:HE	1.37	0.72
2:X:336:GLY:HA3	2:X:398:ARG:HA	1.71	0.72
1:D:41:ARG:HE	1:D:46:ARG:HE	1.37	0.72
2:S:272:TYR:CE2	2:S:275:ALA:HA	2.24	0.72
2:V:336:GLY:HA3	2:V:398:ARG:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:LEU:HD12	1:F:395:LYS:HD3	1.71	0.72
2:V:272:TYR:CE2	2:V:275:ALA:HA	2.24	0.72
2:X:532:VAL:HG22	2:X:543:VAL:HG22	1.72	0.72
1:D:86:ASP:O	1:D:118:ASN:ND2	2.22	0.72
1:F:86:ASP:O	1:F:118:ASN:ND2	2.23	0.71
1:H:86:ASP:O	1:H:118:ASN:ND2	2.22	0.71
2:X:627:LEU:HD21	2:X:656:GLU:HG3	1.72	0.71
2:Z:532:VAL:HG22	2:Z:543:VAL:HG22	1.72	0.71
1:E:86:ASP:O	1:E:118:ASN:ND2	2.22	0.71
2:V:84:PRO:HD3	2:V:107:VAL:HB	1.73	0.71
2:Z:627:LEU:HD21	2:Z:656:GLU:HG3	1.72	0.71
1:E:395:LYS:HD3	1:G:522:LEU:HD12	1.71	0.71
2:X:84:PRO:HD3	2:X:107:VAL:HB	1.73	0.71
2:Z:348:PRO:HA	2:Z:352:TYR:HD1	1.55	0.71
2:S:336:GLY:HA3	2:S:398:ARG:HA	1.71	0.71
2:V:91:GLU:HA	2:V:106:PHE:HZ	1.55	0.71
2:V:159:VAL:HG13	2:V:161:ILE:HG13	1.70	0.71
1:C:86:ASP:O	1:C:118:ASN:ND2	2.22	0.71
1:E:41:ARG:HE	1:E:46:ARG:HE	1.37	0.71
1:G:74:HIS:HA	1:G:79:GLU:HG3	1.73	0.71
1:H:74:HIS:HA	1:H:79:GLU:HG3	1.73	0.71
1:E:522:LEU:HD12	1:G:395:LYS:HD3	1.72	0.71
2:X:348:PRO:HA	2:X:352:TYR:HD1	1.55	0.71
2:Z:84:PRO:HD3	2:Z:107:VAL:HB	1.73	0.71
1:E:74:HIS:HA	1:E:79:GLU:HG3	1.73	0.70
2:Z:159:VAL:CG1	2:Z:161:ILE:HG13	2.20	0.70
1:C:74:HIS:HA	1:C:79:GLU:HG3	1.73	0.70
2:S:84:PRO:HD3	2:S:107:VAL:HB	1.73	0.70
2:S:627:LEU:HD21	2:S:656:GLU:HG3	1.72	0.70
2:V:348:PRO:HA	2:V:352:TYR:HD1	1.55	0.70
1:H:41:ARG:HE	1:H:46:ARG:HE	1.37	0.70
2:V:532:VAL:HG22	2:V:543:VAL:HG22	1.72	0.70
2:S:159:VAL:CG1	2:S:161:ILE:HG13	2.20	0.70
1:D:74:HIS:HA	1:D:79:GLU:HG3	1.73	0.70
1:F:74:HIS:HA	1:F:79:GLU:HG3	1.73	0.70
1:G:86:ASP:O	1:G:118:ASN:ND2	2.22	0.70
2:X:159:VAL:CG1	2:X:161:ILE:HG13	2.21	0.70
1:C:162:LEU:HD11	1:H:429:ARG:HG3	1.74	0.70
2:V:159:VAL:CG1	2:V:161:ILE:HG13	2.21	0.70
1:C:522:LEU:HD12	1:H:395:LYS:HD3	1.73	0.70
2:S:91:GLU:HA	2:S:106:PHE:HZ	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:348:PRO:HA	2:S:352:TYR:HD1	1.55	0.70
2:Z:91:GLU:HA	2:Z:106:PHE:HZ	1.55	0.69
1:D:162:LEU:HD11	1:F:429:ARG:HG3	1.74	0.69
2:V:627:LEU:HD21	2:V:656:GLU:HG3	1.72	0.69
2:Z:89:LEU:H	2:Z:89:LEU:HD23	1.58	0.69
2:S:532:VAL:HG22	2:S:543:VAL:HG22	1.72	0.69
2:V:89:LEU:HD23	2:V:89:LEU:H	1.58	0.69
2:X:91:GLU:HA	2:X:106:PHE:HZ	1.55	0.69
1:E:429:ARG:HG3	1:G:162:LEU:HD11	1.75	0.69
2:X:89:LEU:H	2:X:89:LEU:HD23	1.58	0.69
2:V:135:ILE:HD12	2:V:136:PRO:HD2	1.75	0.68
2:S:89:LEU:H	2:S:89:LEU:HD23	1.58	0.68
1:D:429:ARG:HG3	1:F:162:LEU:HD11	1.76	0.68
2:Z:135:ILE:HD12	2:Z:136:PRO:HD2	1.75	0.68
2:X:135:ILE:HD12	2:X:136:PRO:HD2	1.75	0.68
1:E:162:LEU:HD11	1:G:429:ARG:HG3	1.75	0.68
2:S:135:ILE:HD12	2:S:136:PRO:HD2	1.75	0.68
1:C:429:ARG:HG3	1:H:162:LEU:HD11	1.76	0.67
1:E:380:PRO:HD3	3:E:801:BTI:H63	1.75	0.67
1:D:116:ARG:HB2	1:D:152:ASP:HB3	1.78	0.66
2:S:605:GLY:HA3	2:S:627:LEU:HD23	1.77	0.66
1:F:116:ARG:HB2	1:F:152:ASP:HB3	1.78	0.66
2:S:296:ARG:NH2	2:S:298:GLN:HA	2.11	0.65
2:Z:605:GLY:HA3	2:Z:627:LEU:HD23	1.77	0.65
2:V:296:ARG:NH2	2:V:298:GLN:HA	2.11	0.65
1:G:116:ARG:HB2	1:G:152:ASP:HB3	1.78	0.65
1:H:116:ARG:HB2	1:H:152:ASP:HB3	1.78	0.65
1:H:380:PRO:CD	3:H:801:BTI:H63	2.26	0.65
1:C:116:ARG:HB2	1:C:152:ASP:HB3	1.78	0.65
1:C:215:VAL:HG11	1:H:380:PRO:HG2	1.77	0.65
1:E:215:VAL:HG11	1:G:380:PRO:HG2	1.79	0.65
2:S:159:VAL:HB	2:S:175:ALA:HB3	1.79	0.65
2:X:605:GLY:HA3	2:X:627:LEU:HD23	1.77	0.65
2:Z:296:ARG:NH2	2:Z:298:GLN:HA	2.11	0.65
1:D:215:VAL:HG11	1:F:380:PRO:HG2	1.79	0.64
2:Z:155:ILE:HB	2:Z:157:TYR:CD2	2.33	0.64
2:V:605:GLY:HA3	2:V:627:LEU:HD23	1.77	0.64
2:X:155:ILE:HB	2:X:157:TYR:CD2	2.33	0.64
2:V:155:ILE:HB	2:V:157:TYR:CD2	2.33	0.64
2:X:296:ARG:NH2	2:X:298:GLN:HA	2.11	0.64
1:E:116:ARG:HB2	1:E:152:ASP:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:155:ILE:HB	2:S:157:TYR:CD2	2.33	0.64
1:C:380:PRO:HG2	1:H:215:VAL:HG11	1.80	0.64
2:X:302:PRO:O	2:X:306:GLU:HG3	1.98	0.64
2:Z:302:PRO:O	2:Z:306:GLU:HG3	1.98	0.64
1:E:41:ARG:HE	1:E:46:ARG:NE	1.97	0.63
1:C:507:ARG:NH2	1:E:261:LEU:HD13	2.11	0.63
2:Z:159:VAL:HB	2:Z:175:ALA:HB3	1.80	0.63
1:E:380:PRO:HG2	1:G:215:VAL:HG11	1.79	0.63
1:G:507:ARG:NH2	1:H:261:LEU:HD13	2.12	0.63
2:V:159:VAL:HB	2:V:175:ALA:HB3	1.79	0.63
1:H:41:ARG:HE	1:H:46:ARG:NE	1.97	0.63
1:C:261:LEU:HD13	1:D:507:ARG:NH2	2.12	0.63
1:G:41:ARG:HE	1:G:46:ARG:NE	1.97	0.63
1:F:378:PHE:O	3:F:801:BTI:C6	2.47	0.63
2:X:159:VAL:HB	2:X:175:ALA:HB3	1.79	0.63
1:C:41:ARG:HE	1:C:46:ARG:NE	1.97	0.62
1:D:41:ARG:HE	1:D:46:ARG:NE	1.97	0.62
1:D:380:PRO:HG2	1:F:215:VAL:HG11	1.81	0.62
1:F:41:ARG:HE	1:F:46:ARG:NE	1.97	0.62
2:V:302:PRO:O	2:V:306:GLU:HG3	1.98	0.62
2:S:91:GLU:HA	2:S:106:PHE:CZ	2.34	0.62
2:S:246:ALA:HB3	2:S:247:PRO:HD3	1.82	0.62
2:Z:246:ALA:HB3	2:Z:247:PRO:HD3	1.82	0.62
2:X:336:GLY:CA	2:X:398:ARG:HA	2.30	0.62
2:Z:336:GLY:CA	2:Z:398:ARG:HA	2.30	0.62
2:V:246:ALA:HB3	2:V:247:PRO:HD3	1.82	0.62
2:X:246:ALA:HB3	2:X:247:PRO:HD3	1.82	0.62
2:Z:490:GLU:OE1	2:Z:510:ARG:NH1	2.33	0.61
2:S:490:GLU:OE1	2:S:510:ARG:NH1	2.33	0.61
2:Z:205:ARG:NH1	2:Z:206:PHE:O	2.32	0.61
2:X:91:GLU:HA	2:X:106:PHE:CZ	2.34	0.61
2:Z:91:GLU:HA	2:Z:106:PHE:CZ	2.34	0.61
2:X:277:THR:HG21	2:X:298:GLN:NE2	2.15	0.61
2:Z:277:THR:HG21	2:Z:298:GLN:NE2	2.15	0.61
2:S:302:PRO:O	2:S:306:GLU:HG3	1.98	0.61
2:X:490:GLU:OE1	2:X:510:ARG:NH1	2.33	0.61
2:S:336:GLY:CA	2:S:398:ARG:HA	2.30	0.61
2:V:205:ARG:NH1	2:V:206:PHE:O	2.32	0.61
2:V:490:GLU:OE1	2:V:510:ARG:NH1	2.33	0.61
2:X:205:ARG:NH1	2:X:206:PHE:O	2.32	0.61
2:S:226:VAL:HG13	2:S:329:GLN:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:337:HIS:NE2	2:V:400:ARG:HD2	2.16	0.61
2:V:20:ARG:NH2	2:V:301:HIS:HE1	1.99	0.61
2:V:277:THR:HG21	2:V:298:GLN:NE2	2.15	0.61
2:V:226:VAL:HG13	2:V:329:GLN:HG3	1.83	0.60
2:V:336:GLY:CA	2:V:398:ARG:HA	2.30	0.60
1:D:261:LEU:HD13	1:E:507:ARG:NH2	2.11	0.60
2:Z:226:VAL:HA	2:Z:329:GLN:HE21	1.66	0.60
2:V:91:GLU:HA	2:V:106:PHE:CZ	2.34	0.60
2:X:109:PRO:CG	2:X:274:SER:HB3	2.31	0.60
2:X:337:HIS:NE2	2:X:400:ARG:HD2	2.16	0.60
2:Z:337:HIS:NE2	2:Z:400:ARG:HD2	2.16	0.60
2:X:226:VAL:HA	2:X:329:GLN:HE21	1.66	0.60
1:D:135:PRO:HB3	1:D:172:PRO:HG2	1.84	0.60
1:F:135:PRO:HB3	1:F:172:PRO:HG2	1.84	0.60
2:S:226:VAL:HA	2:S:329:GLN:HE21	1.66	0.60
2:S:277:THR:HG21	2:S:298:GLN:NE2	2.15	0.60
2:S:20:ARG:NH2	2:S:301:HIS:HE1	1.99	0.60
1:G:272:THR:HG22	1:G:274:ASP:H	1.67	0.60
2:S:337:HIS:NE2	2:S:400:ARG:HD2	2.16	0.60
2:V:226:VAL:HA	2:V:329:GLN:HE21	1.66	0.60
2:X:157:TYR:HD1	2:X:159:VAL:H	1.50	0.60
2:X:226:VAL:HG13	2:X:329:GLN:HG3	1.83	0.60
1:C:135:PRO:HB3	1:C:172:PRO:HG2	1.84	0.60
1:C:272:THR:HG22	1:C:274:ASP:H	1.67	0.60
2:Z:226:VAL:HG13	2:Z:329:GLN:HG3	1.83	0.60
1:F:380:PRO:CD	3:F:801:BTI:H63	2.19	0.60
2:S:109:PRO:CG	2:S:274:SER:HB3	2.31	0.60
2:V:157:TYR:HD1	2:V:159:VAL:H	1.50	0.60
2:Z:157:TYR:HD1	2:Z:159:VAL:H	1.50	0.60
2:X:512:LEU:HD23	2:X:518:GLU:HG3	1.84	0.59
1:G:135:PRO:HB3	1:G:172:PRO:HG2	1.84	0.59
2:V:109:PRO:CG	2:V:274:SER:HB3	2.31	0.59
2:Z:512:LEU:HD23	2:Z:518:GLU:HG3	1.85	0.59
2:S:464:GLN:O	2:S:468:GLU:HG2	2.02	0.59
2:X:20:ARG:NH2	2:X:301:HIS:HE1	2.00	0.59
2:Z:20:ARG:NH2	2:Z:301:HIS:HE1	1.99	0.59
2:Z:464:GLN:O	2:Z:468:GLU:HG2	2.02	0.59
1:D:272:THR:HG22	1:D:274:ASP:H	1.67	0.59
2:X:303:ILE:HD11	2:X:340:GLU:HB3	1.85	0.59
2:Z:303:ILE:HD11	2:Z:340:GLU:HB3	1.85	0.59
2:S:157:TYR:HD1	2:S:159:VAL:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:LEU:HD23	1:E:132:ILE:HD11	1.85	0.59
1:E:272:THR:HG22	1:E:274:ASP:H	1.67	0.59
1:H:135:PRO:HB3	1:H:172:PRO:HG2	1.84	0.59
2:V:303:ILE:HD11	2:V:340:GLU:HB3	1.85	0.59
2:V:307:ILE:HG13	2:V:308:THR:HG23	1.85	0.59
2:X:464:GLN:O	2:X:468:GLU:HG2	2.02	0.59
1:E:135:PRO:HB3	1:E:172:PRO:HG2	1.84	0.58
1:F:272:THR:HG22	1:F:274:ASP:H	1.67	0.58
2:V:464:GLN:O	2:V:468:GLU:HG2	2.02	0.58
1:C:70:GLU:OE1	1:D:481:ARG:HG2	2.04	0.58
1:F:261:LEU:HD13	1:H:507:ARG:NH2	2.13	0.58
2:S:10:LEU:HD11	2:S:35:VAL:HG13	1.85	0.58
2:V:512:LEU:HD23	2:V:518:GLU:HG3	1.85	0.58
1:D:132:ILE:HD11	1:E:505:LEU:HD23	1.85	0.58
2:X:307:ILE:HG13	2:X:308:THR:HG23	1.85	0.58
1:D:376:PRO:O	3:D:801:BTI:H4	2.02	0.58
1:F:507:ARG:NH2	1:G:261:LEU:HD13	2.14	0.58
1:H:272:THR:HG22	1:H:274:ASP:H	1.67	0.58
2:V:10:LEU:HD11	2:V:35:VAL:HG13	1.85	0.58
2:Z:109:PRO:CG	2:Z:274:SER:HB3	2.31	0.58
2:S:28:LEU:CD1	2:S:317:LEU:HD21	2.34	0.58
2:S:512:LEU:HD23	2:S:518:GLU:HG3	1.85	0.58
2:S:205:ARG:NH1	2:S:206:PHE:O	2.32	0.58
2:S:303:ILE:HD11	2:S:340:GLU:HB3	1.85	0.58
2:Z:307:ILE:HG13	2:Z:308:THR:HG23	1.85	0.58
2:V:298:GLN:OE1	2:V:300:GLU:CD	2.42	0.58
1:C:132:ILE:HD11	1:D:505:LEU:HD23	1.86	0.58
1:H:380:PRO:HD3	3:H:801:BTI:C6	2.29	0.58
2:V:28:LEU:CD1	2:V:317:LEU:HD21	2.34	0.58
2:X:28:LEU:CD1	2:X:317:LEU:HD21	2.34	0.58
2:X:641:ASP:OD2	2:X:664:LEU:HD23	2.04	0.58
2:Z:641:ASP:OD2	2:Z:664:LEU:HD23	2.04	0.58
2:S:364:GLU:OE2	2:S:540:ILE:HD11	2.04	0.57
2:Z:28:LEU:CD1	2:Z:317:LEU:HD21	2.34	0.57
2:V:364:GLU:OE2	2:V:540:ILE:HD11	2.04	0.57
2:Z:298:GLN:OE1	2:Z:300:GLU:CD	2.42	0.57
1:G:505:LEU:HD23	1:H:132:ILE:HD11	1.87	0.57
2:V:173:ARG:NH2	2:V:191:GLU:OE1	2.37	0.57
2:X:10:LEU:HD11	2:X:35:VAL:HG13	1.85	0.57
2:S:173:ARG:NH2	2:S:191:GLU:OE1	2.37	0.57
2:S:298:GLN:OE1	2:S:300:GLU:CD	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:14:ARG:HD3	2:V:386:TYR:CE1	2.40	0.57
2:V:641:ASP:OD2	2:V:664:LEU:HD23	2.04	0.57
2:X:298:GLN:OE1	2:X:300:GLU:CD	2.42	0.57
2:S:307:ILE:HG13	2:S:308:THR:HG23	1.85	0.57
1:E:298:ARG:NH2	1:E:312:GLU:OE1	2.38	0.57
2:V:158:PRO:HB2	2:V:206:PHE:HD2	1.70	0.57
2:V:376:ILE:HD12	2:V:390:ILE:HA	1.87	0.57
2:Z:364:GLU:OE2	2:Z:540:ILE:HD11	2.04	0.57
1:F:481:ARG:HG2	1:G:70:GLU:OE1	2.05	0.57
1:G:298:ARG:NH2	1:G:312:GLU:OE1	2.38	0.57
1:H:298:ARG:NH2	1:H:312:GLU:OE1	2.38	0.57
2:Z:173:ARG:NH2	2:Z:191:GLU:OE1	2.37	0.57
2:X:376:ILE:HD12	2:X:390:ILE:HA	1.87	0.57
2:Z:10:LEU:HD11	2:Z:35:VAL:HG13	1.85	0.57
2:Z:14:ARG:HD3	2:Z:386:TYR:CE1	2.40	0.57
2:Z:158:PRO:HB2	2:Z:206:PHE:HD2	1.70	0.57
2:X:14:ARG:HD3	2:X:386:TYR:CE1	2.40	0.56
2:X:158:PRO:HB2	2:X:206:PHE:HD2	1.70	0.56
2:Z:376:ILE:HD12	2:Z:390:ILE:HA	1.87	0.56
1:C:298:ARG:NH2	1:C:312:GLU:OE1	2.38	0.56
1:C:481:ARG:HG2	1:E:70:GLU:OE1	2.04	0.56
2:S:14:ARG:HD3	2:S:386:TYR:CE1	2.40	0.56
2:S:158:PRO:HB2	2:S:206:PHE:HD2	1.70	0.56
2:X:364:GLU:OE2	2:X:540:ILE:HD11	2.04	0.56
1:D:70:GLU:OE1	1:E:481:ARG:HG2	2.05	0.56
1:F:132:ILE:HD11	1:H:505:LEU:HD23	1.87	0.56
1:F:505:LEU:HD23	1:G:132:ILE:HD11	1.87	0.56
2:S:376:ILE:HD12	2:S:390:ILE:HA	1.87	0.56
2:X:173:ARG:NH2	2:X:191:GLU:OE1	2.37	0.56
2:Z:255:THR:O	2:Z:259:MET:HG2	2.06	0.56
2:S:255:THR:O	2:S:259:MET:HG2	2.06	0.56
2:S:641:ASP:OD2	2:S:664:LEU:HD23	2.04	0.56
2:S:158:PRO:HD2	2:S:206:PHE:O	2.06	0.56
2:V:644:VAL:HG12	2:V:664:LEU:HG	1.88	0.56
1:F:378:PHE:O	3:F:801:BTI:H5	2.04	0.56
2:V:158:PRO:HD2	2:V:206:PHE:O	2.06	0.56
2:X:255:THR:O	2:X:259:MET:HG2	2.06	0.56
1:D:298:ARG:NH2	1:D:312:GLU:OE1	2.38	0.56
1:F:298:ARG:NH2	1:F:312:GLU:OE1	2.38	0.56
2:S:644:VAL:HG12	2:S:664:LEU:HG	1.88	0.56
2:Z:355:SER:HB3	2:Z:358:ARG:CZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:644:VAL:HG12	2:X:664:LEU:HG	1.88	0.56
2:S:160:MET:HB2	2:S:206:PHE:HB2	1.88	0.56
2:V:255:THR:O	2:V:259:MET:HG2	2.06	0.56
2:V:306:GLU:HB3	2:V:396:TRP:HD1	1.71	0.56
2:V:355:SER:HB3	2:V:358:ARG:CZ	2.36	0.56
2:V:479:ARG:NH1	2:V:488:PRO:O	2.39	0.56
2:X:355:SER:HB3	2:X:358:ARG:CZ	2.36	0.56
2:Z:644:VAL:HG12	2:Z:664:LEU:HG	1.88	0.56
2:X:160:MET:HB2	2:X:206:PHE:HB2	1.88	0.55
2:Z:479:ARG:NH1	2:Z:488:PRO:O	2.39	0.55
2:X:161:ILE:O	2:X:172:MET:HA	2.06	0.55
2:Z:158:PRO:HB2	2:Z:206:PHE:CD2	2.41	0.55
2:Z:161:ILE:O	2:Z:172:MET:HA	2.06	0.55
1:G:481:ARG:HG2	1:H:70:GLU:OE1	2.06	0.55
2:X:158:PRO:HB2	2:X:206:PHE:CD2	2.41	0.55
2:X:158:PRO:HD2	2:X:206:PHE:O	2.06	0.55
2:Z:158:PRO:HD2	2:Z:206:PHE:O	2.06	0.55
2:Z:160:MET:HB2	2:Z:206:PHE:HB2	1.88	0.55
2:S:355:SER:HB3	2:S:358:ARG:CZ	2.36	0.55
2:S:479:ARG:NH1	2:S:488:PRO:O	2.39	0.55
2:V:432:GLU:HG3	2:V:434:ARG:H	1.71	0.55
2:X:479:ARG:NH1	2:X:488:PRO:O	2.39	0.55
2:X:337:HIS:CE1	2:X:400:ARG:HD2	2.42	0.55
2:S:306:GLU:HB3	2:S:396:TRP:HD1	1.71	0.55
2:S:348:PRO:HA	2:S:352:TYR:CD1	2.40	0.55
2:X:306:GLU:HB3	2:X:396:TRP:HD1	1.71	0.55
1:F:70:GLU:OE1	1:H:481:ARG:HG2	2.06	0.55
2:S:161:ILE:O	2:S:172:MET:HA	2.06	0.55
2:V:158:PRO:HB2	2:V:206:PHE:CD2	2.41	0.55
2:Z:337:HIS:CE1	2:Z:400:ARG:HD2	2.42	0.55
2:Z:432:GLU:HG3	2:Z:434:ARG:H	1.71	0.55
2:S:215:ILE:HD13	2:S:259:MET:HB3	1.89	0.55
2:X:215:ILE:HD13	2:X:259:MET:HB3	1.89	0.55
1:D:296:ASP:OD1	1:D:339:GLN:NE2	2.40	0.55
2:S:337:HIS:CE1	2:S:400:ARG:HD2	2.42	0.55
2:S:432:GLU:HG3	2:S:434:ARG:H	1.71	0.55
2:V:161:ILE:O	2:V:172:MET:HA	2.06	0.55
2:S:33:VAL:HG13	2:S:51:GLU:HB2	1.90	0.54
2:X:611:LYS:HG2	2:X:623:GLU:HG2	1.89	0.54
2:Z:611:LYS:HG2	2:Z:623:GLU:HG2	1.89	0.54
2:Z:306:GLU:HB3	2:Z:396:TRP:HD1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:606:VAL:O	2:Z:627:LEU:HA	2.07	0.54
1:F:296:ASP:OD1	1:F:339:GLN:NE2	2.40	0.54
2:V:160:MET:HB2	2:V:206:PHE:HB2	1.88	0.54
2:V:606:VAL:O	2:V:627:LEU:HA	2.08	0.54
2:Z:215:ILE:HD13	2:Z:259:MET:HB3	1.89	0.54
1:H:296:ASP:OD1	1:H:339:GLN:NE2	2.40	0.54
2:V:337:HIS:CE1	2:V:400:ARG:HD2	2.42	0.54
2:Z:33:VAL:HG13	2:Z:51:GLU:HB2	1.90	0.54
2:V:33:VAL:HG13	2:V:51:GLU:HB2	1.89	0.54
2:V:159:VAL:HG13	2:V:161:ILE:H	1.73	0.54
2:V:611:LYS:HG2	2:V:623:GLU:HG2	1.89	0.54
2:X:33:VAL:HG13	2:X:51:GLU:HB2	1.90	0.54
2:X:432:GLU:HG3	2:X:434:ARG:H	1.71	0.54
1:E:296:ASP:OD1	1:E:339:GLN:NE2	2.40	0.54
1:G:376:PRO:HB2	3:G:801:BTI:H4	1.89	0.54
2:S:159:VAL:HG13	2:S:161:ILE:H	1.73	0.54
2:S:611:LYS:HG2	2:S:623:GLU:HG2	1.89	0.54
2:X:399:ASP:HB2	2:X:402:GLU:HG2	1.89	0.54
2:X:606:VAL:O	2:X:627:LEU:HA	2.08	0.54
2:S:158:PRO:HB2	2:S:206:PHE:CD2	2.41	0.54
2:V:97:SER:O	2:V:101:LYS:HG2	2.08	0.54
2:V:348:PRO:HA	2:V:352:TYR:CD1	2.40	0.54
2:X:159:VAL:HG13	2:X:161:ILE:H	1.73	0.54
2:S:606:VAL:O	2:S:627:LEU:HA	2.08	0.54
2:V:399:ASP:HB2	2:V:402:GLU:HG2	1.89	0.54
2:Z:399:ASP:HB2	2:Z:402:GLU:HG2	1.89	0.54
2:S:9:VAL:HA	2:S:81:ALA:O	2.08	0.54
2:Z:159:VAL:HG13	2:Z:161:ILE:H	1.73	0.54
2:V:86:TYR:HD2	2:V:296:ARG:HD3	1.73	0.53
1:C:296:ASP:OD1	1:C:339:GLN:NE2	2.40	0.53
1:G:296:ASP:OD1	1:G:339:GLN:NE2	2.40	0.53
2:V:109:PRO:HB3	2:V:272:TYR:HE1	1.73	0.53
2:X:86:TYR:HD2	2:X:296:ARG:HD3	1.73	0.53
2:S:97:SER:O	2:S:101:LYS:HG2	2.08	0.53
2:Z:86:TYR:HD2	2:Z:296:ARG:HD3	1.73	0.53
2:Z:152:ALA:HA	2:Z:157:TYR:CE1	2.44	0.53
2:S:152:ALA:HA	2:S:157:TYR:CE1	2.44	0.53
2:V:9:VAL:HA	2:V:81:ALA:O	2.08	0.53
2:V:215:ILE:HD13	2:V:259:MET:HB3	1.89	0.53
2:X:97:SER:O	2:X:101:LYS:HG2	2.08	0.53
2:X:152:ALA:HA	2:X:157:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:159:VAL:CB	2:Z:175:ALA:HB3	2.39	0.53
2:S:399:ASP:HB2	2:S:402:GLU:HG2	1.89	0.53
2:S:553:GLN:HB2	2:S:565:GLN:HB3	1.91	0.53
2:Z:221:ARG:HG2	2:Z:273:VAL:HG13	1.90	0.53
2:Z:348:PRO:HA	2:Z:352:TYR:CD1	2.40	0.53
2:Z:553:GLN:HB2	2:Z:565:GLN:HB3	1.91	0.53
1:D:140:ASN:ND2	1:D:189:PRO:HG3	2.24	0.52
2:V:221:ARG:HG2	2:V:273:VAL:HG13	1.90	0.52
2:X:348:PRO:HA	2:X:352:TYR:CD1	2.40	0.52
2:Z:97:SER:O	2:Z:101:LYS:HG2	2.08	0.52
1:F:140:ASN:ND2	1:F:189:PRO:HG3	2.25	0.52
2:S:623:GLU:HA	2:S:637:HIS:HD2	1.75	0.52
2:X:553:GLN:HB2	2:X:565:GLN:HB3	1.91	0.52
2:Z:598:GLN:HA	2:Z:663:GLU:HA	1.92	0.52
2:S:10:LEU:O	2:S:82:VAL:HG13	2.10	0.52
2:S:159:VAL:CB	2:S:175:ALA:HB3	2.39	0.52
2:V:10:LEU:O	2:V:82:VAL:HG13	2.09	0.52
2:X:159:VAL:CB	2:X:175:ALA:HB3	2.39	0.52
2:X:598:GLN:HA	2:X:663:GLU:HA	1.92	0.52
2:Z:9:VAL:HA	2:Z:81:ALA:O	2.08	0.52
2:V:541:ILE:HD11	2:V:554:PHE:HB2	1.92	0.52
2:X:623:GLU:HA	2:X:637:HIS:HD2	1.75	0.52
2:Z:10:LEU:O	2:Z:82:VAL:HG13	2.10	0.52
1:E:381:GLY:HA3	1:E:383:GLN:HE22	1.75	0.52
2:S:541:ILE:HD11	2:S:554:PHE:HB2	1.92	0.52
2:V:159:VAL:CB	2:V:175:ALA:HB3	2.39	0.52
2:X:221:ARG:HG2	2:X:273:VAL:HG13	1.90	0.52
2:Z:623:GLU:HA	2:Z:637:HIS:HD2	1.75	0.52
1:C:140:ASN:ND2	1:C:189:PRO:HG3	2.24	0.52
2:V:152:ALA:HA	2:V:157:TYR:CE1	2.44	0.52
1:G:140:ASN:ND2	1:G:189:PRO:HG3	2.25	0.52
2:S:86:TYR:HD2	2:S:296:ARG:HD3	1.73	0.52
2:X:9:VAL:HA	2:X:81:ALA:O	2.08	0.52
2:Z:109:PRO:HB3	2:Z:272:TYR:HE1	1.73	0.52
2:Z:237:ARG:HG2	2:Z:238:ARG:HG2	1.92	0.52
1:H:140:ASN:ND2	1:H:189:PRO:HG3	2.24	0.52
2:V:623:GLU:HA	2:V:637:HIS:HD2	1.75	0.52
2:X:10:LEU:O	2:X:82:VAL:HG13	2.09	0.52
1:H:189:PRO:O	1:H:192:THR:OG1	2.26	0.52
2:X:237:ARG:HG2	2:X:238:ARG:HG2	1.92	0.52
1:H:439:ALA:O	1:H:476:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:109:PRO:HB3	2:S:272:TYR:HE1	1.73	0.52
2:V:598:GLN:HA	2:V:663:GLU:HA	1.92	0.52
1:E:439:ALA:O	1:E:476:PRO:HD3	2.10	0.51
1:H:381:GLY:HA3	1:H:383:GLN:HE22	1.75	0.51
2:S:221:ARG:HG2	2:S:273:VAL:HG13	1.90	0.51
2:X:541:ILE:HD11	2:X:554:PHE:HB2	1.92	0.51
1:F:381:GLY:HA3	1:F:383:GLN:HE22	1.75	0.51
2:S:315:GLN:HB3	2:S:325:LEU:HD22	1.92	0.51
1:E:189:PRO:O	1:E:192:THR:OG1	2.26	0.51
2:V:252:ASP:OD1	2:V:252:ASP:N	2.43	0.51
2:V:553:GLN:HB2	2:V:565:GLN:HB3	1.91	0.51
2:X:109:PRO:HB3	2:X:272:TYR:HE1	1.73	0.51
2:X:623:GLU:HA	2:X:637:HIS:CD2	2.46	0.51
2:Z:541:ILE:HD11	2:Z:554:PHE:HB2	1.92	0.51
1:D:381:GLY:HA3	1:D:383:GLN:HE22	1.75	0.51
2:S:226:VAL:HA	2:S:329:GLN:NE2	2.26	0.51
2:S:598:GLN:HA	2:S:663:GLU:HA	1.92	0.51
2:Z:623:GLU:HA	2:Z:637:HIS:CD2	2.46	0.51
1:E:140:ASN:ND2	1:E:189:PRO:HG3	2.25	0.51
2:S:277:THR:HG22	2:S:294:ASN:HB3	1.93	0.51
2:S:623:GLU:HA	2:S:637:HIS:CD2	2.46	0.51
2:V:315:GLN:HB3	2:V:325:LEU:HD22	1.92	0.51
2:V:226:VAL:HA	2:V:329:GLN:NE2	2.26	0.51
1:D:283:LEU:HD21	1:D:303:PRO:HG2	1.93	0.51
1:F:283:LEU:HD21	1:F:303:PRO:HG2	1.93	0.51
1:F:378:PHE:O	3:F:801:BTI:N3	2.43	0.51
1:H:457:GLU:OE2	1:H:465:ARG:NH2	2.44	0.51
2:V:623:GLU:HA	2:V:637:HIS:CD2	2.46	0.51
2:Z:226:VAL:HA	2:Z:329:GLN:NE2	2.26	0.51
1:F:439:ALA:O	1:F:476:PRO:HD3	2.10	0.51
1:G:381:GLY:HA3	1:G:383:GLN:HE22	1.75	0.51
1:G:439:ALA:O	1:G:476:PRO:HD3	2.10	0.51
2:S:237:ARG:HG2	2:S:238:ARG:HG2	1.92	0.51
2:V:157:TYR:CG	2:V:205:ARG:HA	2.46	0.51
2:V:277:THR:HG22	2:V:294:ASN:HB3	1.93	0.51
2:X:157:TYR:CG	2:X:205:ARG:HA	2.46	0.51
2:X:226:VAL:HA	2:X:329:GLN:NE2	2.26	0.51
2:Z:75:LYS:CE	2:Z:102:ASN:HD21	2.24	0.51
1:C:439:ALA:O	1:C:476:PRO:HD3	2.10	0.51
1:F:292:LYS:HE2	2:S:631:LYS:HA	1.93	0.51
1:F:457:GLU:OE2	1:F:465:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:21:VAL:O	2:V:24:THR:HG22	2.11	0.51
2:V:160:MET:HB3	2:V:204:GLU:O	2.11	0.51
2:Z:157:TYR:CG	2:Z:205:ARG:HA	2.46	0.51
1:E:457:GLU:OE2	1:E:465:ARG:NH2	2.44	0.50
2:V:75:LYS:CE	2:V:102:ASN:HD21	2.24	0.50
2:V:76:LYS:N	2:V:76:LYS:HD2	2.27	0.50
2:V:237:ARG:HG2	2:V:238:ARG:HG2	1.92	0.50
2:X:75:LYS:CE	2:X:102:ASN:HD21	2.24	0.50
2:Z:277:THR:HG22	2:Z:294:ASN:HB3	1.93	0.50
2:S:160:MET:SD	2:S:206:PHE:HD1	2.34	0.50
2:X:277:THR:HG22	2:X:294:ASN:HB3	1.93	0.50
2:Z:160:MET:SD	2:Z:206:PHE:HD1	2.34	0.50
1:D:189:PRO:O	1:D:192:THR:OG1	2.26	0.50
1:D:439:ALA:O	1:D:476:PRO:HD3	2.10	0.50
2:V:160:MET:SD	2:V:206:PHE:HD1	2.34	0.50
2:V:428:ASP:OD2	2:V:449:TYR:OH	2.28	0.50
1:C:292:LYS:HE2	2:V:631:LYS:HA	1.92	0.50
2:S:75:LYS:CE	2:S:102:ASN:HD21	2.24	0.50
2:X:21:VAL:O	2:X:24:THR:HG22	2.11	0.50
1:C:380:PRO:HD3	3:V:801:BTI:H63	1.94	0.50
2:S:10:LEU:HB3	2:S:82:VAL:HG22	1.93	0.50
2:V:10:LEU:HB3	2:V:82:VAL:HG22	1.93	0.50
2:X:76:LYS:N	2:X:76:LYS:HD2	2.27	0.50
2:Z:315:GLN:HB3	2:Z:325:LEU:HD22	1.92	0.50
1:C:193:ASP:OD1	1:H:519:ASN:ND2	2.45	0.50
1:D:457:GLU:OE2	1:D:465:ARG:NH2	2.44	0.50
2:S:160:MET:HB3	2:S:204:GLU:O	2.12	0.50
2:S:287:GLN:N	2:S:287:GLN:OE1	2.44	0.50
2:X:160:MET:SD	2:X:206:PHE:HD1	2.34	0.50
2:Z:287:GLN:N	2:Z:287:GLN:OE1	2.44	0.50
1:H:283:LEU:HD21	1:H:303:PRO:HG2	1.93	0.50
2:S:76:LYS:HD2	2:S:76:LYS:N	2.27	0.50
2:X:247:PRO:HD2	2:X:337:HIS:HB2	1.94	0.50
2:X:287:GLN:N	2:X:287:GLN:OE1	2.44	0.50
2:X:315:GLN:HB3	2:X:325:LEU:HD22	1.92	0.50
2:Z:21:VAL:O	2:Z:24:THR:HG22	2.11	0.50
1:C:381:GLY:HA3	1:C:383:GLN:HE22	1.75	0.50
2:S:21:VAL:O	2:S:24:THR:HG22	2.11	0.50
2:S:157:TYR:CG	2:S:205:ARG:HA	2.46	0.50
2:S:247:PRO:HD2	2:S:337:HIS:HB2	1.94	0.50
2:S:277:THR:CG2	2:S:294:ASN:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:247:PRO:HD2	2:V:337:HIS:HB2	1.94	0.50
2:Z:247:PRO:HD2	2:Z:337:HIS:HB2	1.94	0.50
1:C:283:LEU:HD21	1:C:303:PRO:HG2	1.93	0.50
2:S:158:PRO:O	2:S:159:VAL:HG12	2.12	0.50
2:S:159:VAL:HG13	2:S:161:ILE:N	2.27	0.50
1:C:519:ASN:ND2	1:H:193:ASP:OD1	2.45	0.49
1:G:283:LEU:HD21	1:G:303:PRO:HG2	1.93	0.49
2:V:158:PRO:O	2:V:159:VAL:HG12	2.12	0.49
2:V:277:THR:CG2	2:V:294:ASN:HB3	2.42	0.49
2:X:34:ALA:O	2:X:52:SER:HA	2.12	0.49
1:H:211:VAL:O	1:H:215:VAL:HG12	2.12	0.49
2:Z:76:LYS:HD2	2:Z:76:LYS:N	2.27	0.49
1:E:283:LEU:HD21	1:E:303:PRO:HG2	1.93	0.49
1:F:189:PRO:O	1:F:192:THR:OG1	2.26	0.49
2:X:157:TYR:CB	2:X:205:ARG:HA	2.42	0.49
2:Z:34:ALA:O	2:Z:52:SER:HA	2.13	0.49
1:C:457:GLU:OE2	1:C:465:ARG:NH2	2.44	0.49
1:E:292:LYS:HE2	2:X:631:LYS:HA	1.93	0.49
2:V:157:TYR:CB	2:V:205:ARG:HA	2.42	0.49
2:X:10:LEU:HB3	2:X:82:VAL:HG22	1.93	0.49
2:X:160:MET:HB3	2:X:204:GLU:O	2.11	0.49
2:Z:601:SER:O	2:Z:658:ASN:ND2	2.39	0.49
1:E:519:ASN:ND2	1:G:193:ASP:OD1	2.45	0.49
1:G:457:GLU:OE2	1:G:465:ARG:NH2	2.44	0.49
2:S:601:SER:O	2:S:658:ASN:ND2	2.39	0.49
1:E:132:ILE:HG22	1:E:134:VAL:HG23	1.95	0.49
2:Z:10:LEU:HB3	2:Z:82:VAL:HG22	1.93	0.49
2:Z:159:VAL:HG13	2:Z:161:ILE:N	2.27	0.49
2:Z:160:MET:HB3	2:Z:204:GLU:O	2.11	0.49
2:S:34:ALA:O	2:S:52:SER:HA	2.13	0.49
2:X:159:VAL:HG13	2:X:161:ILE:N	2.27	0.49
2:X:601:SER:O	2:X:658:ASN:ND2	2.39	0.49
2:Z:157:TYR:CB	2:Z:205:ARG:HA	2.42	0.49
1:C:397:LEU:HD21	1:H:161:PHE:HB3	1.95	0.49
1:H:132:ILE:HG22	1:H:134:VAL:HG23	1.95	0.49
2:V:34:ALA:O	2:V:52:SER:HA	2.13	0.49
1:E:211:VAL:O	1:E:215:VAL:HG12	2.13	0.49
2:S:303:ILE:HG23	2:S:338:ALA:HB3	1.95	0.49
2:V:59:ALA:HB3	2:V:62:GLU:OE2	2.13	0.49
2:V:287:GLN:OE1	2:V:287:GLN:N	2.44	0.49
1:E:193:ASP:OD1	1:G:519:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:ARG:HG2	1:G:48:THR:HG22	1.95	0.49
1:H:292:LYS:HE2	2:Z:631:LYS:HA	1.93	0.49
2:S:216:GLN:OE1	2:S:231:ARG:NH1	2.45	0.49
2:S:428:ASP:OD2	2:S:449:TYR:OH	2.28	0.49
2:V:303:ILE:HG23	2:V:338:ALA:HB3	1.95	0.49
2:S:88:PHE:HB3	2:S:89:LEU:HD23	1.95	0.48
2:V:88:PHE:HB3	2:V:89:LEU:HD23	1.95	0.48
2:V:159:VAL:HG13	2:V:161:ILE:N	2.27	0.48
2:Z:88:PHE:HB3	2:Z:89:LEU:HD23	1.95	0.48
1:F:211:VAL:O	1:F:215:VAL:HG12	2.12	0.48
1:G:132:ILE:HG22	1:G:134:VAL:HG23	1.95	0.48
2:S:157:TYR:CB	2:S:205:ARG:HA	2.42	0.48
2:Z:158:PRO:O	2:Z:159:VAL:HG12	2.12	0.48
1:C:41:ARG:HG2	1:C:48:THR:HG22	1.96	0.48
1:C:151:VAL:HG12	1:H:484:PHE:HE2	1.77	0.48
2:X:301:HIS:O	2:X:302:PRO:C	2.51	0.48
2:Z:428:ASP:OD2	2:Z:449:TYR:OH	2.28	0.48
1:D:211:VAL:O	1:D:215:VAL:HG12	2.13	0.48
1:G:211:VAL:O	1:G:215:VAL:HG12	2.13	0.48
2:X:277:THR:CG2	2:X:294:ASN:HB3	2.42	0.48
1:E:151:VAL:HG12	1:G:484:PHE:HE2	1.78	0.48
1:F:41:ARG:HG2	1:F:48:THR:HG22	1.96	0.48
2:S:360:THR:O	2:S:361:MET:C	2.52	0.48
2:Z:277:THR:CG2	2:Z:294:ASN:HB3	2.42	0.48
1:C:132:ILE:HG22	1:C:134:VAL:HG23	1.95	0.48
1:C:211:VAL:O	1:C:215:VAL:HG12	2.13	0.48
2:S:655:VAL:HG13	2:S:656:GLU:H	1.79	0.48
2:V:655:VAL:HG13	2:V:656:GLU:H	1.79	0.48
2:X:59:ALA:HB3	2:X:62:GLU:OE2	2.13	0.48
2:X:88:PHE:HB3	2:X:89:LEU:HD23	1.95	0.48
2:X:158:PRO:O	2:X:159:VAL:HG12	2.12	0.48
2:X:160:MET:CE	2:X:206:PHE:HA	2.44	0.48
2:X:428:ASP:OD2	2:X:449:TYR:OH	2.28	0.48
2:Z:301:HIS:O	2:Z:302:PRO:C	2.51	0.48
1:D:519:ASN:ND2	1:F:193:ASP:OD1	2.47	0.48
2:S:308:THR:HB	2:S:310:VAL:HG23	1.96	0.48
2:Z:160:MET:CE	2:Z:206:PHE:HA	2.44	0.48
1:D:132:ILE:HG22	1:D:134:VAL:HG23	1.95	0.48
1:D:428:LEU:HA	1:F:162:LEU:HD12	1.95	0.48
2:S:160:MET:CE	2:S:206:PHE:HA	2.44	0.48
2:Z:59:ALA:HB3	2:Z:62:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:136:PRO:HD3	2:Z:289:TYR:HE1	1.79	0.48
1:D:41:ARG:HG2	1:D:48:THR:HG22	1.96	0.48
2:X:136:PRO:HD3	2:X:289:TYR:HE1	1.79	0.48
2:Z:303:ILE:HG23	2:Z:338:ALA:HB3	1.95	0.48
1:D:193:ASP:OD1	1:F:519:ASN:ND2	2.47	0.47
1:E:397:LEU:HD21	1:G:161:PHE:HB3	1.96	0.47
2:S:366:THR:HG22	2:S:414:TYR:HD1	1.80	0.47
2:X:283:ASN:ND2	2:X:285:GLN:OE1	2.47	0.47
1:D:162:LEU:HD12	1:F:428:LEU:HA	1.95	0.47
1:E:41:ARG:HG2	1:E:48:THR:HG22	1.96	0.47
1:E:161:PHE:HB3	1:G:397:LEU:HD21	1.96	0.47
2:V:25:CYS:O	2:V:29:GLY:N	2.47	0.47
2:X:655:VAL:HG13	2:X:656:GLU:H	1.79	0.47
2:Z:25:CYS:O	2:Z:29:GLY:N	2.47	0.47
2:Z:216:GLN:OE1	2:Z:231:ARG:NH1	2.45	0.47
1:D:401:ALA:HB3	1:F:165:THR:HG21	1.96	0.47
2:S:241:LYS:HD2	2:S:300:GLU:OE1	2.14	0.47
2:X:303:ILE:HG23	2:X:338:ALA:HB3	1.95	0.47
2:Z:117:MET:CE	2:Z:270:VAL:HG21	2.44	0.47
1:F:132:ILE:HG22	1:F:134:VAL:HG23	1.95	0.47
2:V:159:VAL:HG12	2:V:175:ALA:H	1.79	0.47
2:V:160:MET:CE	2:V:206:PHE:HA	2.44	0.47
2:Z:283:ASN:ND2	2:Z:285:GLN:OE1	2.47	0.47
1:C:214:ALA:HB1	3:H:801:BTI:H11	1.96	0.47
1:D:151:VAL:HG12	1:F:484:PHE:HE2	1.79	0.47
2:V:283:ASN:ND2	2:V:285:GLN:OE1	2.47	0.47
2:V:360:THR:O	2:V:361:MET:C	2.52	0.47
2:V:366:THR:HG22	2:V:414:TYR:HD1	1.79	0.47
2:V:601:SER:O	2:V:658:ASN:ND2	2.39	0.47
2:X:132:VAL:CG1	2:X:290:PHE:HD2	2.28	0.47
2:Z:132:VAL:CG1	2:Z:290:PHE:HD2	2.27	0.47
2:Z:655:VAL:HG13	2:Z:656:GLU:H	1.79	0.47
1:E:114:LEU:HD22	1:E:157:TYR:CE1	2.50	0.47
2:S:132:VAL:CG1	2:S:290:PHE:HD2	2.28	0.47
2:V:534:TRP:CD1	2:V:541:ILE:HG12	2.50	0.47
2:Z:655:VAL:HG13	2:Z:656:GLU:N	2.30	0.47
1:D:397:LEU:HD12	1:D:422:VAL:HG22	1.97	0.47
1:E:461:GLN:HA	1:E:464:GLN:HE22	1.80	0.47
1:E:484:PHE:HE2	1:G:151:VAL:HG12	1.79	0.47
1:G:461:GLN:HA	1:G:464:GLN:HE22	1.80	0.47
1:H:41:ARG:HG2	1:H:48:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:LEU:HD22	1:H:157:TYR:CE1	2.50	0.47
1:H:397:LEU:HD12	1:H:422:VAL:HG22	1.97	0.47
2:S:136:PRO:HD3	2:S:289:TYR:HE1	1.79	0.47
2:S:211:ARG:NH2	2:S:248:SER:HB3	2.29	0.47
2:S:283:ASN:ND2	2:S:285:GLN:OE1	2.47	0.47
2:S:534:TRP:CD1	2:S:541:ILE:HG12	2.50	0.47
2:V:33:VAL:HG22	2:V:51:GLU:HB2	1.96	0.47
2:V:132:VAL:CG1	2:V:290:PHE:HD2	2.27	0.47
2:V:301:HIS:O	2:V:302:PRO:C	2.51	0.47
2:V:655:VAL:HG13	2:V:656:GLU:N	2.30	0.47
2:X:25:CYS:O	2:X:29:GLY:N	2.47	0.47
2:X:216:GLN:OE1	2:X:231:ARG:NH1	2.45	0.47
2:X:534:TRP:CD1	2:X:541:ILE:HG12	2.50	0.47
2:X:655:VAL:HG13	2:X:656:GLU:N	2.30	0.47
2:Z:241:LYS:HD2	2:Z:300:GLU:OE1	2.14	0.47
2:Z:366:THR:HG22	2:Z:414:TYR:HD1	1.79	0.47
1:C:461:GLN:HA	1:C:464:GLN:HE22	1.80	0.47
1:D:278:ARG:NH1	1:D:303:PRO:O	2.40	0.47
1:E:397:LEU:HD12	1:E:422:VAL:HG22	1.97	0.47
2:V:278:VAL:HA	2:V:293:MET:HG2	1.97	0.47
2:X:159:VAL:HG12	2:X:175:ALA:H	1.79	0.47
2:Z:534:TRP:CD1	2:Z:541:ILE:HG12	2.50	0.47
1:F:278:ARG:NH1	1:F:303:PRO:O	2.40	0.47
1:G:114:LEU:HD22	1:G:157:TYR:CE1	2.50	0.47
1:G:189:PRO:O	1:G:192:THR:OG1	2.26	0.47
2:S:25:CYS:O	2:S:29:GLY:N	2.47	0.47
2:S:278:VAL:HA	2:S:293:MET:HG2	1.97	0.47
2:S:655:VAL:HG13	2:S:656:GLU:N	2.30	0.47
2:V:136:PRO:HD3	2:V:289:TYR:HE1	1.79	0.47
2:V:158:PRO:CB	2:V:206:PHE:HB3	2.36	0.47
2:V:308:THR:HB	2:V:310:VAL:HG23	1.96	0.47
2:Z:33:VAL:HG22	2:Z:51:GLU:HB2	1.96	0.47
2:Z:129:ARG:HD3	2:Z:129:ARG:C	2.36	0.47
2:Z:278:VAL:HA	2:Z:293:MET:HG2	1.97	0.47
2:Z:308:THR:HB	2:Z:310:VAL:HG23	1.96	0.47
1:C:161:PHE:HB3	1:H:397:LEU:HD21	1.96	0.47
1:C:484:PHE:HE2	1:H:151:VAL:HG12	1.80	0.47
1:D:114:LEU:HD22	1:D:157:TYR:CE1	2.50	0.47
1:D:165:THR:HG21	1:F:401:ALA:HB3	1.97	0.47
1:H:461:GLN:HA	1:H:464:GLN:HE22	1.80	0.47
2:S:59:ALA:HB3	2:S:62:GLU:OE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:532:VAL:HG22	2:V:543:VAL:CG2	2.44	0.47
2:X:117:MET:CE	2:X:270:VAL:HG21	2.45	0.47
2:X:278:VAL:HA	2:X:293:MET:HG2	1.97	0.47
2:X:301:HIS:N	2:X:302:PRO:HD2	2.30	0.47
1:F:397:LEU:HD12	1:F:422:VAL:HG22	1.97	0.46
2:X:33:VAL:HG22	2:X:51:GLU:HB2	1.96	0.46
2:Z:301:HIS:N	2:Z:302:PRO:HD2	2.31	0.46
1:C:189:PRO:O	1:C:192:THR:OG1	2.26	0.46
1:C:428:LEU:HA	1:H:162:LEU:HD12	1.96	0.46
2:X:129:ARG:HD3	2:X:129:ARG:C	2.36	0.46
2:X:211:ARG:NH2	2:X:248:SER:HB3	2.29	0.46
2:X:366:THR:HG22	2:X:414:TYR:HD1	1.79	0.46
2:Z:159:VAL:HG12	2:Z:175:ALA:H	1.79	0.46
2:Z:211:ARG:NH2	2:Z:248:SER:HB3	2.29	0.46
1:C:114:LEU:HD22	1:C:157:TYR:CE1	2.50	0.46
1:E:428:LEU:HA	1:G:162:LEU:HD12	1.98	0.46
1:F:114:LEU:HD22	1:F:157:TYR:CE1	2.50	0.46
2:S:33:VAL:HG22	2:S:51:GLU:HB2	1.96	0.46
2:V:117:MET:CE	2:V:270:VAL:HG21	2.44	0.46
2:V:129:ARG:C	2:V:129:ARG:HD3	2.36	0.46
2:V:211:ARG:NH2	2:V:248:SER:HB3	2.29	0.46
2:S:117:MET:CE	2:S:270:VAL:HG21	2.45	0.46
2:X:241:LYS:HD2	2:X:300:GLU:OE1	2.14	0.46
2:X:308:THR:HB	2:X:310:VAL:HG23	1.96	0.46
2:V:99:LEU:HD21	2:V:106:PHE:CD1	2.51	0.46
2:V:241:LYS:HD2	2:V:300:GLU:OE1	2.14	0.46
1:C:162:LEU:HD12	1:H:428:LEU:HA	1.98	0.46
1:G:446:ALA:HA	1:G:469:TYR:CE2	2.51	0.46
2:S:301:HIS:O	2:S:302:PRO:C	2.52	0.46
1:C:446:ALA:HA	1:C:469:TYR:CE2	2.51	0.46
2:S:99:LEU:HD21	2:S:106:PHE:CD1	2.51	0.46
2:S:517:PHE:O	2:S:529:LYS:HA	2.15	0.46
2:X:158:PRO:CB	2:X:206:PHE:HB3	2.36	0.46
2:Z:517:PHE:O	2:Z:529:LYS:HA	2.15	0.46
1:F:446:ALA:HA	1:F:469:TYR:CE2	2.51	0.46
2:S:129:ARG:HD3	2:S:129:ARG:C	2.36	0.46
2:V:301:HIS:N	2:V:302:PRO:HD2	2.31	0.46
2:X:360:THR:O	2:X:361:MET:C	2.52	0.46
2:S:252:ASP:OD1	2:S:252:ASP:N	2.43	0.46
1:D:461:GLN:HA	1:D:464:GLN:HE22	1.80	0.45
1:E:162:LEU:HD12	1:G:428:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:PRO:HB3	1:E:203:TYR:CZ	2.51	0.45
1:G:397:LEU:HD12	1:G:422:VAL:HG22	1.97	0.45
1:H:180:PRO:HB3	1:H:203:TYR:CZ	2.51	0.45
1:C:397:LEU:HD12	1:C:422:VAL:HG22	1.97	0.45
1:E:446:ALA:HA	1:E:469:TYR:CE2	2.51	0.45
2:S:159:VAL:HG12	2:S:175:ALA:H	1.79	0.45
2:S:301:HIS:N	2:S:302:PRO:HD2	2.31	0.45
2:X:517:PHE:O	2:X:529:LYS:HA	2.16	0.45
2:Z:304:THR:HA	2:Z:307:ILE:HG12	1.98	0.45
1:G:180:PRO:HB3	1:G:203:TYR:CZ	2.51	0.45
2:Z:360:THR:O	2:Z:361:MET:C	2.52	0.45
1:D:397:LEU:HD21	1:F:161:PHE:HB3	1.97	0.45
1:D:446:ALA:HA	1:D:469:TYR:CE2	2.51	0.45
1:F:461:GLN:HA	1:F:464:GLN:HE22	1.80	0.45
1:H:446:ALA:HA	1:H:469:TYR:CE2	2.51	0.45
2:X:510:ARG:HB3	2:X:518:GLU:HB2	1.99	0.45
1:C:180:PRO:HB3	1:C:203:TYR:CZ	2.51	0.45
1:C:401:ALA:HB3	1:H:165:THR:HG21	1.97	0.45
1:D:151:VAL:HG13	1:D:154:LEU:HD12	1.99	0.45
1:D:484:PHE:HE2	1:F:151:VAL:HG12	1.81	0.45
1:F:151:VAL:HG13	1:F:154:LEU:HD12	1.99	0.45
2:S:142:VAL:HG11	2:S:148:LEU:HB2	1.99	0.45
2:X:304:THR:HA	2:X:307:ILE:HG12	1.98	0.45
2:Z:158:PRO:CB	2:Z:206:PHE:HB3	2.36	0.45
2:Z:510:ARG:HB3	2:Z:518:GLU:HB2	1.99	0.45
2:S:161:ILE:HG21	2:S:188:CYS:SG	2.57	0.45
1:D:161:PHE:HB3	1:F:397:LEU:HD21	1.98	0.45
1:D:180:PRO:HB3	1:D:203:TYR:CZ	2.51	0.45
2:Z:99:LEU:HD21	2:Z:106:PHE:CD1	2.51	0.45
2:S:25:CYS:HB3	2:S:30:ILE:O	2.18	0.45
2:V:75:LYS:HB2	2:V:76:LYS:NZ	2.32	0.45
2:V:517:PHE:O	2:V:529:LYS:HA	2.15	0.45
2:X:356:ILE:HG23	2:X:357:GLY:N	2.32	0.45
1:D:155:ALA:HB2	1:F:484:PHE:CZ	2.51	0.44
2:S:226:VAL:HG13	2:S:329:GLN:CG	2.46	0.44
2:V:510:ARG:HB3	2:V:518:GLU:HB2	1.99	0.44
2:X:44:LYS:HD2	2:X:377:ILE:HG23	2.00	0.44
1:E:401:ALA:HB3	1:G:165:THR:HG21	1.99	0.44
2:V:304:THR:HA	2:V:307:ILE:HG12	1.98	0.44
2:X:75:LYS:HB2	2:X:76:LYS:NZ	2.32	0.44
2:X:99:LEU:HD21	2:X:106:PHE:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:PRO:HB3	1:F:203:TYR:CZ	2.51	0.44
2:V:161:ILE:HG21	2:V:188:CYS:SG	2.57	0.44
2:V:356:ILE:HG23	2:V:357:GLY:N	2.32	0.44
2:Z:44:LYS:HD2	2:Z:377:ILE:HG23	2.00	0.44
2:Z:75:LYS:HB2	2:Z:76:LYS:NZ	2.33	0.44
2:S:356:ILE:HG23	2:S:357:GLY:N	2.32	0.44
2:S:387:ASP:OD1	2:S:387:ASP:N	2.50	0.44
2:V:356:ILE:HG13	2:V:382:ILE:HG13	2.00	0.44
2:V:536:ALA:O	2:V:538:TYR:HD1	2.01	0.44
2:X:142:VAL:HG11	2:X:148:LEU:HB2	1.99	0.44
2:Z:161:ILE:HG21	2:Z:188:CYS:SG	2.57	0.44
2:Z:356:ILE:HG23	2:Z:357:GLY:N	2.32	0.44
1:G:151:VAL:HG13	1:G:154:LEU:HD12	1.99	0.44
2:S:510:ARG:HB3	2:S:518:GLU:HB2	1.99	0.44
2:V:25:CYS:HB3	2:V:30:ILE:O	2.17	0.44
2:V:216:GLN:OE1	2:V:231:ARG:NH1	2.45	0.44
2:X:66:CYS:SG	2:X:69:LYS:HB2	2.58	0.44
2:Z:25:CYS:HB3	2:Z:30:ILE:O	2.17	0.44
2:Z:66:CYS:SG	2:Z:69:LYS:HB2	2.58	0.44
2:Z:252:ASP:N	2:Z:252:ASP:OD1	2.43	0.44
1:C:165:THR:HG21	1:H:401:ALA:HB3	1.99	0.44
2:S:66:CYS:SG	2:S:69:LYS:HB2	2.58	0.44
2:S:75:LYS:HB2	2:S:76:LYS:NZ	2.32	0.44
2:Z:142:VAL:HG11	2:Z:148:LEU:HB2	1.99	0.44
1:E:151:VAL:HG13	1:E:154:LEU:HD12	1.99	0.44
1:H:151:VAL:HG13	1:H:154:LEU:HD12	1.99	0.44
2:S:304:THR:HA	2:S:307:ILE:HG12	1.98	0.44
2:V:337:HIS:NE2	2:V:400:ARG:HA	2.32	0.44
2:X:536:ALA:O	2:X:538:TYR:HD1	2.01	0.44
1:D:426:LYS:NZ	1:D:486:ASP:OD1	2.44	0.44
2:S:356:ILE:HG13	2:S:382:ILE:HG13	2.00	0.44
2:V:142:VAL:HG11	2:V:148:LEU:HB2	1.98	0.44
2:X:161:ILE:HG21	2:X:188:CYS:SG	2.57	0.44
2:X:283:ASN:OD1	2:X:284:PRO:HD2	2.18	0.44
2:X:532:VAL:HG22	2:X:543:VAL:CG2	2.44	0.44
2:Z:298:GLN:HE21	2:Z:298:GLN:HB2	1.62	0.44
1:C:151:VAL:HG13	1:C:154:LEU:HD12	1.99	0.44
1:D:484:PHE:CZ	1:F:155:ALA:HB2	2.52	0.44
2:S:536:ALA:O	2:S:538:TYR:HD1	2.00	0.44
2:X:25:CYS:HB3	2:X:30:ILE:O	2.17	0.44
2:X:387:ASP:OD1	2:X:387:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:536:ALA:O	2:Z:538:TYR:HD1	2.01	0.44
1:C:461:GLN:HA	1:C:464:GLN:NE2	2.33	0.43
1:E:484:PHE:CZ	1:G:155:ALA:HB2	2.53	0.43
1:G:461:GLN:HA	1:G:464:GLN:NE2	2.33	0.43
2:V:66:CYS:SG	2:V:69:LYS:HB2	2.58	0.43
2:X:252:ASP:OD1	2:X:252:ASP:N	2.43	0.43
2:Z:160:MET:SD	2:Z:162:LYS:HE3	2.58	0.43
2:Z:283:ASN:OD1	2:Z:284:PRO:HD2	2.18	0.43
2:Z:544:LYS:HG3	2:Z:549:GLU:HG2	2.00	0.43
1:C:484:PHE:CZ	1:H:155:ALA:HB2	2.52	0.43
1:E:461:GLN:HA	1:E:464:GLN:NE2	2.33	0.43
1:H:454:TYR:HB3	1:H:457:GLU:HB2	2.00	0.43
2:V:44:LYS:HD2	2:V:377:ILE:HG23	2.00	0.43
2:X:160:MET:SD	2:X:162:LYS:HE3	2.58	0.43
2:X:226:VAL:HG13	2:X:329:GLN:CG	2.46	0.43
2:X:544:LYS:HG3	2:X:549:GLU:HG2	2.00	0.43
2:Z:160:MET:O	2:Z:160:MET:HG3	2.19	0.43
2:Z:528:ARG:HH12	2:Z:530:MET:HE3	1.83	0.43
1:C:92:THR:HG23	1:C:93:GLY:H	1.83	0.43
1:C:155:ALA:HB2	1:H:484:PHE:CZ	2.53	0.43
2:S:160:MET:SD	2:S:162:LYS:HE3	2.58	0.43
2:V:226:VAL:HG13	2:V:329:GLN:CG	2.46	0.43
2:X:67:ILE:O	2:X:71:VAL:HG22	2.18	0.43
2:X:160:MET:O	2:X:160:MET:HG3	2.19	0.43
2:Z:226:VAL:HG13	2:Z:329:GLN:CG	2.46	0.43
2:S:160:MET:O	2:S:160:MET:HG3	2.19	0.43
2:V:397:GLY:HA3	2:V:403:CYS:HB2	2.00	0.43
2:X:26:ARG:NE	2:X:26:ARG:HA	2.33	0.43
2:Z:19:CYS:HA	2:Z:22:MET:HG2	2.00	0.43
2:Z:532:VAL:HG22	2:Z:543:VAL:CG2	2.44	0.43
1:G:92:THR:HG23	1:G:93:GLY:H	1.83	0.43
1:G:92:THR:HG23	1:G:93:GLY:N	2.34	0.43
1:G:454:TYR:HB3	1:G:457:GLU:HB2	2.00	0.43
1:H:461:GLN:HA	1:H:464:GLN:NE2	2.33	0.43
2:S:19:CYS:HA	2:S:22:MET:HG2	2.00	0.43
2:S:597:LYS:O	2:S:664:LEU:HB2	2.19	0.43
2:V:544:LYS:HG3	2:V:549:GLU:HG2	2.00	0.43
2:V:597:LYS:O	2:V:664:LEU:HB2	2.18	0.43
2:X:337:HIS:NE2	2:X:400:ARG:HA	2.33	0.43
2:Z:26:ARG:NE	2:Z:26:ARG:HA	2.33	0.43
1:D:454:TYR:HB3	1:D:457:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:337:HIS:NE2	2:S:400:ARG:HA	2.32	0.43
2:Z:67:ILE:O	2:Z:71:VAL:HG22	2.18	0.43
2:Z:356:ILE:HG13	2:Z:382:ILE:HG13	2.00	0.43
1:C:92:THR:HG23	1:C:93:GLY:N	2.34	0.43
1:C:454:TYR:HB3	1:C:457:GLU:HB2	2.00	0.43
3:D:801:BTI:HN2	3:D:801:BTI:H72	1.73	0.43
1:E:165:THR:HG21	1:G:401:ALA:HB3	1.99	0.43
1:E:454:TYR:HB3	1:E:457:GLU:HB2	2.00	0.43
1:G:376:PRO:O	3:G:801:BTI:H4	2.19	0.43
2:S:283:ASN:OD1	2:S:284:PRO:HD2	2.18	0.43
2:V:67:ILE:O	2:V:71:VAL:HG22	2.18	0.43
2:X:301:HIS:N	2:X:302:PRO:CD	2.82	0.43
1:F:454:TYR:HB3	1:F:457:GLU:HB2	2.00	0.43
1:H:92:THR:HG23	1:H:93:GLY:N	2.34	0.43
2:S:64:TYR:HB2	2:S:88:PHE:CE1	2.54	0.43
2:S:158:PRO:CB	2:S:206:PHE:HB3	2.36	0.43
2:S:301:HIS:N	2:S:302:PRO:CD	2.82	0.43
2:V:387:ASP:OD1	2:V:387:ASP:N	2.50	0.43
2:Z:75:LYS:HE3	2:Z:102:ASN:HD21	1.84	0.43
2:Z:301:HIS:N	2:Z:302:PRO:CD	2.82	0.43
2:S:397:GLY:HA3	2:S:403:CYS:HB2	2.00	0.43
2:V:160:MET:SD	2:V:162:LYS:HE3	2.58	0.43
2:X:64:TYR:HB2	2:X:88:PHE:CE1	2.54	0.43
2:X:75:LYS:HE3	2:X:102:ASN:HD21	1.84	0.43
2:X:356:ILE:HG13	2:X:382:ILE:HG13	1.99	0.43
2:X:624:LEU:HD21	2:X:638:ALA:HB2	2.01	0.43
1:E:92:THR:HG23	1:E:93:GLY:N	2.34	0.43
1:H:92:THR:HG23	1:H:93:GLY:H	1.83	0.43
2:S:44:LYS:HD2	2:S:377:ILE:HG23	2.00	0.43
2:Z:64:TYR:HB2	2:Z:88:PHE:CE1	2.54	0.43
2:Z:337:HIS:NE2	2:Z:400:ARG:HA	2.33	0.43
1:C:214:ALA:CB	3:H:801:BTI:H11	2.49	0.42
1:E:92:THR:HG23	1:E:93:GLY:H	1.83	0.42
2:S:544:LYS:HG3	2:S:549:GLU:HG2	2.00	0.42
2:V:160:MET:O	2:V:160:MET:HG3	2.19	0.42
2:V:301:HIS:N	2:V:302:PRO:CD	2.82	0.42
2:V:328:THR:HG23	2:V:330:ASP:H	1.84	0.42
2:V:358:ARG:HB2	2:V:419:LEU:HB3	2.02	0.42
2:X:160:MET:HE2	2:X:206:PHE:HA	2.01	0.42
2:X:231:ARG:NH2	2:X:300:GLU:HB2	2.34	0.42
2:X:363:GLN:O	2:X:363:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:461:GLN:HA	1:F:464:GLN:NE2	2.33	0.42
2:S:26:ARG:NE	2:S:26:ARG:HA	2.33	0.42
2:Z:160:MET:HE2	2:Z:206:PHE:HA	2.01	0.42
2:Z:231:ARG:NH2	2:Z:300:GLU:HB2	2.34	0.42
2:Z:363:GLN:O	2:Z:363:GLN:HG3	2.19	0.42
2:Z:397:GLY:HA3	2:Z:403:CYS:HB2	2.00	0.42
1:C:237:VAL:HG22	1:H:391:ARG:HG3	2.02	0.42
1:C:278:ARG:NH1	1:C:303:PRO:O	2.40	0.42
1:E:155:ALA:HB2	1:G:484:PHE:CZ	2.53	0.42
2:S:328:THR:HG23	2:S:330:ASP:H	1.84	0.42
2:V:363:GLN:O	2:V:363:GLN:HG3	2.19	0.42
2:X:19:CYS:HA	2:X:22:MET:HG2	2.00	0.42
2:X:328:THR:HG23	2:X:330:ASP:H	1.84	0.42
2:X:597:LYS:O	2:X:664:LEU:HB2	2.18	0.42
2:Z:624:LEU:HD21	2:Z:638:ALA:HB2	2.01	0.42
2:Z:631:LYS:N	2:Z:631:LYS:HD2	2.35	0.42
1:D:461:GLN:HA	1:D:464:GLN:NE2	2.33	0.42
1:G:278:ARG:NH1	1:G:303:PRO:O	2.40	0.42
2:S:358:ARG:HB2	2:S:419:LEU:HB3	2.02	0.42
2:V:26:ARG:NE	2:V:26:ARG:HA	2.33	0.42
2:V:296:ARG:HE	2:V:296:ARG:HB3	1.75	0.42
2:X:604:PRO:HA	2:X:656:GLU:HB3	2.02	0.42
2:Z:358:ARG:HB2	2:Z:419:LEU:HB3	2.02	0.42
2:Z:597:LYS:O	2:Z:664:LEU:HB2	2.18	0.42
1:D:457:GLU:HG2	1:D:458:THR:N	2.35	0.42
1:F:92:THR:HG23	1:F:93:GLY:N	2.34	0.42
2:S:17:ILE:HG21	2:S:86:TYR:HD1	1.85	0.42
2:S:67:ILE:O	2:S:71:VAL:HG22	2.18	0.42
2:V:17:ILE:HG21	2:V:86:TYR:HD1	1.85	0.42
2:X:358:ARG:HB2	2:X:419:LEU:HB3	2.02	0.42
2:Z:604:PRO:HA	2:Z:656:GLU:HB3	2.02	0.42
1:C:475:THR:OG1	1:C:476:PRO:HD2	2.20	0.42
1:G:475:THR:OG1	1:G:476:PRO:HD2	2.20	0.42
2:S:231:ARG:NH2	2:S:300:GLU:HB2	2.34	0.42
2:X:631:LYS:HD2	2:X:631:LYS:N	2.35	0.42
2:Z:106:PHE:CE2	2:Z:108:GLY:HA3	2.55	0.42
2:Z:328:THR:HG23	2:Z:330:ASP:H	1.84	0.42
1:D:188:SER:OG	1:D:189:PRO:HD3	2.20	0.42
1:E:188:SER:OG	1:E:189:PRO:HD3	2.20	0.42
1:G:58:ASP:HB2	1:G:61:THR:OG1	2.20	0.42
1:H:188:SER:OG	1:H:189:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:28:LEU:HD13	2:S:317:LEU:HD21	2.01	0.42
2:S:631:LYS:N	2:S:631:LYS:HD2	2.35	0.42
2:V:283:ASN:OD1	2:V:284:PRO:HD2	2.18	0.42
2:V:624:LEU:HD21	2:V:638:ALA:HB2	2.01	0.42
2:V:631:LYS:HD2	2:V:631:LYS:N	2.35	0.42
2:Z:614:PRO:HA	2:Z:648:LYS:HZ3	1.83	0.42
1:C:58:ASP:HB2	1:C:61:THR:OG1	2.20	0.42
1:D:92:THR:HG23	1:D:93:GLY:N	2.34	0.42
1:F:457:GLU:HG2	1:F:458:THR:N	2.35	0.42
1:H:457:GLU:HG2	1:H:458:THR:N	2.35	0.42
2:S:153:ARG:O	2:S:154:GLU:C	2.57	0.42
2:S:572:ASP:N	2:S:572:ASP:OD1	2.53	0.42
2:V:64:TYR:HB2	2:V:88:PHE:CE1	2.54	0.42
2:V:132:VAL:HG11	2:V:290:PHE:HD2	1.85	0.42
2:X:106:PHE:CE2	2:X:108:GLY:HA3	2.55	0.42
2:X:397:GLY:HA3	2:X:403:CYS:HB2	2.00	0.42
1:E:278:ARG:NH1	1:E:303:PRO:O	2.40	0.42
1:F:188:SER:OG	1:F:189:PRO:HD3	2.20	0.42
2:S:604:PRO:HA	2:S:656:GLU:HB3	2.02	0.42
2:V:159:VAL:HG11	2:V:161:ILE:HG13	2.01	0.42
2:V:344:TYR:CE1	2:V:389:LEU:HG	2.55	0.42
2:V:512:LEU:HD23	2:V:518:GLU:CG	2.49	0.42
2:X:512:LEU:HD23	2:X:518:GLU:CG	2.49	0.42
2:Z:280:ASN:HD22	2:Z:289:TYR:H	1.68	0.42
1:D:58:ASP:HB2	1:D:61:THR:OG1	2.20	0.42
3:G:801:BTI:HN2	3:G:801:BTI:H72	1.73	0.42
1:H:58:ASP:HB2	1:H:61:THR:OG1	2.20	0.42
2:S:106:PHE:CE2	2:S:108:GLY:HA3	2.55	0.42
2:V:75:LYS:HE3	2:V:102:ASN:HD21	1.84	0.42
2:V:604:PRO:HA	2:V:656:GLU:HB3	2.02	0.42
2:X:231:ARG:HG2	2:X:246:ALA:HA	2.02	0.42
2:Z:572:ASP:OD1	2:Z:572:ASP:N	2.53	0.42
1:C:188:SER:OG	1:C:189:PRO:HD3	2.20	0.41
1:C:391:ARG:HG3	1:H:237:VAL:HG22	2.02	0.41
1:F:378:PHE:O	3:F:801:BTI:H63	2.17	0.41
1:F:475:THR:OG1	1:F:476:PRO:HD2	2.20	0.41
2:V:19:CYS:HA	2:V:22:MET:HG2	2.00	0.41
2:V:231:ARG:NH2	2:V:300:GLU:HB2	2.34	0.41
2:X:344:TYR:CE1	2:X:389:LEU:HG	2.55	0.41
1:D:269:VAL:HG22	1:D:331:ARG:HB3	2.02	0.41
1:D:475:THR:OG1	1:D:476:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ASP:HB2	1:E:61:THR:OG1	2.20	0.41
1:E:237:VAL:HG22	1:G:391:ARG:HG3	2.03	0.41
1:G:188:SER:OG	1:G:189:PRO:HD3	2.20	0.41
1:H:475:THR:OG1	1:H:476:PRO:HD2	2.20	0.41
2:S:231:ARG:HG2	2:S:246:ALA:HA	2.02	0.41
2:S:280:ASN:HD22	2:S:289:TYR:H	1.68	0.41
2:S:532:VAL:HG22	2:S:543:VAL:CG2	2.44	0.41
2:V:109:PRO:HB3	2:V:272:TYR:CE1	2.55	0.41
2:X:93:GLY:C	2:X:95:PHE:N	2.73	0.41
2:Z:44:LYS:HD3	2:Z:375:GLY:HA2	2.02	0.41
2:Z:93:GLY:C	2:Z:95:PHE:N	2.73	0.41
2:Z:153:ARG:O	2:Z:154:GLU:C	2.57	0.41
2:Z:231:ARG:HG2	2:Z:246:ALA:HA	2.01	0.41
2:Z:296:ARG:HE	2:Z:296:ARG:HB3	1.75	0.41
1:E:457:GLU:HG2	1:E:458:THR:N	2.35	0.41
1:F:58:ASP:HB2	1:F:61:THR:OG1	2.20	0.41
1:F:269:VAL:HG22	1:F:331:ARG:HB3	2.02	0.41
1:G:239:ALA:HA	1:G:314:GLN:HG3	2.03	0.41
2:S:132:VAL:HG11	2:S:290:PHE:HD2	1.85	0.41
2:S:162:LYS:O	2:S:202:LEU:HG	2.20	0.41
2:X:17:ILE:HG21	2:X:86:TYR:HD1	1.85	0.41
2:X:136:PRO:HD3	2:X:289:TYR:CE1	2.55	0.41
2:X:280:ASN:HD22	2:X:289:TYR:H	1.68	0.41
2:Z:28:LEU:HD13	2:Z:317:LEU:HD21	2.01	0.41
1:C:269:VAL:HG22	1:C:331:ARG:HB3	2.02	0.41
1:C:457:GLU:HG2	1:C:458:THR:N	2.35	0.41
1:D:376:PRO:HB2	3:D:801:BTI:C4	2.46	0.41
1:F:92:THR:HG23	1:F:93:GLY:H	1.83	0.41
1:H:380:PRO:HG3	3:H:801:BTI:H63	2.02	0.41
2:V:162:LYS:O	2:V:202:LEU:HG	2.20	0.41
2:X:572:ASP:N	2:X:572:ASP:OD1	2.53	0.41
2:Z:344:TYR:CE1	2:Z:389:LEU:HG	2.55	0.41
1:E:239:ALA:HA	1:E:314:GLN:HG3	2.03	0.41
1:E:391:ARG:HG3	1:G:237:VAL:HG22	2.03	0.41
1:F:426:LYS:NZ	1:F:486:ASP:OD1	2.44	0.41
1:G:269:VAL:HG22	1:G:331:ARG:HB3	2.02	0.41
1:G:457:GLU:HG2	1:G:458:THR:N	2.35	0.41
2:S:296:ARG:HD2	2:S:297:LEU:N	2.35	0.41
2:S:363:GLN:O	2:S:363:GLN:HG3	2.19	0.41
2:S:512:LEU:HD23	2:S:518:GLU:CG	2.49	0.41
2:S:624:LEU:HD21	2:S:638:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:280:ASN:HD22	2:V:289:TYR:H	1.68	0.41
2:X:44:LYS:HD3	2:X:375:GLY:HA2	2.02	0.41
2:X:153:ARG:O	2:X:154:GLU:C	2.57	0.41
2:Z:17:ILE:HG21	2:Z:86:TYR:HD1	1.85	0.41
2:V:92:ASN:O	2:V:96:GLN:N	2.44	0.41
2:V:106:PHE:CE2	2:V:108:GLY:HA3	2.55	0.41
2:V:136:PRO:HD3	2:V:289:TYR:CE1	2.55	0.41
3:V:801:BTI:HN2	3:V:801:BTI:H72	1.73	0.41
2:X:296:ARG:HE	2:X:296:ARG:HB3	1.75	0.41
2:X:613:GLN:C	2:X:648:LYS:HZ3	2.24	0.41
2:Z:359:LEU:HA	2:Z:380:SER:O	2.20	0.41
2:Z:512:LEU:HD23	2:Z:518:GLU:CG	2.49	0.41
1:E:475:THR:OG1	1:E:476:PRO:HD2	2.20	0.41
1:H:239:ALA:HA	1:H:314:GLN:HG3	2.03	0.41
2:S:359:LEU:HA	2:S:380:SER:O	2.20	0.41
2:V:44:LYS:HD3	2:V:375:GLY:HA2	2.02	0.41
2:X:44:LYS:O	2:X:47:LYS:HG2	2.21	0.41
2:X:417:ARG:HH21	2:X:555:TRP:HA	1.86	0.41
2:Z:44:LYS:O	2:Z:47:LYS:HG2	2.21	0.41
2:Z:296:ARG:HD2	2:Z:297:LEU:N	2.35	0.41
1:C:292:LYS:O	2:V:633:ARG:HG2	2.21	0.41
1:D:92:THR:HG23	1:D:93:GLY:H	1.83	0.41
2:S:67:ILE:HG23	2:S:68:ASP:N	2.36	0.41
2:X:109:PRO:HB3	2:X:272:TYR:CE1	2.55	0.41
2:X:160:MET:N	2:X:206:PHE:HB2	2.36	0.41
2:X:359:LEU:HA	2:X:380:SER:O	2.20	0.41
2:Z:136:PRO:HD3	2:Z:289:TYR:CE1	2.55	0.41
2:Z:162:LYS:O	2:Z:202:LEU:HG	2.20	0.41
1:C:239:ALA:HA	1:C:314:GLN:HG3	2.03	0.41
1:D:397:LEU:HD22	1:F:191:ILE:HD11	2.02	0.41
1:E:39:ASP:O	1:E:43:LYS:HG3	2.21	0.41
1:H:39:ASP:O	1:H:43:LYS:HG3	2.21	0.41
2:S:44:LYS:HD3	2:S:375:GLY:HA2	2.02	0.41
2:S:75:LYS:HE3	2:S:102:ASN:HD21	1.84	0.41
2:S:232:GLU:OE2	2:S:234:SER:HB2	2.21	0.41
2:S:344:TYR:CE1	2:S:389:LEU:HG	2.55	0.41
2:V:44:LYS:O	2:V:47:LYS:HG2	2.21	0.41
2:V:160:MET:HE2	2:V:206:PHE:HA	2.03	0.41
2:V:417:ARG:HH21	2:V:555:TRP:HA	1.86	0.41
2:X:28:LEU:HD13	2:X:317:LEU:HD21	2.01	0.41
2:X:232:GLU:OE2	2:X:234:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:646:GLU:HB3	2:X:663:GLU:HB2	2.03	0.41
2:Z:109:PRO:HB3	2:Z:272:TYR:CE1	2.55	0.41
2:Z:160:MET:N	2:Z:206:PHE:HB2	2.36	0.41
2:Z:220:ASP:OD1	2:Z:221:ARG:N	2.54	0.41
2:Z:232:GLU:OE2	2:Z:234:SER:HB2	2.21	0.41
2:Z:417:ARG:HH21	2:Z:555:TRP:HA	1.86	0.41
2:Z:646:GLU:HB3	2:Z:663:GLU:HB2	2.03	0.41
2:V:28:LEU:HD13	2:V:317:LEU:HD21	2.01	0.41
2:V:160:MET:N	2:V:206:PHE:HB2	2.36	0.41
2:V:232:GLU:OE2	2:V:234:SER:HB2	2.21	0.41
2:V:359:LEU:HA	2:V:380:SER:O	2.20	0.41
2:X:67:ILE:HG23	2:X:68:ASP:N	2.36	0.41
2:X:162:LYS:O	2:X:202:LEU:HG	2.20	0.41
2:X:220:ASP:OD1	2:X:221:ARG:N	2.54	0.41
1:D:376:PRO:HB2	3:D:801:BTI:H2	2.01	0.40
1:G:39:ASP:O	1:G:43:LYS:HG3	2.22	0.40
2:S:136:PRO:HD3	2:S:289:TYR:CE1	2.55	0.40
2:S:159:VAL:HG11	2:S:161:ILE:HG13	2.01	0.40
2:S:231:ARG:HH11	2:S:304:THR:HG23	1.87	0.40
2:S:238:ARG:O	2:S:240:GLN:NE2	2.54	0.40
2:S:530:MET:HB3	2:S:530:MET:HE2	1.90	0.40
2:V:55:ILE:CG2	2:V:69:LYS:HD3	2.51	0.40
2:V:153:ARG:O	2:V:154:GLU:C	2.57	0.40
2:V:238:ARG:O	2:V:240:GLN:NE2	2.54	0.40
2:X:216:GLN:HB2	2:X:228:LEU:HB2	2.04	0.40
2:X:296:ARG:HD2	2:X:297:LEU:N	2.36	0.40
2:Z:67:ILE:HG23	2:Z:68:ASP:N	2.36	0.40
1:C:39:ASP:O	1:C:43:LYS:HG3	2.22	0.40
1:F:41:ARG:NE	1:F:46:ARG:HE	2.12	0.40
2:S:159:VAL:CG1	2:S:175:ALA:H	2.35	0.40
2:S:623:GLU:H	2:S:623:GLU:CD	2.25	0.40
2:V:18:ALA:O	2:V:22:MET:HG2	2.22	0.40
2:V:646:GLU:HB3	2:V:663:GLU:HB2	2.03	0.40
2:X:238:ARG:O	2:X:240:GLN:NE2	2.54	0.40
2:Z:55:ILE:CG2	2:Z:69:LYS:HD3	2.51	0.40
2:Z:216:GLN:HB2	2:Z:228:LEU:HB2	2.04	0.40
2:Z:238:ARG:O	2:Z:240:GLN:NE2	2.54	0.40
1:C:41:ARG:NE	1:C:46:ARG:HE	2.12	0.40
1:E:451:LYS:HE3	1:E:451:LYS:HB3	1.92	0.40
1:H:269:VAL:HG22	1:H:331:ARG:HB3	2.02	0.40
2:S:109:PRO:HB3	2:S:272:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:611:LYS:NZ	2:S:623:GLU:HG3	2.36	0.40
2:V:231:ARG:HH11	2:V:304:THR:HG23	1.86	0.40
2:X:159:VAL:CG1	2:X:175:ALA:H	2.34	0.40
2:Z:132:VAL:HG11	2:Z:290:PHE:HD2	1.85	0.40
1:D:191:ILE:HD11	1:F:397:LEU:HD22	2.02	0.40
1:E:269:VAL:HG22	1:E:331:ARG:HB3	2.02	0.40
1:H:278:ARG:NH1	1:H:303:PRO:O	2.40	0.40
2:S:300:GLU:C	2:S:302:PRO:HD2	2.42	0.40
2:V:10:LEU:O	2:V:83:HIS:N	2.55	0.40
2:V:67:ILE:HG23	2:V:68:ASP:N	2.36	0.40
2:V:93:GLY:HA2	2:V:96:GLN:HB2	2.04	0.40
2:V:231:ARG:HG2	2:V:246:ALA:HA	2.02	0.40
2:V:282:VAL:HG22	2:V:287:GLN:O	2.22	0.40
2:X:132:VAL:HG11	2:X:290:PHE:HD2	1.85	0.40
1:F:239:ALA:HA	1:F:314:GLN:HG3	2.03	0.40
1:F:254:ARG:O	1:F:257:SER:OG	2.37	0.40
2:S:18:ALA:O	2:S:22:MET:HG2	2.22	0.40
2:S:44:LYS:O	2:S:47:LYS:HG2	2.21	0.40
2:S:160:MET:N	2:S:206:PHE:HB2	2.36	0.40
2:S:282:VAL:HG22	2:S:287:GLN:O	2.22	0.40
2:S:417:ARG:HH21	2:S:555:TRP:HA	1.86	0.40
2:V:296:ARG:HD2	2:V:297:LEU:N	2.35	0.40
2:V:300:GLU:C	2:V:302:PRO:HD2	2.42	0.40
2:X:55:ILE:CG2	2:X:69:LYS:HD3	2.51	0.40
2:X:93:GLY:HA2	2:X:96:GLN:HB2	2.04	0.40
2:Z:159:VAL:CG1	2:Z:175:ALA:H	2.34	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	C	487/489 (100%)	469 (96%)	18 (4%)	0	100	100
1	D	487/489 (100%)	469 (96%)	18 (4%)	0	100	100
1	E	487/489 (100%)	469 (96%)	18 (4%)	0	100	100
1	F	487/489 (100%)	468 (96%)	19 (4%)	0	100	100
1	G	487/489 (100%)	469 (96%)	18 (4%)	0	100	100
1	H	487/489 (100%)	469 (96%)	18 (4%)	0	100	100
2	S	655/657 (100%)	588 (90%)	66 (10%)	1 (0%)	47	81
2	V	655/657 (100%)	588 (90%)	66 (10%)	1 (0%)	47	81
2	X	655/657 (100%)	588 (90%)	66 (10%)	1 (0%)	47	81
2	Z	655/657 (100%)	588 (90%)	66 (10%)	1 (0%)	47	81
All	All	5542/5562 (100%)	5165 (93%)	373 (7%)	4 (0%)	54	86

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	539	PRO
2	V	539	PRO
2	X	539	PRO
2	Z	539	PRO

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	C	400/400 (100%)	400 (100%)	0	100	100
1	D	400/400 (100%)	400 (100%)	0	100	100
1	E	400/400 (100%)	400 (100%)	0	100	100
1	F	400/400 (100%)	400 (100%)	0	100	100
1	G	400/400 (100%)	400 (100%)	0	100	100
1	H	400/400 (100%)	400 (100%)	0	100	100
2	S	553/553 (100%)	547 (99%)	6 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	V	553/553 (100%)	547 (99%)	6 (1%)	73 84
2	X	553/553 (100%)	547 (99%)	6 (1%)	73 84
2	Z	553/553 (100%)	547 (99%)	6 (1%)	73 84
All	All	4612/4612 (100%)	4588 (100%)	24 (0%)	89 93

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	91	GLU
2	S	157	TYR
2	S	159	VAL
2	S	272	TYR
2	S	363	GLN
2	S	627	LEU
2	V	91	GLU
2	V	157	TYR
2	V	159	VAL
2	V	272	TYR
2	V	363	GLN
2	V	627	LEU
2	X	91	GLU
2	X	157	TYR
2	X	159	VAL
2	X	272	TYR
2	X	363	GLN
2	X	627	LEU
2	Z	91	GLU
2	Z	157	TYR
2	Z	159	VAL
2	Z	272	TYR
2	Z	363	GLN
2	Z	627	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	140	ASN
1	F	140	ASN
2	S	80	GLN
2	S	102	ASN

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Mol	Chain	Res	Type
2	S	271	GLN
2	S	301	HIS
2	S	329	GLN
2	S	634	ASN
2	V	80	GLN
2	V	102	ASN
2	V	271	GLN
2	V	301	HIS
2	V	329	GLN
2	V	634	ASN
2	X	80	GLN
2	X	102	ASN
2	X	271	GLN
2	X	301	HIS
2	X	329	GLN
2	X	634	ASN
2	Z	80	GLN
2	Z	102	ASN
2	Z	271	GLN
2	Z	301	HIS
2	Z	329	GLN
2	Z	634	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	V	801	-	16,16,16	1.41	2 (12%)	21,21,21	1.81	7 (33%)
3	BTI	D	801	-	16,16,16	1.42	2 (12%)	21,21,21	1.82	7 (33%)
3	BTI	E	801	-	16,16,16	1.42	2 (12%)	21,21,21	1.82	7 (33%)
3	BTI	H	801	-	16,16,16	1.41	2 (12%)	21,21,21	1.82	7 (33%)
3	BTI	G	801	-	16,16,16	1.41	2 (12%)	21,21,21	1.81	7 (33%)
3	BTI	F	801	-	16,16,16	1.41	2 (12%)	21,21,21	1.81	7 (33%)

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	V	801	-	-	2/5/27/27	0/2/2/2
3	BTI	D	801	-	-	2/5/27/27	0/2/2/2
3	BTI	E	801	-	-	2/5/27/27	0/2/2/2
3	BTI	H	801	-	-	2/5/27/27	0/2/2/2
3	BTI	G	801	-	-	2/5/27/27	0/2/2/2
3	BTI	F	801	-	-	2/5/27/27	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	801	BTI	C2-S1	-4.00	1.76	1.82
3	D	801	BTI	C2-S1	-4.00	1.76	1.82
3	V	801	BTI	C2-S1	-3.98	1.76	1.82
3	E	801	BTI	C2-S1	-3.97	1.76	1.82
3	G	801	BTI	C2-S1	-3.94	1.76	1.82
3	F	801	BTI	C2-S1	-3.91	1.76	1.82
3	F	801	BTI	C3-N2	-2.15	1.31	1.35
3	E	801	BTI	C3-N2	-2.14	1.31	1.35
3	D	801	BTI	C3-N2	-2.12	1.31	1.35
3	G	801	BTI	C3-N2	-2.10	1.31	1.35
3	V	801	BTI	C3-N2	-2.08	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	801	BTI	C3-N2	-2.08	1.31	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	801	BTI	C4-C2-S1	3.76	108.79	105.20
3	V	801	BTI	C4-C2-S1	3.76	108.79	105.20
3	E	801	BTI	C4-C2-S1	3.76	108.79	105.20
3	H	801	BTI	C4-C2-S1	3.76	108.78	105.20
3	G	801	BTI	C4-C2-S1	3.73	108.76	105.20
3	F	801	BTI	C4-C2-S1	3.72	108.75	105.20
3	H	801	BTI	C6-S1-C2	2.78	95.60	89.89
3	G	801	BTI	C6-S1-C2	2.77	95.58	89.89
3	E	801	BTI	C6-S1-C2	2.77	95.58	89.89
3	V	801	BTI	C6-S1-C2	2.77	95.58	89.89
3	D	801	BTI	C6-S1-C2	2.77	95.57	89.89
3	F	801	BTI	C6-S1-C2	2.76	95.57	89.89
3	E	801	BTI	C6-C5-C4	2.60	110.91	108.66
3	H	801	BTI	C6-C5-C4	2.57	110.89	108.66
3	F	801	BTI	C6-C5-C4	2.57	110.89	108.66
3	D	801	BTI	C6-C5-C4	2.55	110.87	108.66
3	G	801	BTI	C6-C5-C4	2.54	110.86	108.66
3	V	801	BTI	C6-C5-C4	2.54	110.86	108.66
3	H	801	BTI	C2-C4-N2	-2.40	110.98	113.13
3	G	801	BTI	C5-C6-S1	2.39	108.36	106.31
3	D	801	BTI	C5-C6-S1	2.39	108.35	106.31
3	F	801	BTI	C2-C4-N2	-2.39	110.99	113.13
3	E	801	BTI	C2-C4-N2	-2.39	110.99	113.13
3	G	801	BTI	C2-C4-N2	-2.38	110.99	113.13
3	V	801	BTI	C2-C4-N2	-2.37	111.00	113.13
3	D	801	BTI	C2-C4-N2	-2.37	111.00	113.13
3	H	801	BTI	C5-C6-S1	2.36	108.33	106.31
3	E	801	BTI	C5-C6-S1	2.36	108.32	106.31
3	F	801	BTI	C5-C6-S1	2.36	108.32	106.31
3	V	801	BTI	C5-C6-S1	2.35	108.31	106.31
3	F	801	BTI	C2-C4-C5	2.31	111.62	108.94
3	E	801	BTI	N2-C3-N3	2.30	110.92	108.76
3	V	801	BTI	C2-C4-C5	2.30	111.60	108.94
3	G	801	BTI	C2-C4-C5	2.28	111.59	108.94
3	H	801	BTI	N2-C3-N3	2.28	110.90	108.76
3	D	801	BTI	N2-C3-N3	2.28	110.90	108.76
3	D	801	BTI	C2-C4-C5	2.26	111.56	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	801	BTI	C2-C4-C5	2.25	111.55	108.94
3	F	801	BTI	N2-C3-N3	2.24	110.86	108.76
3	V	801	BTI	N2-C3-N3	2.23	110.86	108.76
3	E	801	BTI	C2-C4-C5	2.23	111.53	108.94
3	G	801	BTI	N2-C3-N3	2.21	110.84	108.76

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	801	BTI	S1-C2-C7-C8
3	D	801	BTI	C4-C2-C7-C8
3	E	801	BTI	S1-C2-C7-C8
3	E	801	BTI	C4-C2-C7-C8
3	F	801	BTI	S1-C2-C7-C8
3	F	801	BTI	C4-C2-C7-C8
3	G	801	BTI	S1-C2-C7-C8
3	G	801	BTI	C4-C2-C7-C8
3	H	801	BTI	S1-C2-C7-C8
3	H	801	BTI	C4-C2-C7-C8
3	V	801	BTI	S1-C2-C7-C8
3	V	801	BTI	C4-C2-C7-C8

There are no ring outliers.

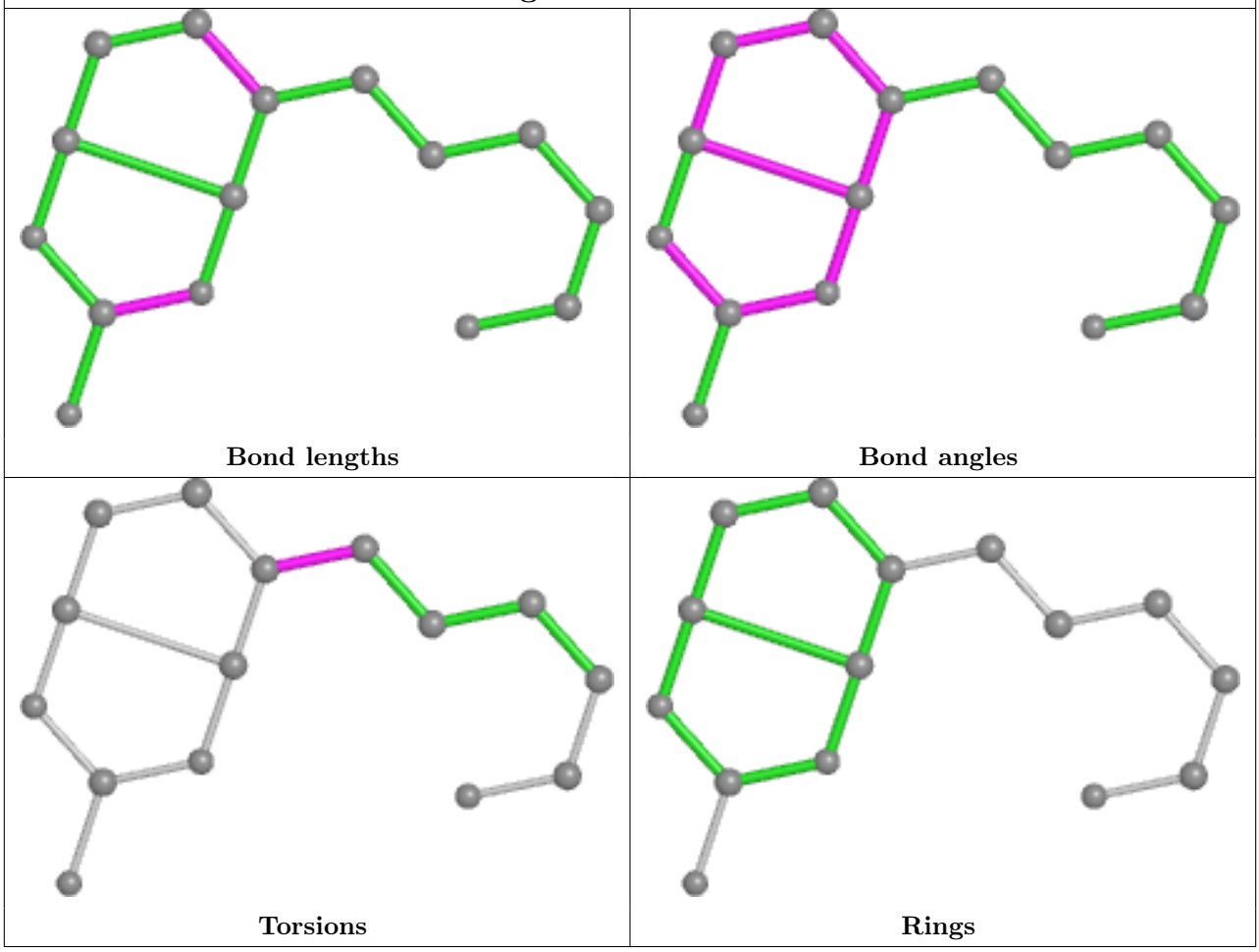
6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	801	BTI	2	0
3	D	801	BTI	5	0
3	E	801	BTI	1	0
3	H	801	BTI	6	0
3	G	801	BTI	3	0
3	F	801	BTI	8	0

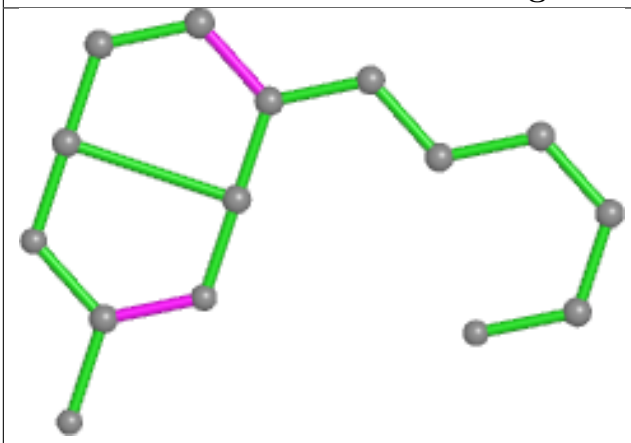
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

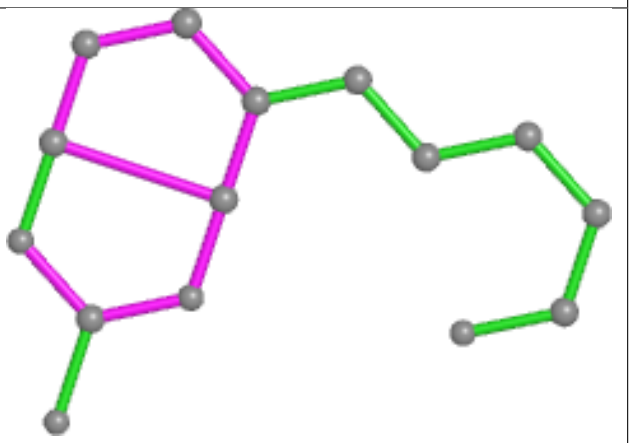
Ligand BTI V 801



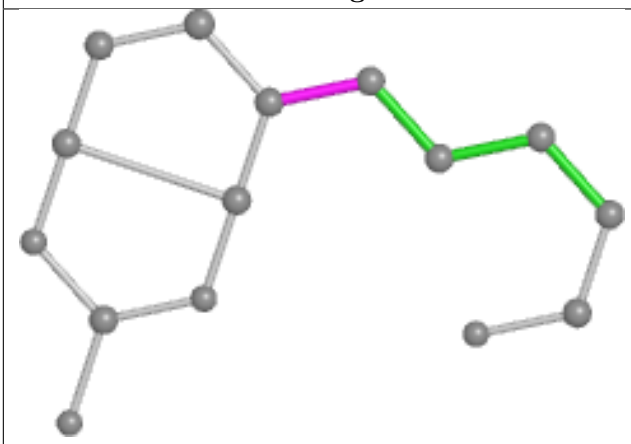
Ligand BTI D 801



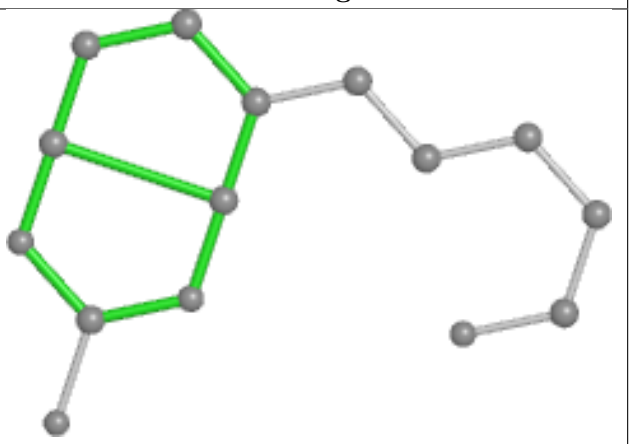
Bond lengths



Bond angles

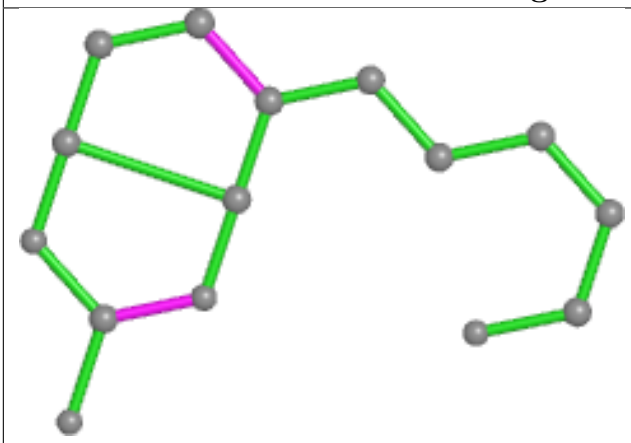


Torsions

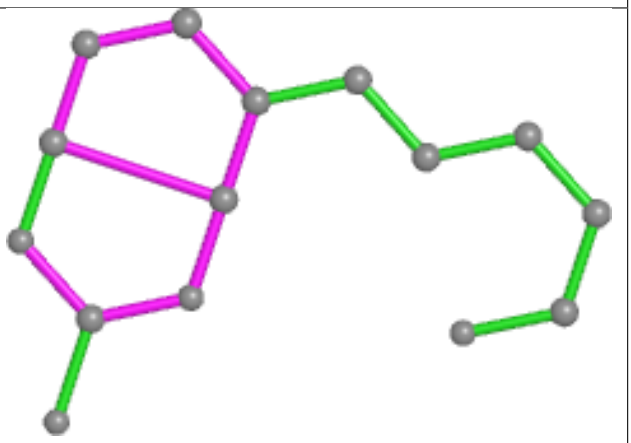


Rings

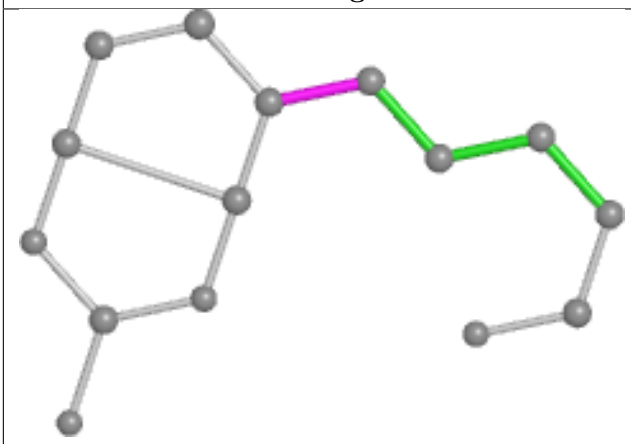
Ligand BTI E 801



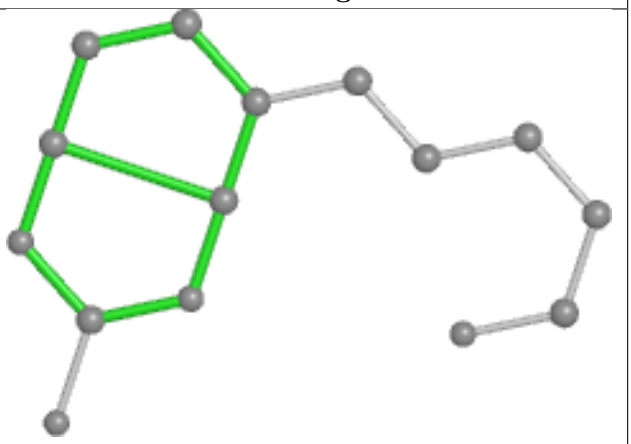
Bond lengths



Bond angles

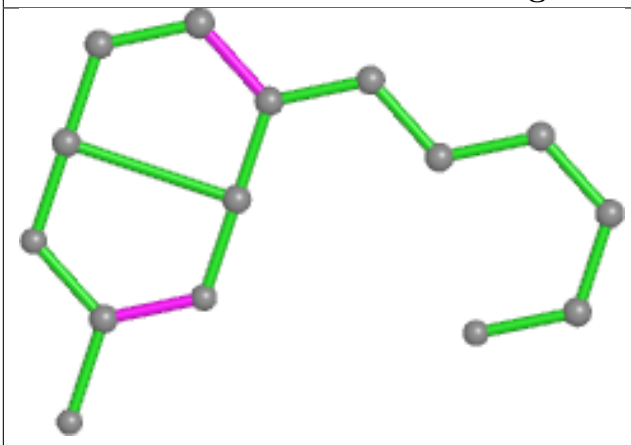


Torsions

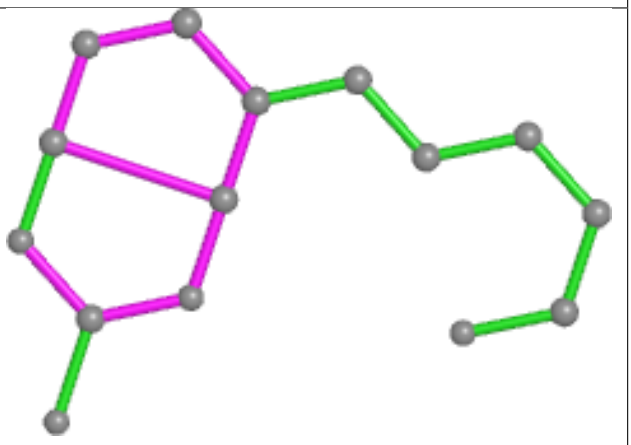


Rings

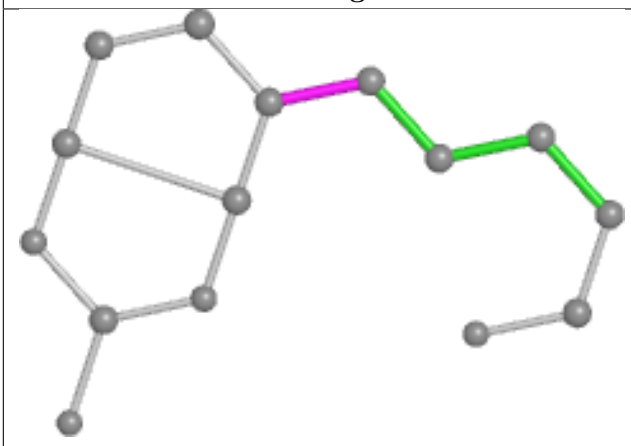
Ligand BTI H 801



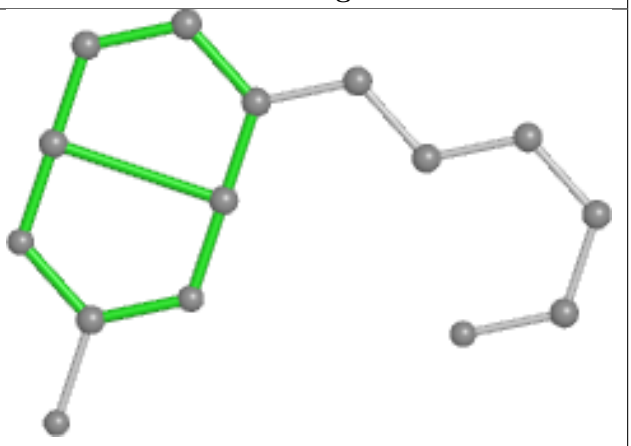
Bond lengths



Bond angles

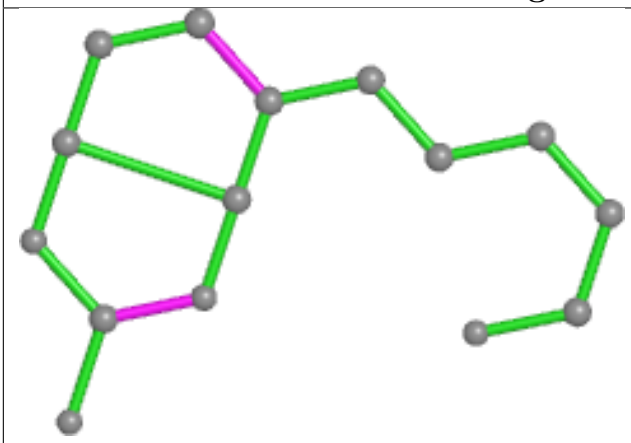


Torsions

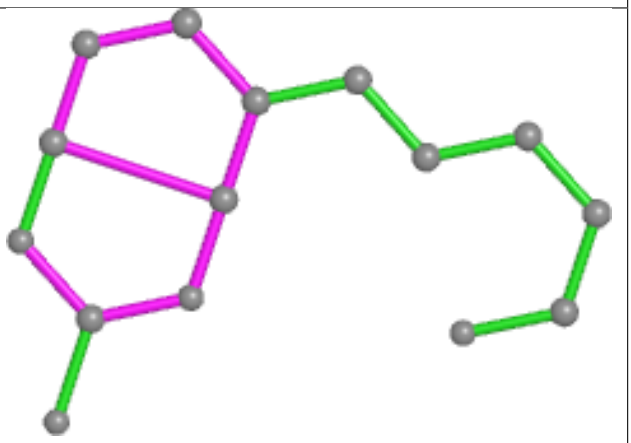


Rings

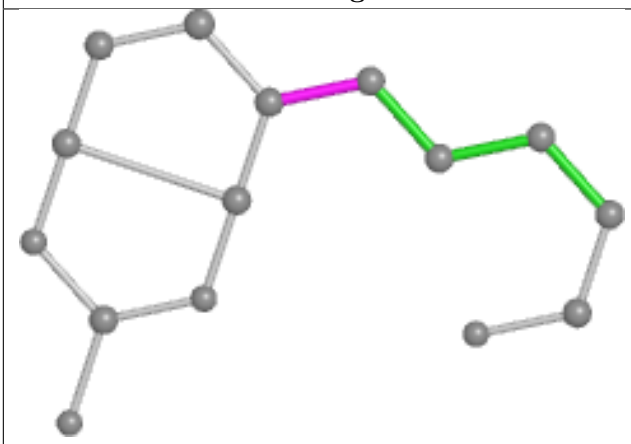
Ligand BTI G 801



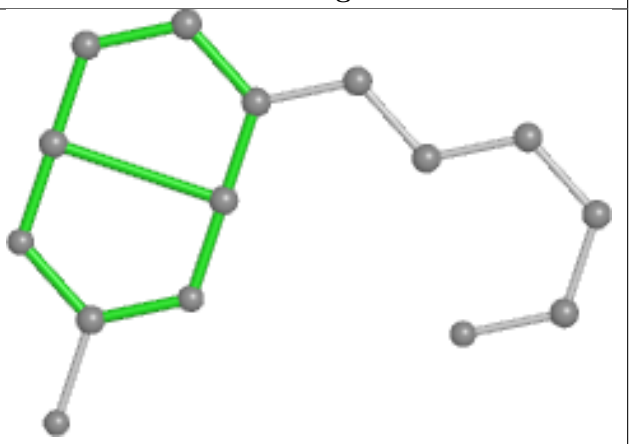
Bond lengths



Bond angles

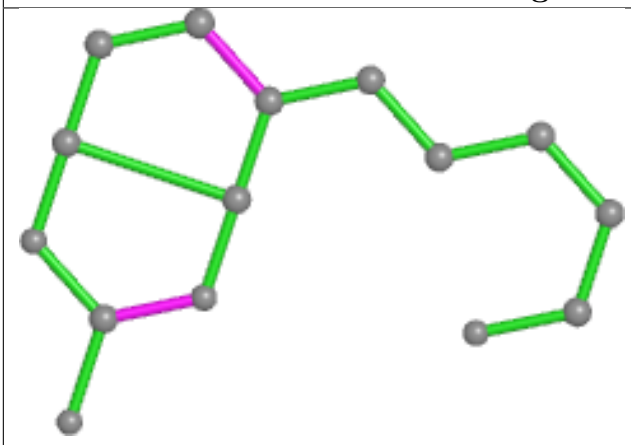


Torsions

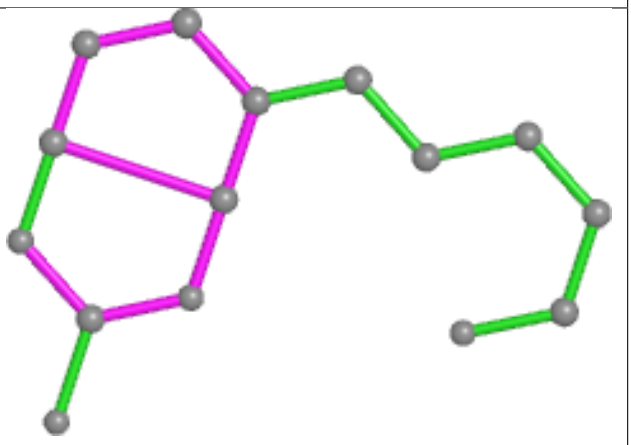


Rings

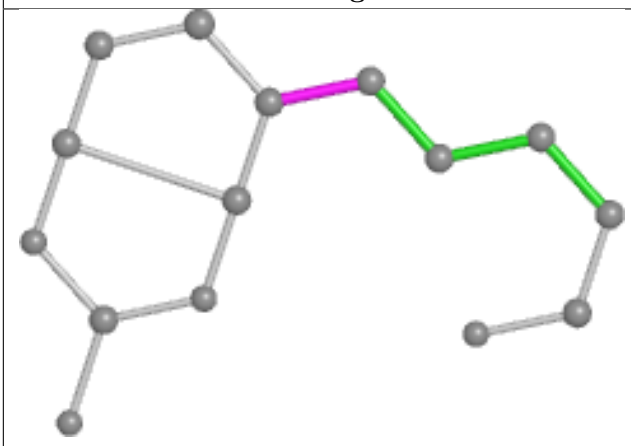
Ligand BTI F 801



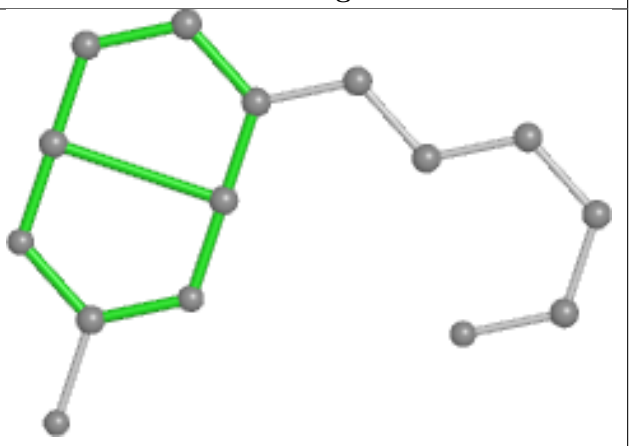
Bond lengths



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.

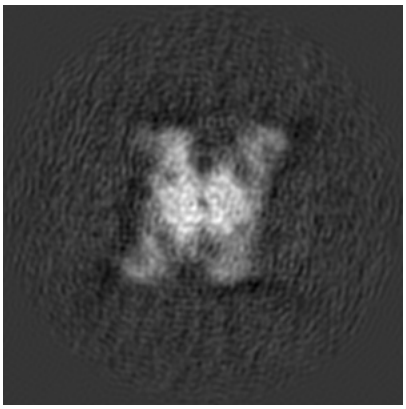
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40472. These allow visual inspection of the internal detail of the map and identification of artifacts.

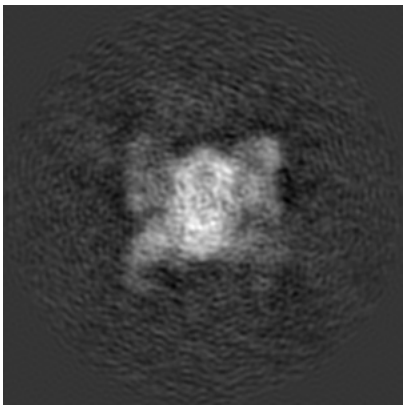
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

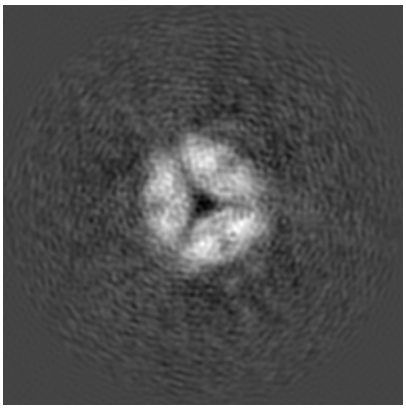
6.1.1 Primary map



X

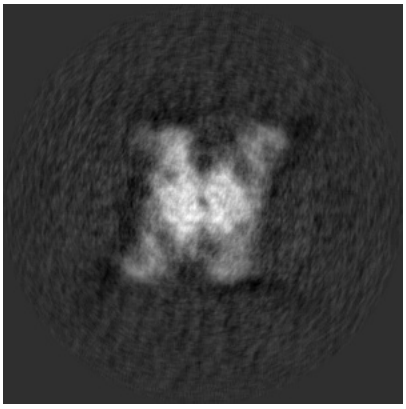


Y

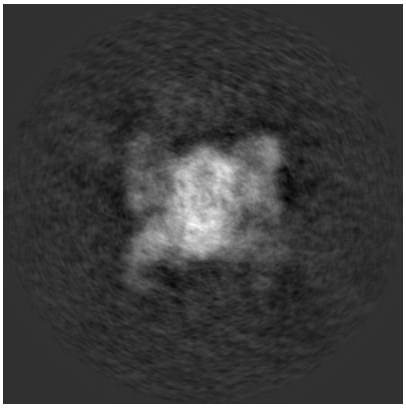


Z

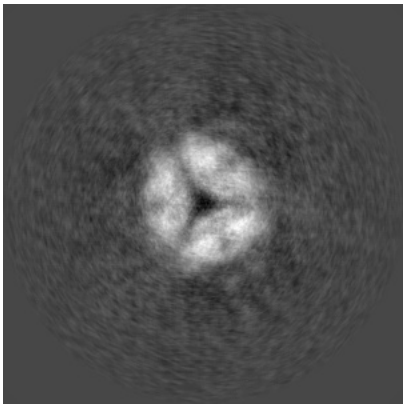
6.1.2 Raw map



X



Y

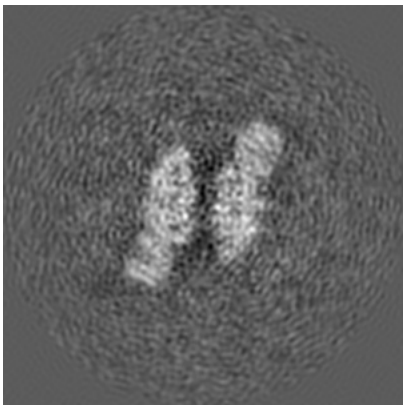


Z

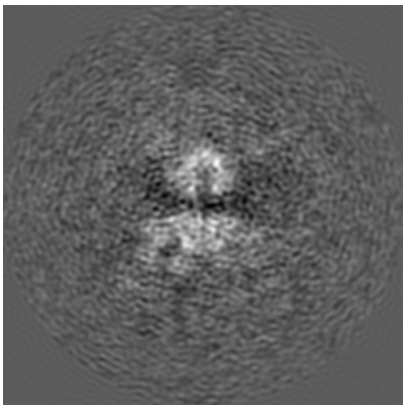
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

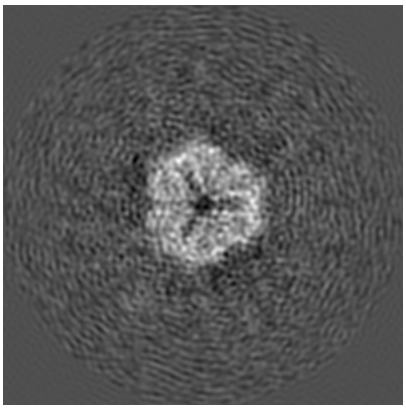
6.2.1 Primary map



X Index: 192

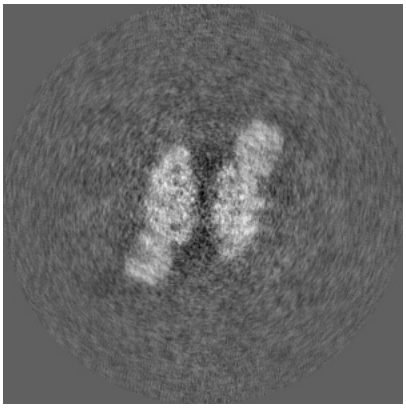


Y Index: 192

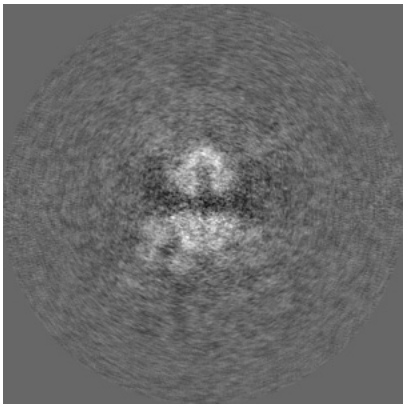


Z Index: 192

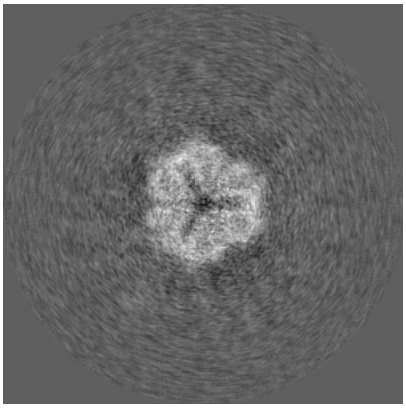
6.2.2 Raw map



X Index: 192



Y Index: 192

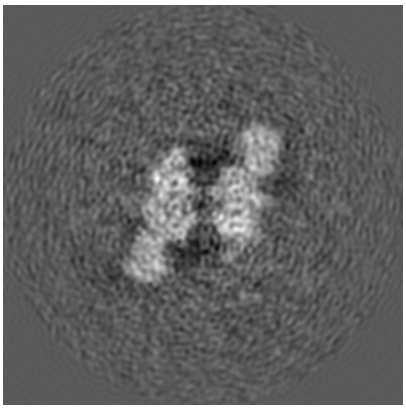


Z Index: 192

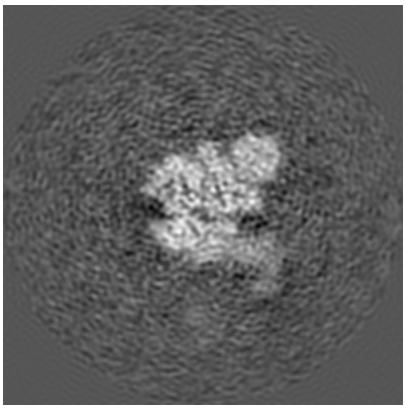
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

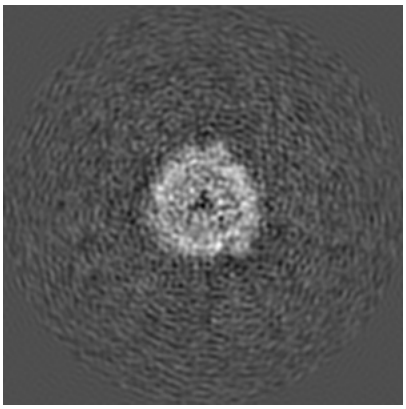
6.3.1 Primary map



X Index: 187

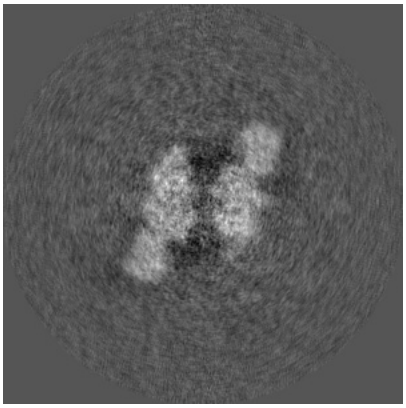


Y Index: 173

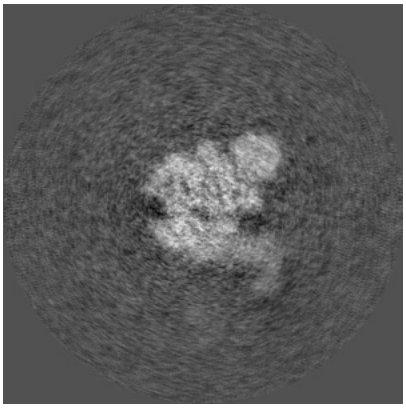


Z Index: 204

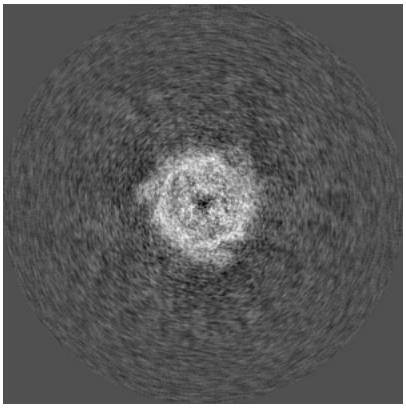
6.3.2 Raw map



X Index: 187



Y Index: 173

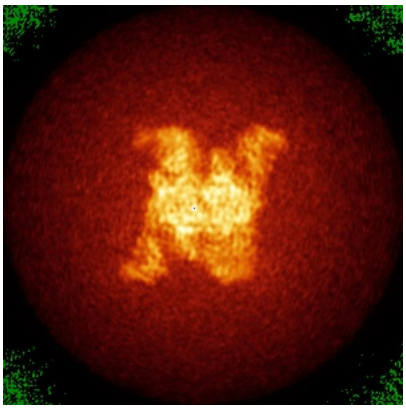


Z Index: 179

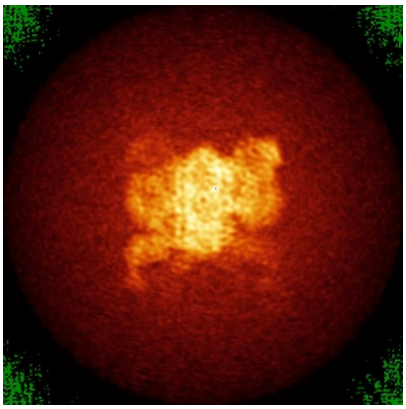
The images above show the largest variance slices of the map in three orthogonal directions.

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

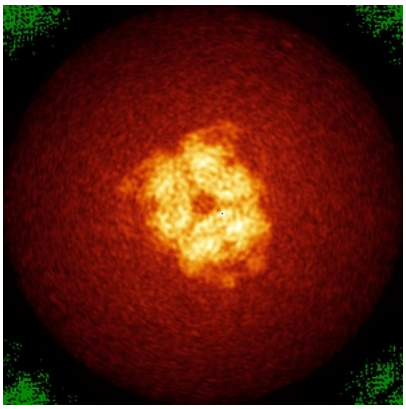
6.4.1 Primary map



X

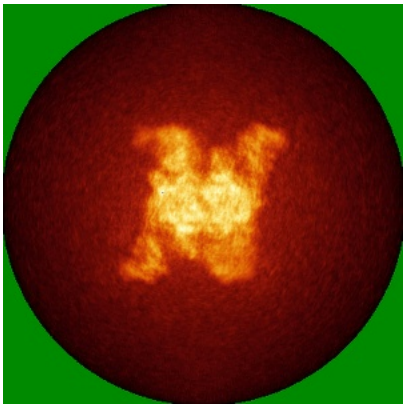


Y

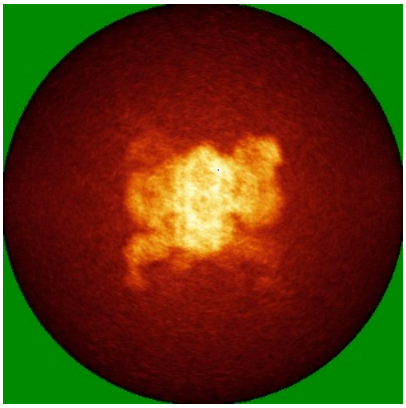


Z

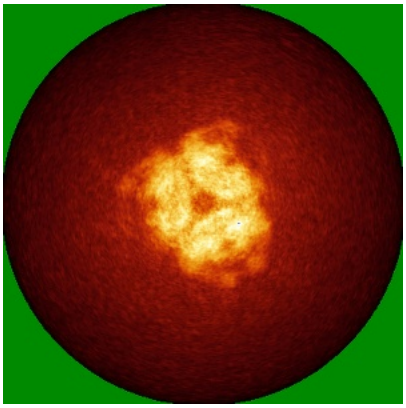
6.4.2 Raw map



X



Y

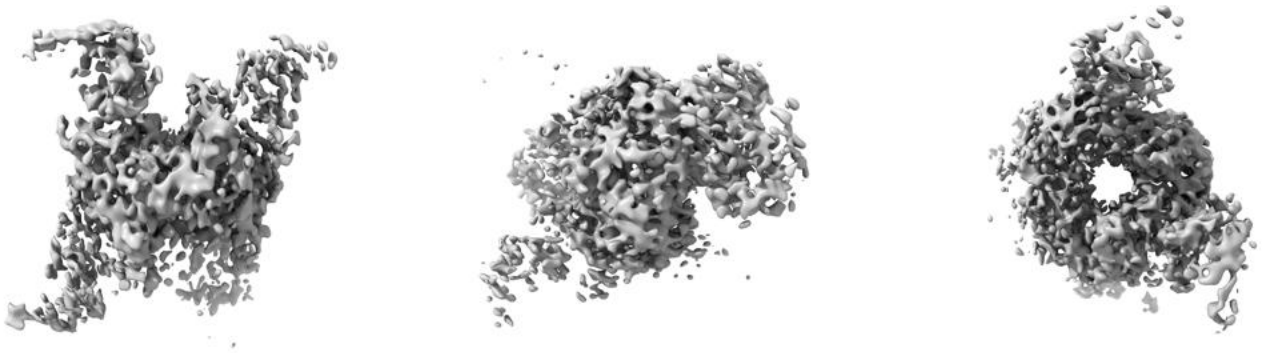


Z

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 0.0121. 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.

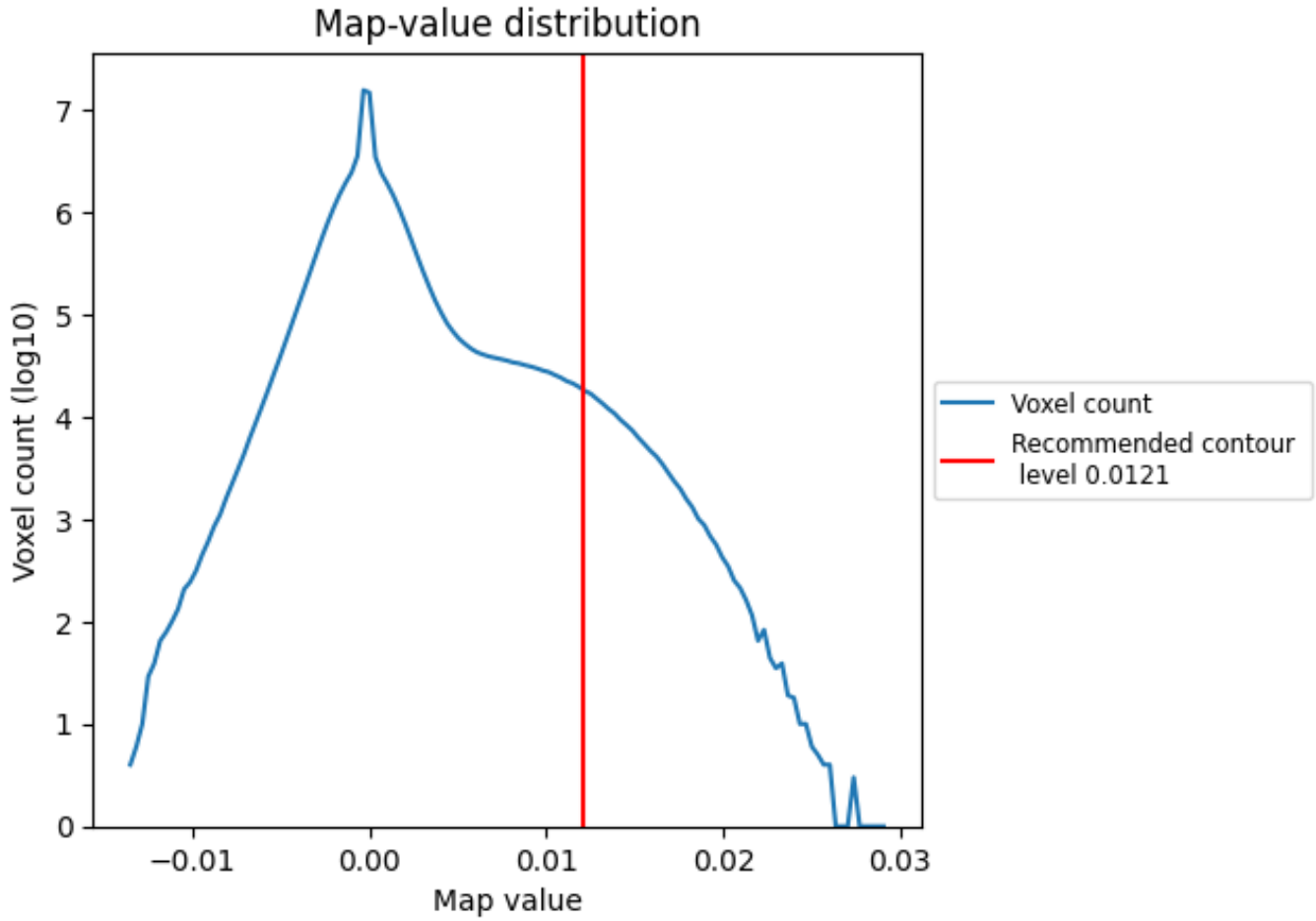
6.6 Mask visualisation (i)

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

7 Map analysis

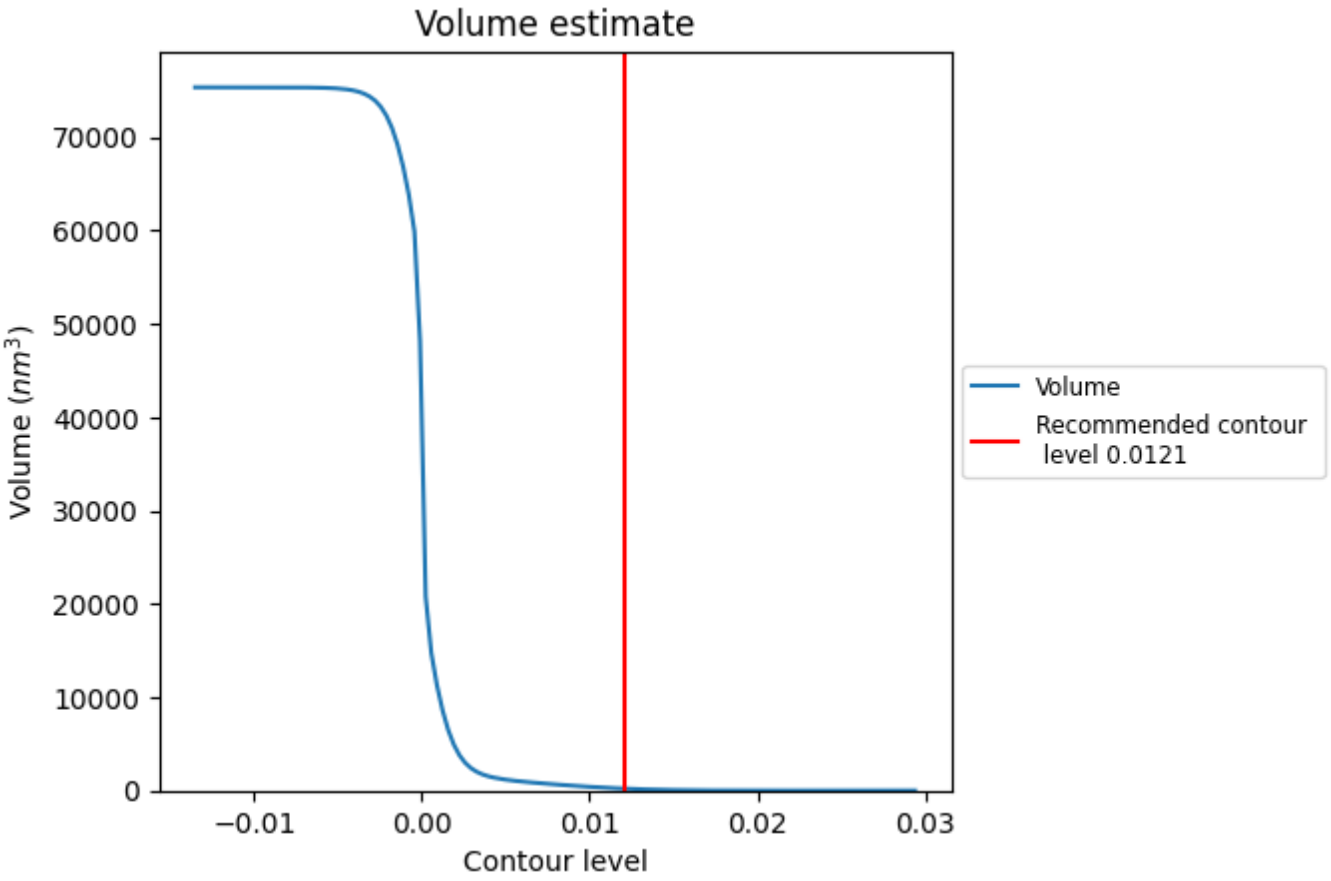
This section contains the results of statistical analysis of the map.

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.

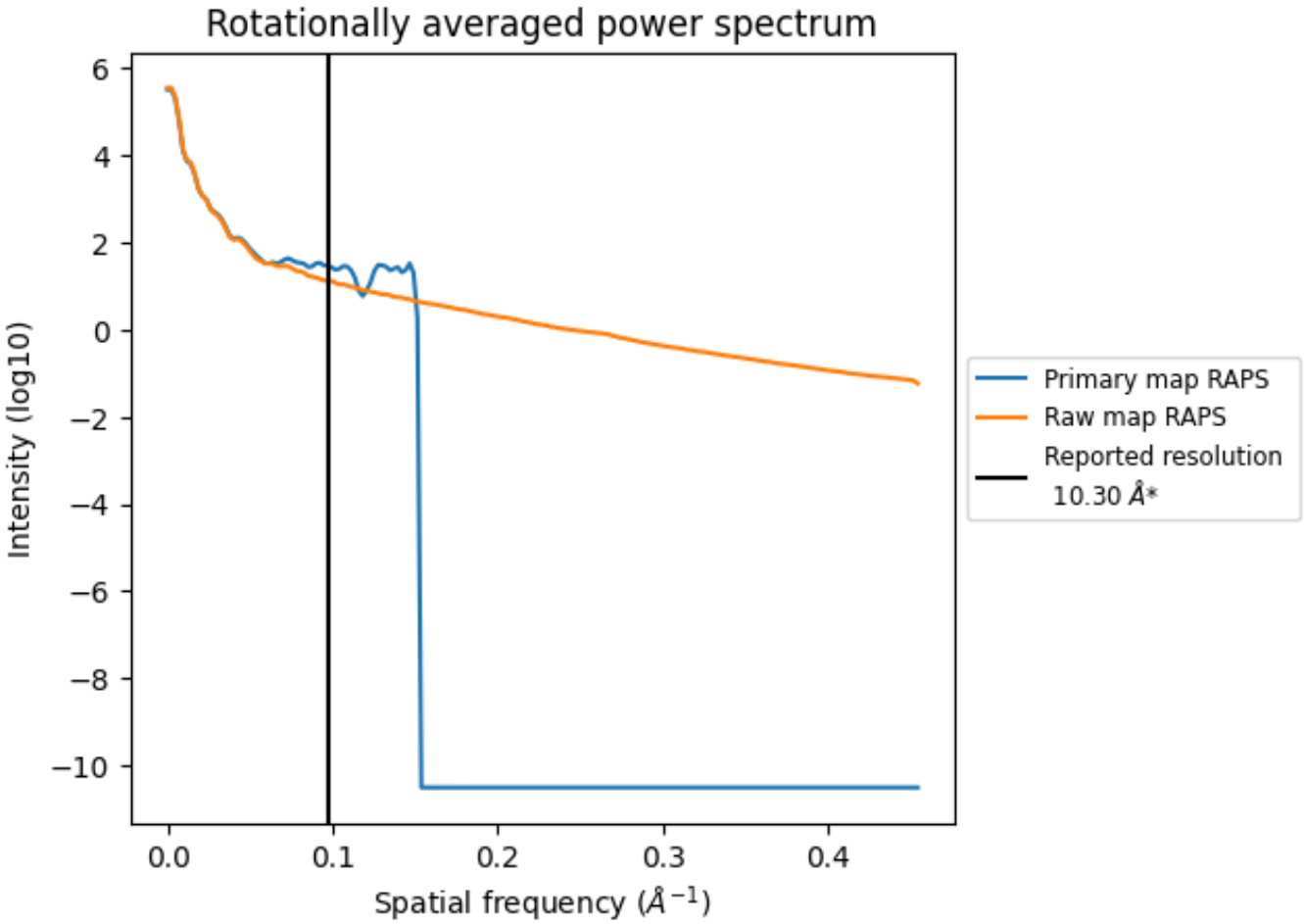
7.2 Volume estimate (i)



The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 184 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)

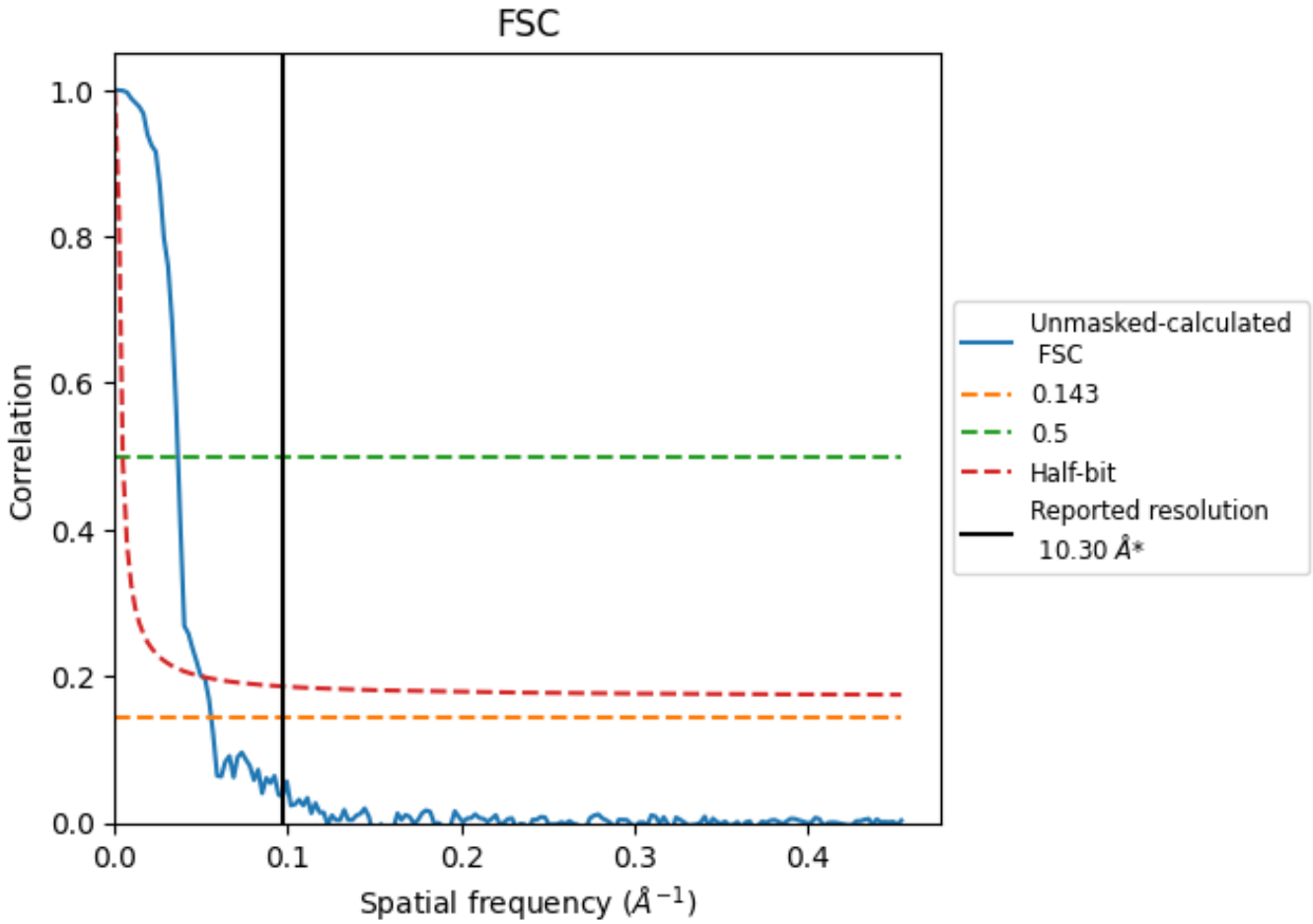


*Reported resolution corresponds to spatial frequency of 0.097 Å^{-1}

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 0.097 Å^{-1}

8.2 Resolution estimates (i)

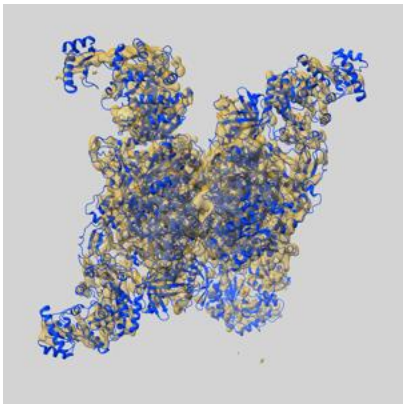
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	17.95	27.40	19.72

*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 17.95 differs from the reported value 10.3 by more than 10 %

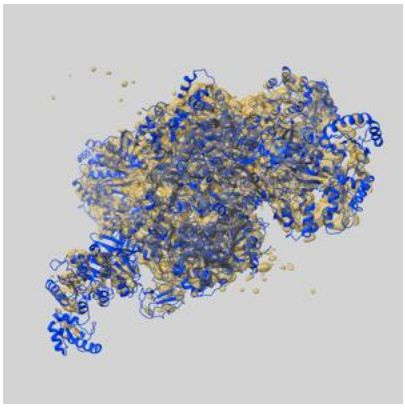
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40472 and PDB model 8SGX. Per-residue inclusion information can be found in section 3 on page 6.

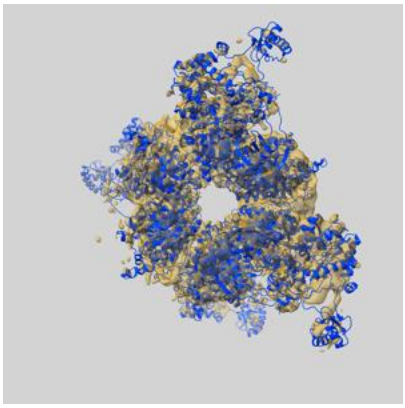
9.1 Map-model overlay



X



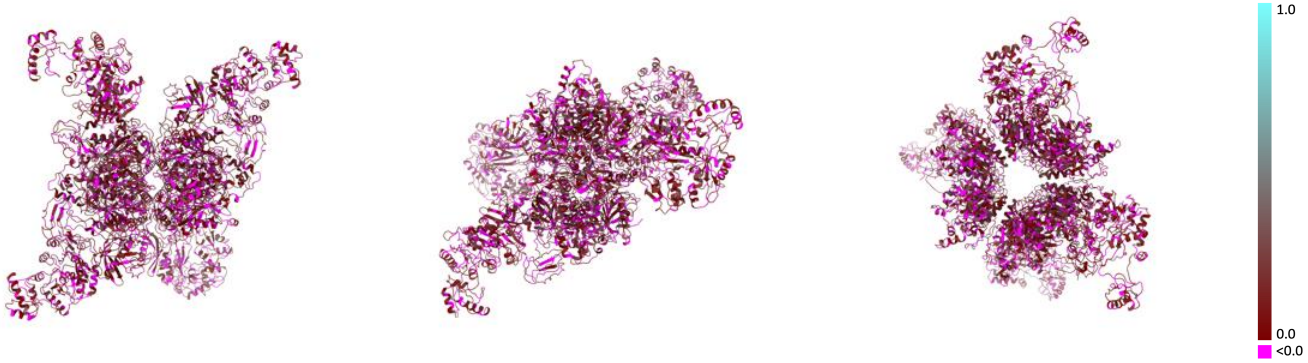
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0121 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.

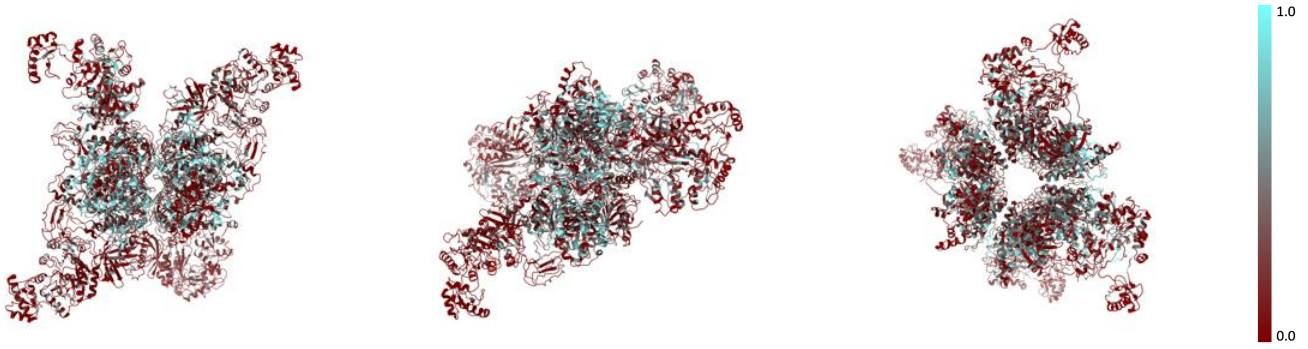
9.2 Q-score mapped to coordinate model (i)



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.

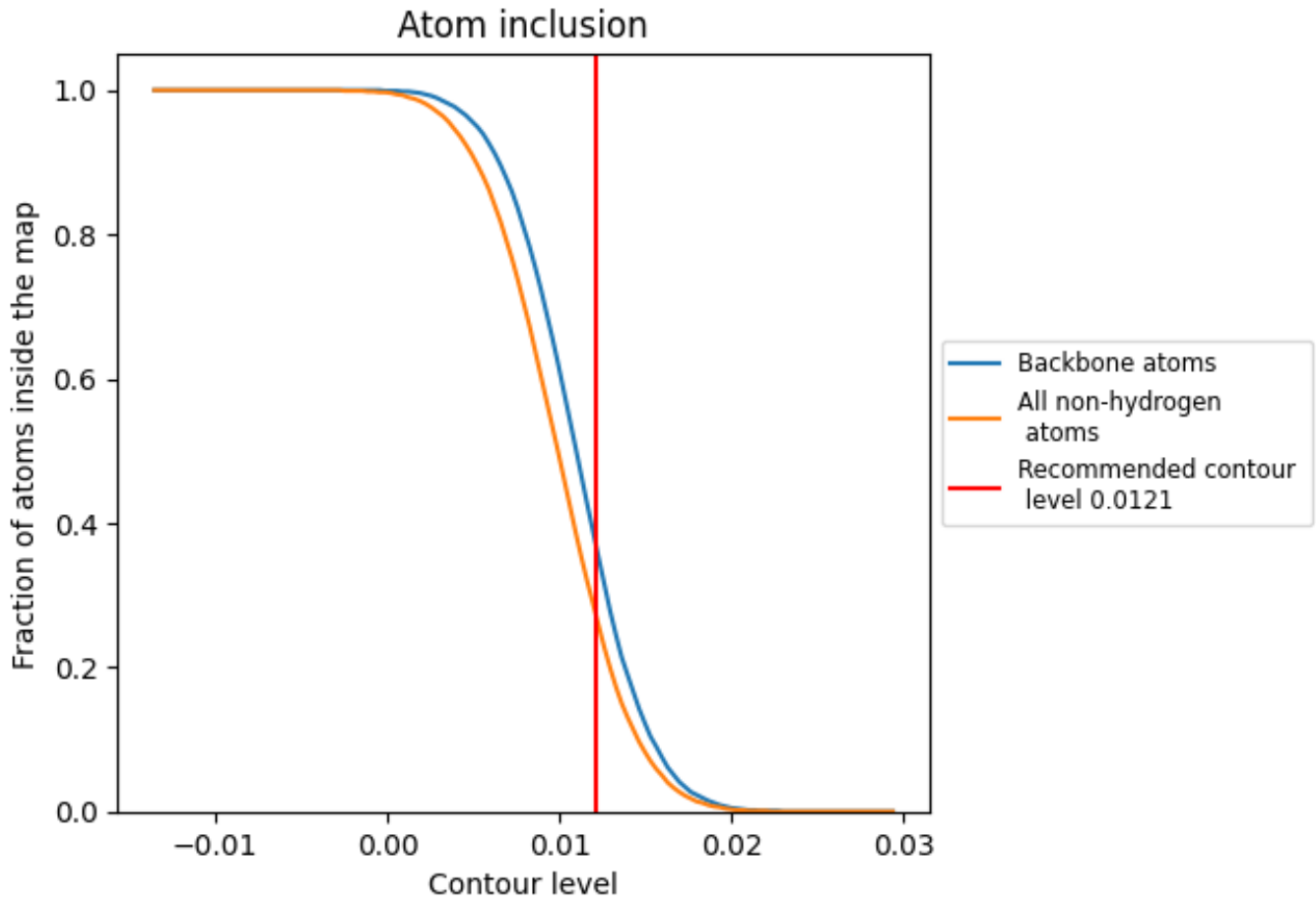
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0121).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 28% 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 (0.0121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2760	0.0890
C	0.4180	0.1080
D	0.2810	0.0790
E	0.4280	0.1100
F	0.3940	0.0980
G	0.3590	0.0810
H	0.4030	0.0970
S	0.0880	0.0790
V	0.2320	0.0830
X	0.1800	0.0860
Z	0.1380	0.0850