



## Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 01:42 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

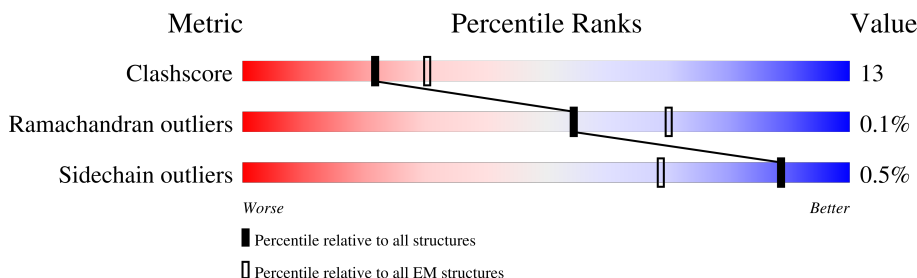
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

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

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Mol	Chain	Length	Quality of chain
2	X	657	<div> <div>82%</div> <div> <div></div> <div>66%</div> <div>33%</div> </div> <div>.</div> </div>
2	Z	657	<div> <div>86%</div> <div> <div></div> <div>67%</div> <div>32%</div> </div> <div>.</div> </div>

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

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.

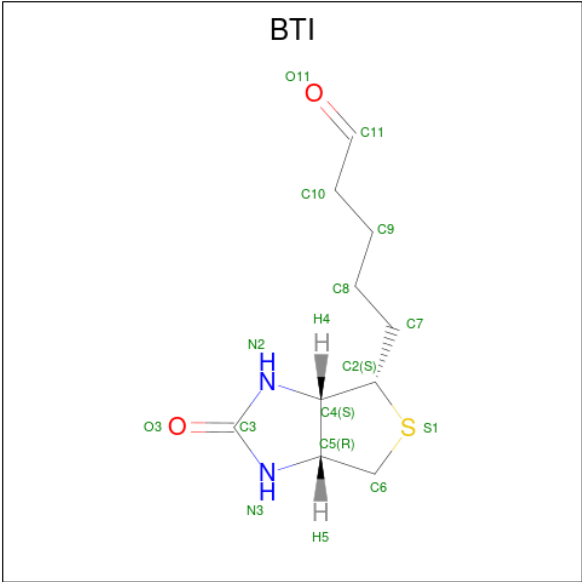
- Molecule 1 is a protein called Propionyl-coa carboxylase beta chain, putative.

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<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S) (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	

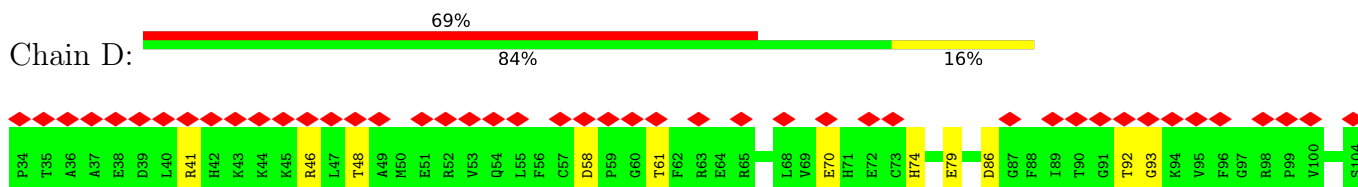
### 3 Residue-property plots

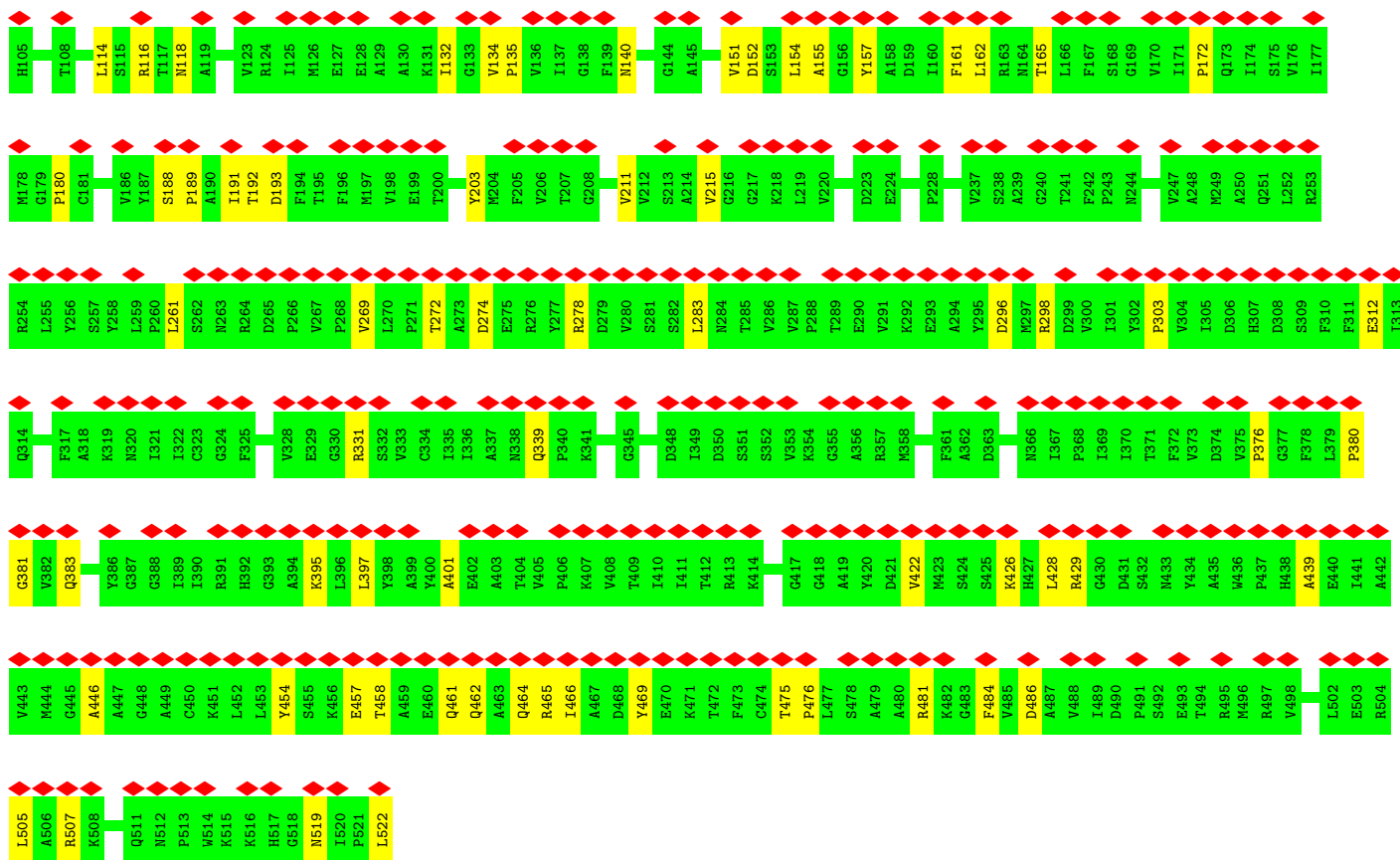
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

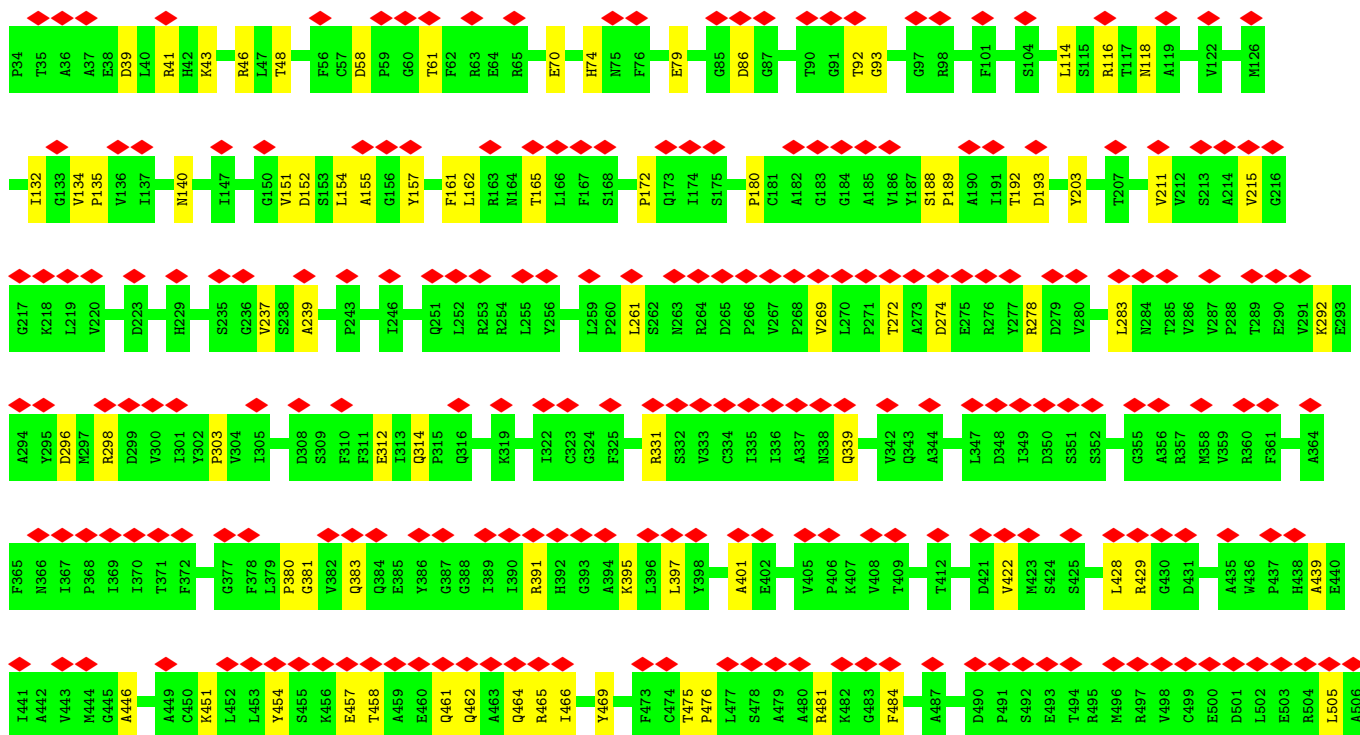
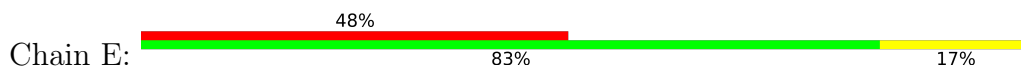


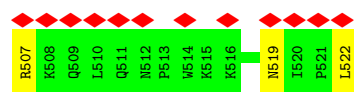
- Molecule 1: Propionyl-coa carboxylase beta chain, putative



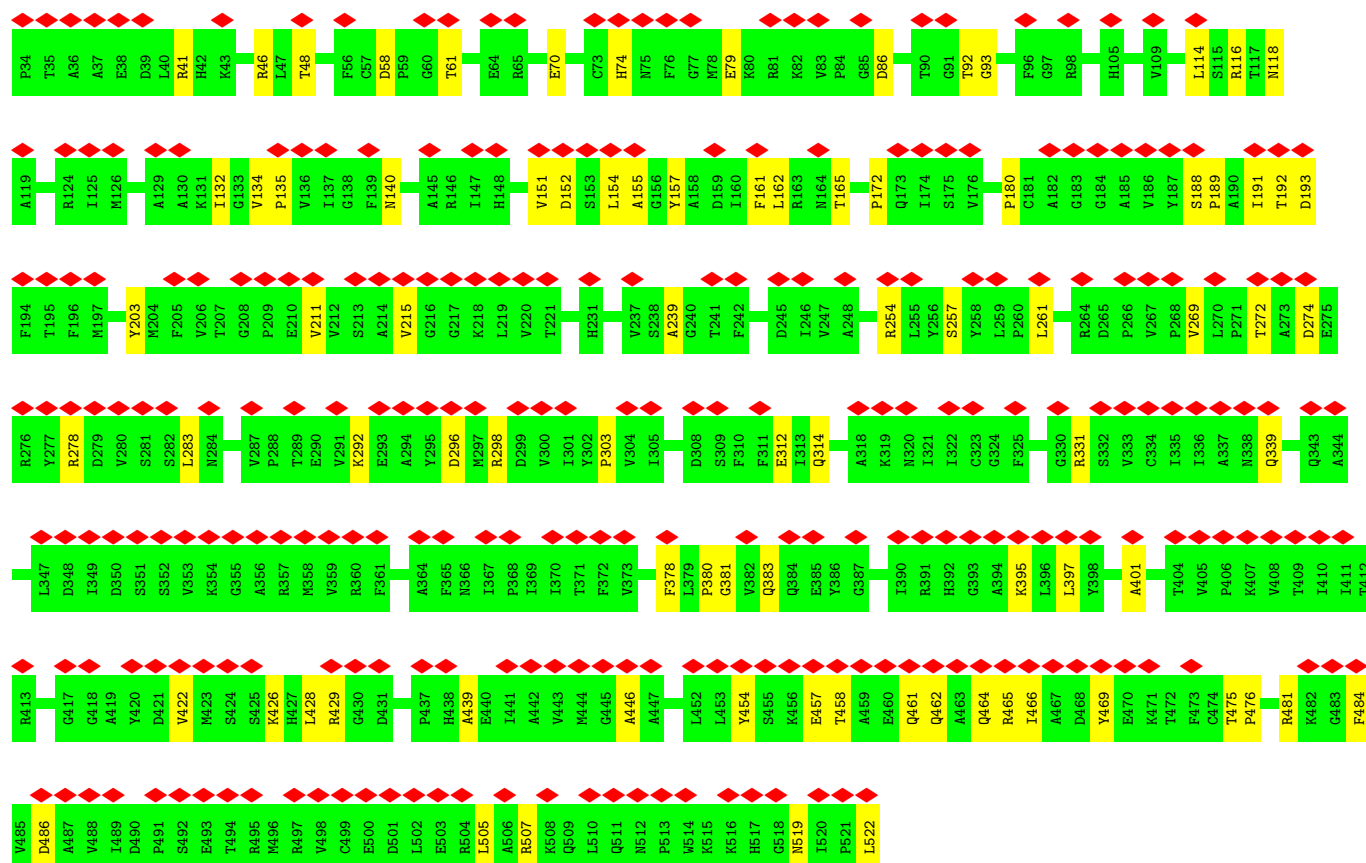
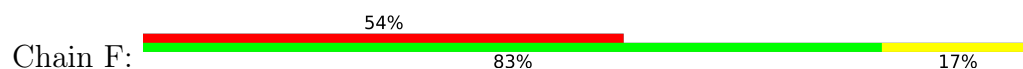


- Molecule 1: Propionyl-coa carboxylase beta chain, putative

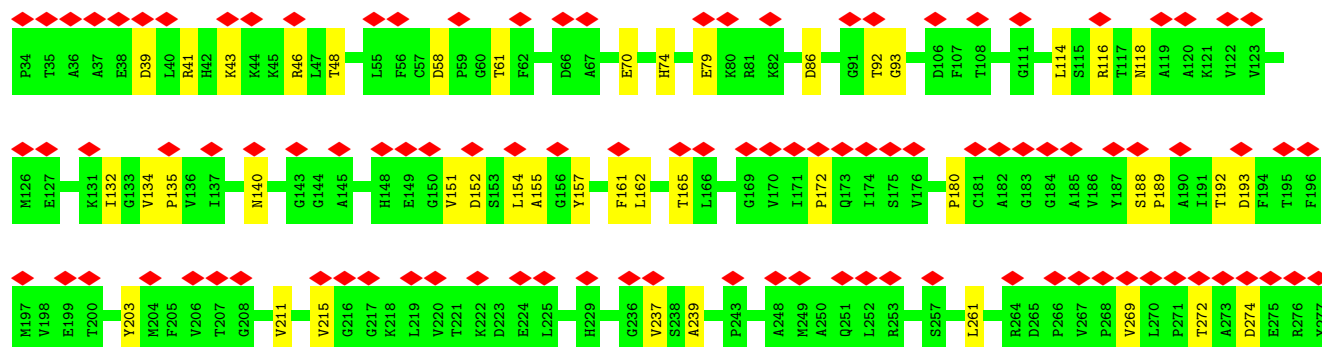
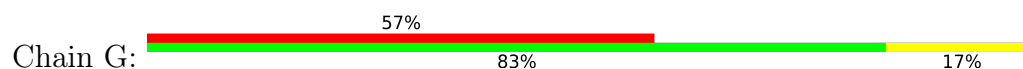




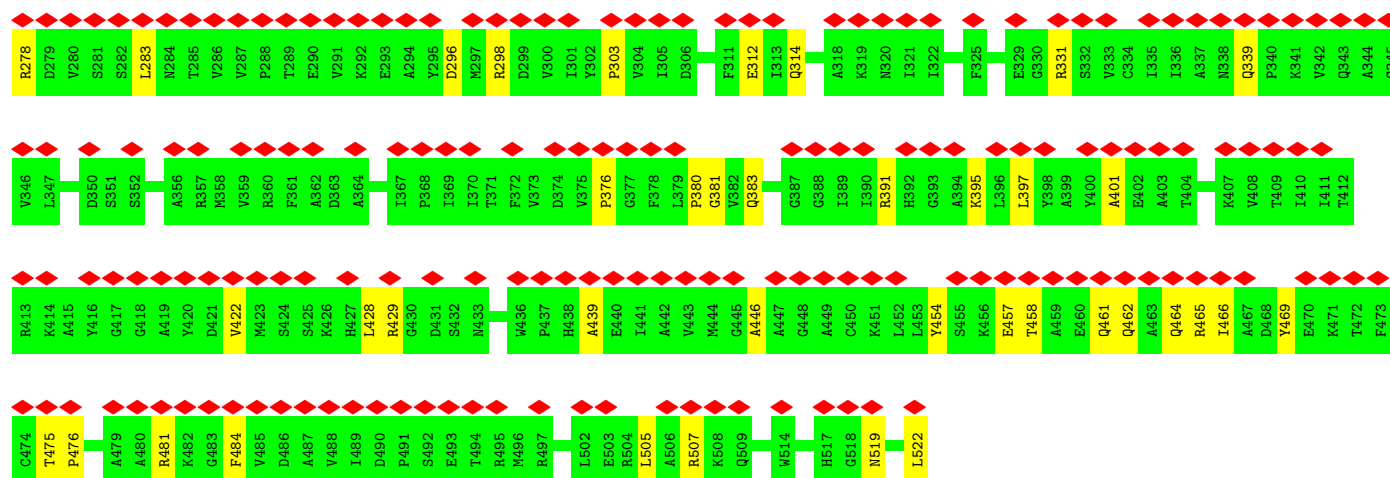
- Molecule 1: Propionyl-coa carboxylase beta chain, putative



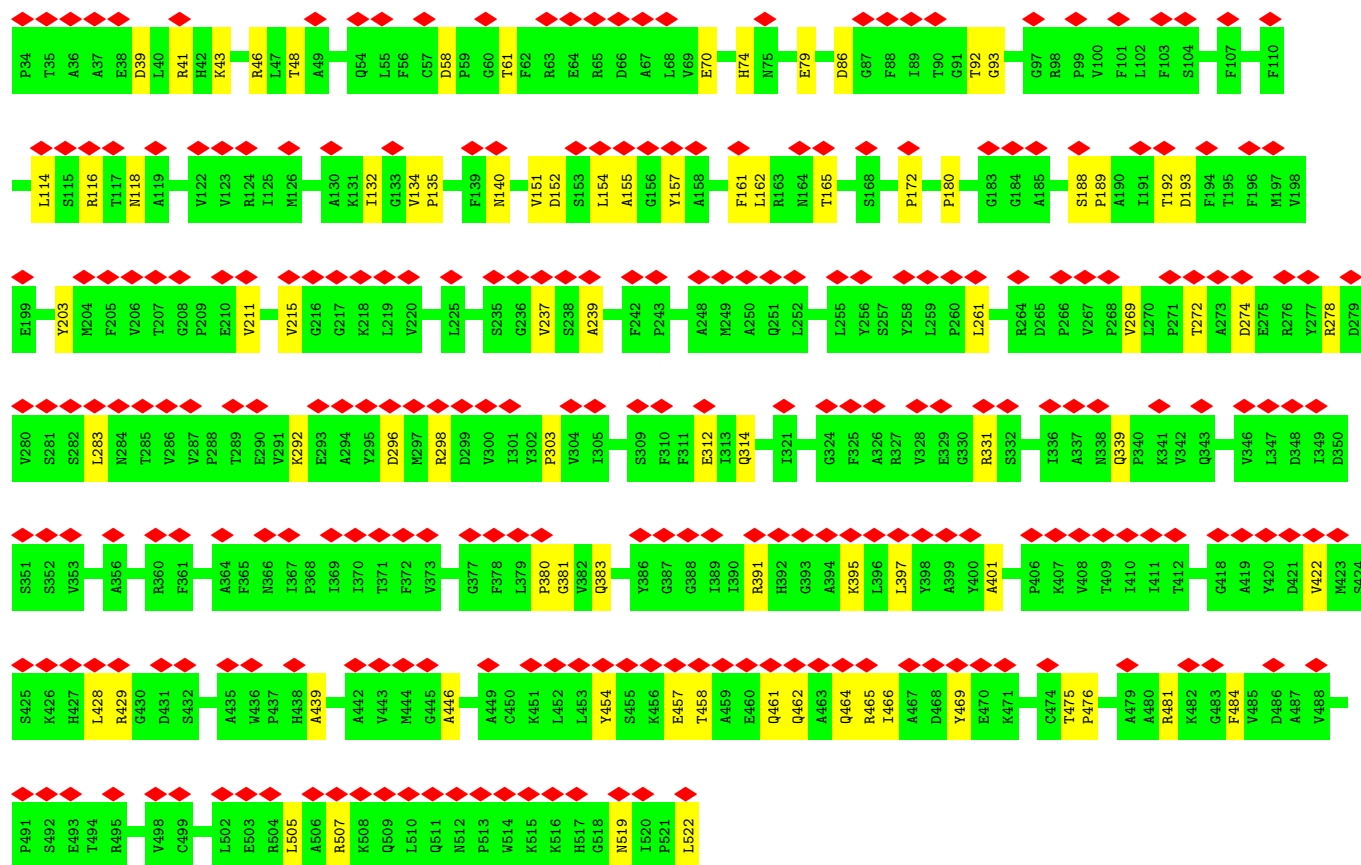
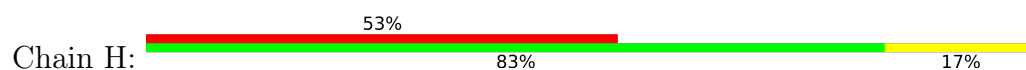
- Molecule 1: Propionyl-coa carboxylase beta chain, putative





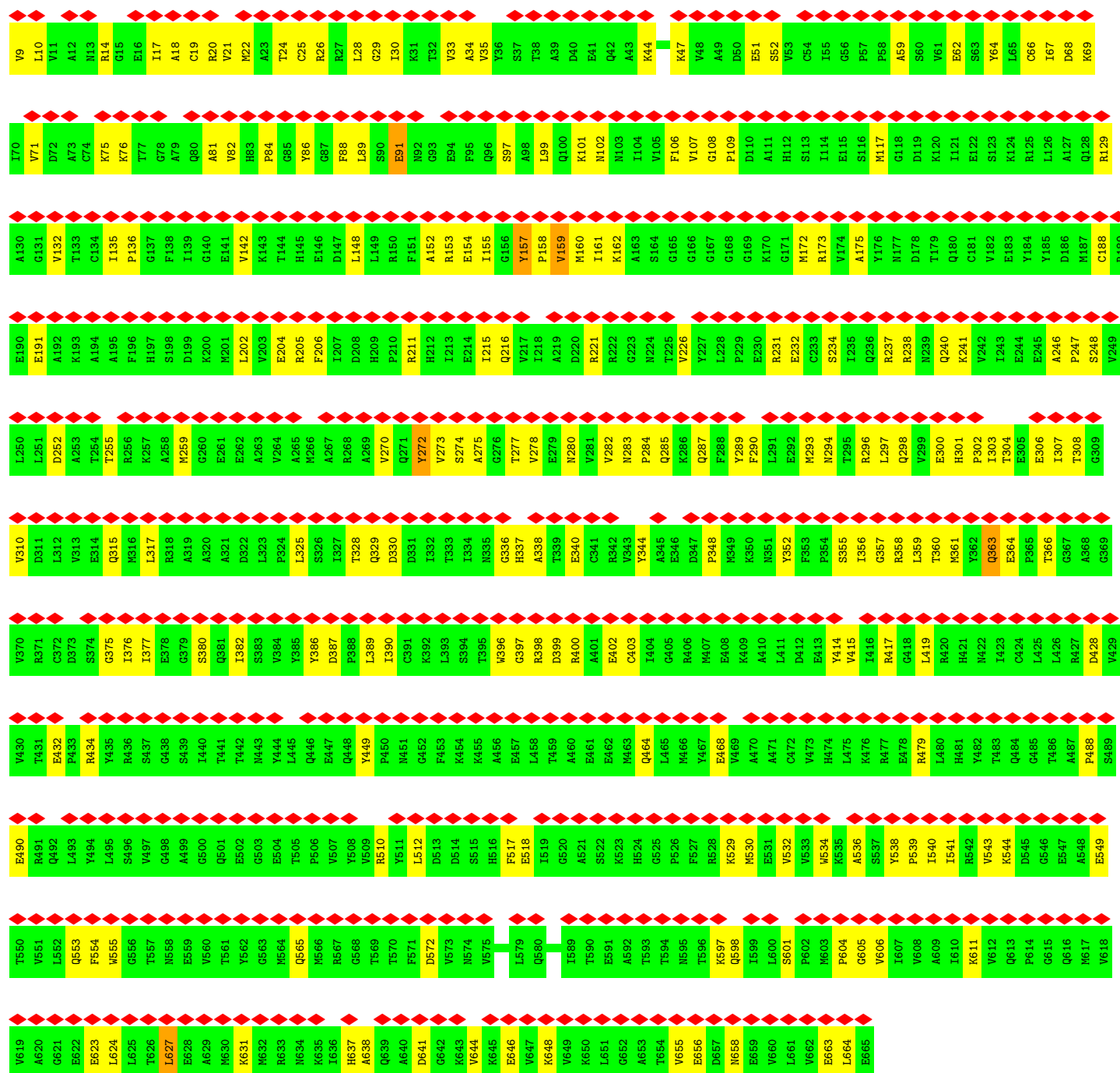


- Molecule 1: Propionyl-coa carboxylase beta chain, putative

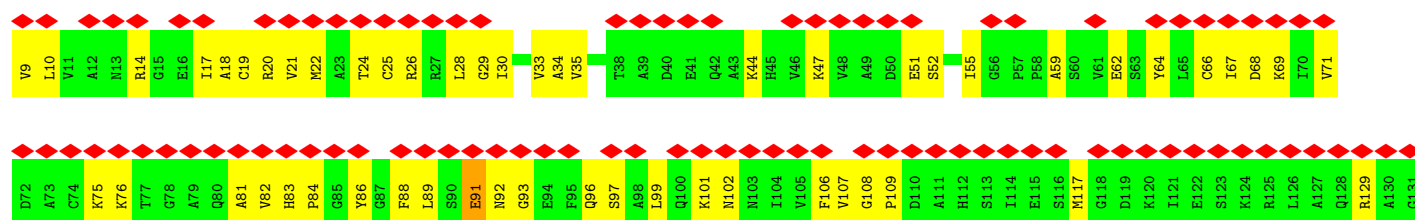
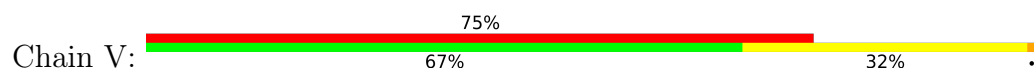


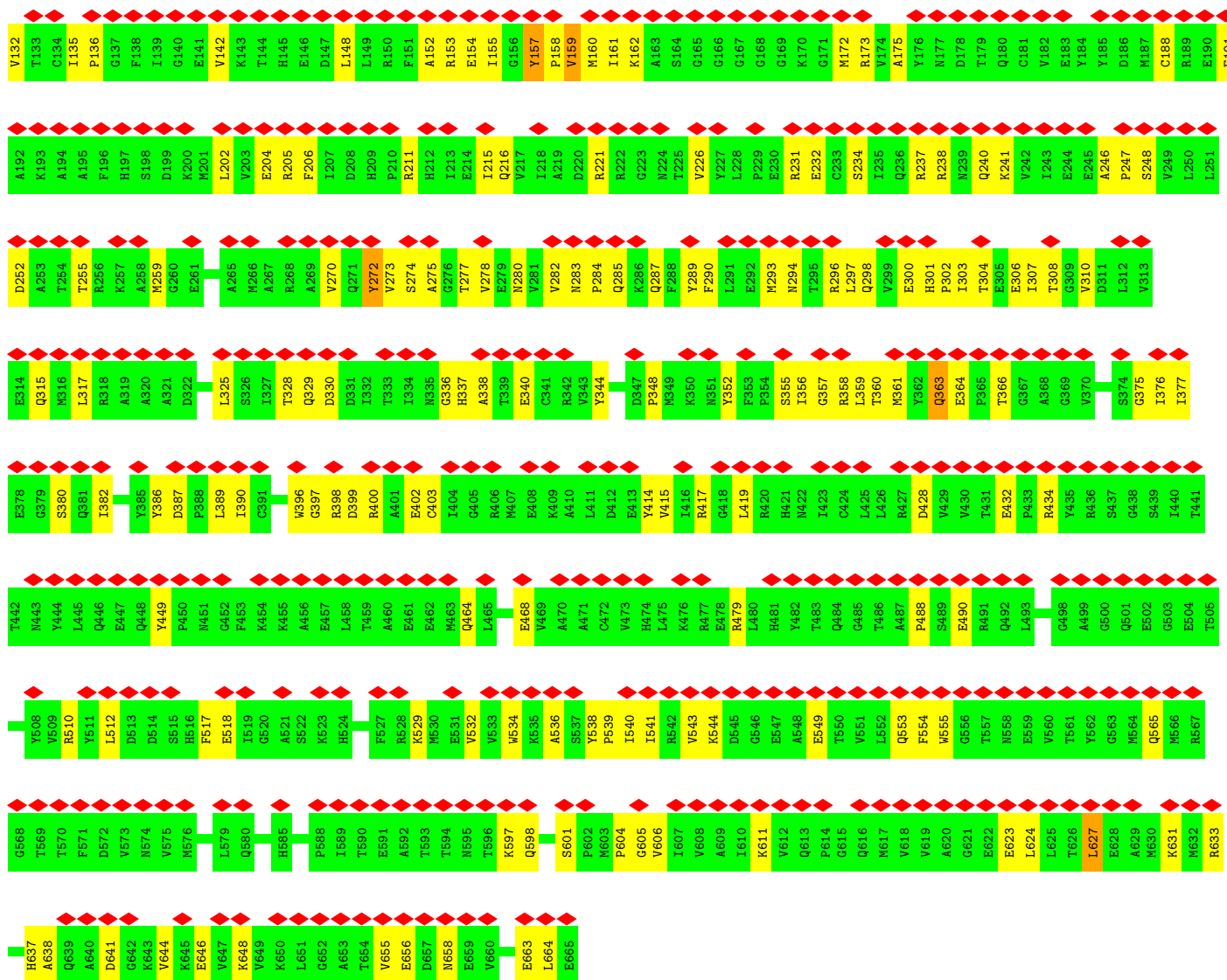
- Molecule 2: propionyl-CoA carboxylase



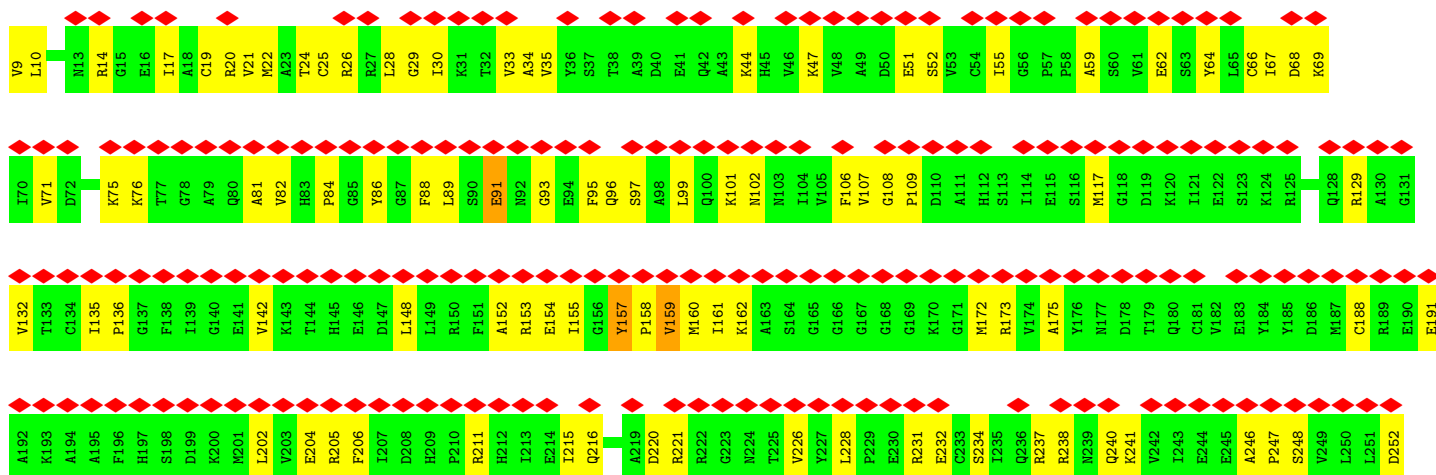
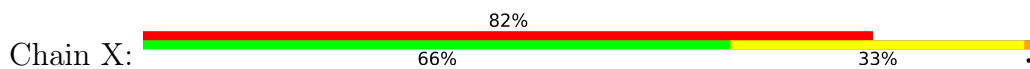


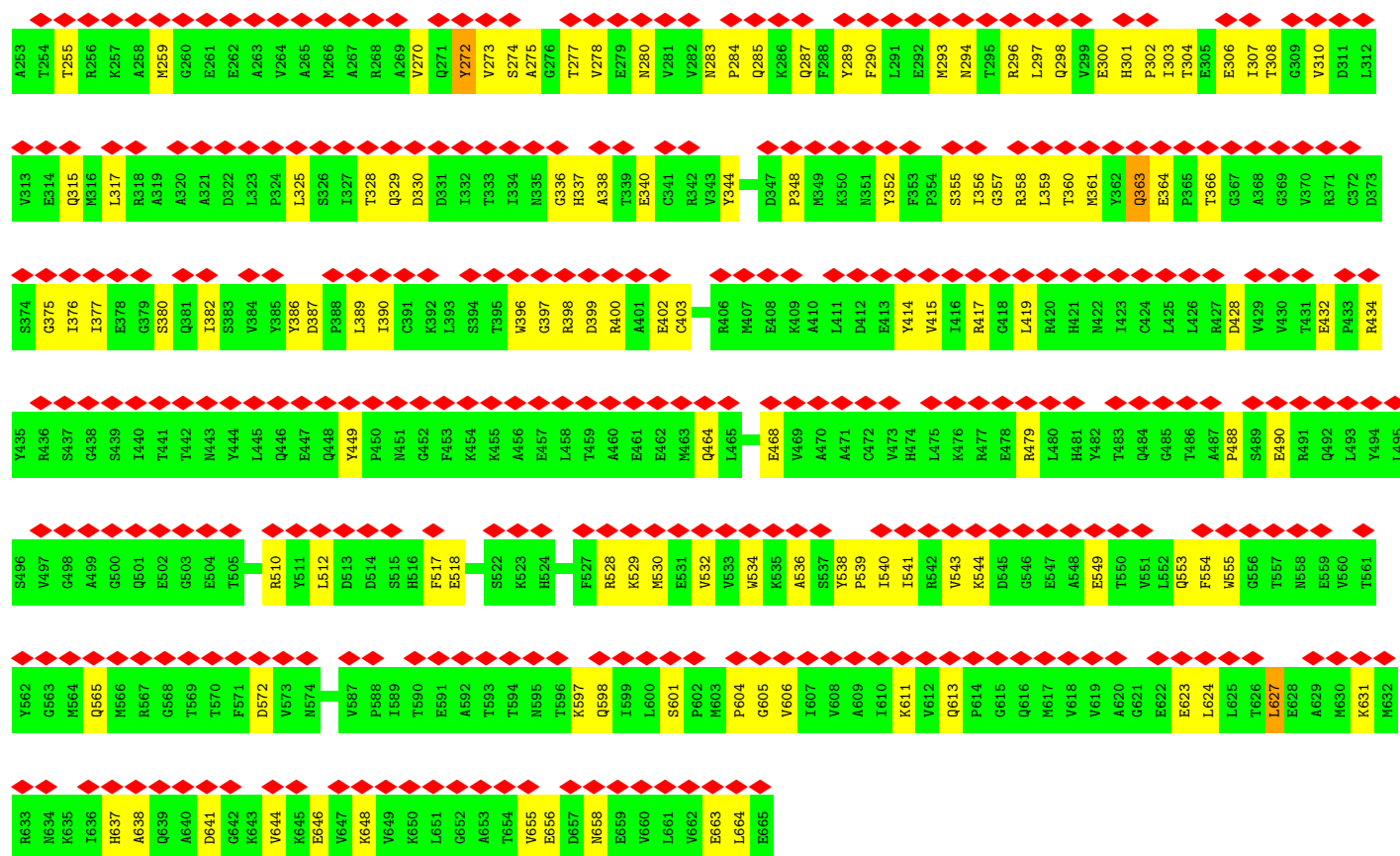
• Molecule 2: propionyl-CoA carboxylase





• Molecule 2: propionyl-CoA carboxylase





M617	F554	L493	E432	C372
V618	W555	Y494	P433	D373
V619	G556	L495	R434	S374
A620	T557	S496	Y435	G375
G621	N558	V497	R436	I376
E622	E559	G498	S437	I377
E623	V560	A499	G438	E378
L624	T561	G500	S439	G379
L625	Y562	Q501	I440	S380
T626	G563	E502	T441	Q381
L627	M564	G503	T442	I382
E628	Q565	E504	M443	S383
A629	M566	T505		V384
M630	R567	P506	Q446	Y385
K631	G568	V507	E447	Y386
M632	T569		Q448	D387
R633	T570		E447	P388
M634	F571	R510	Y449	L389
K635	D572	V511	P450	I390
I636	V573	L512	M451	C391
H637	N574	D513	G452	K392
A638	V575	D514	F453	L393
Q639	M576	S515	K454	S394
A640	S577	H516	K455	T395
D641	D578	F517	A456	W396
G642	L579	E518	E457	G397
K643	Q580	T519	L458	R398
V644	S581	G520	T459	D399
K645		A521	A460	R400
E646	A584	S522	E461	A401
V647	H585	H523	E462	E402
K648		K524	M463	C403
V649	I589	G525	Q464	I404
K650	T590	P526	L465	G405
L651	E591	F527	M466	R406
G652	A592	R528	Y467	M407
A653	T593	K529	E468	E408
T654	T594	M530	V469	K409
V655	N595	E531	A470	A410
E656	T596	V532	A471	L411
D657	K597	V633	C472	D412
M658	Q598	W534	V473	E413
E659	I599	K535	H474	E414
V660	L600	A536	L475	Y414
L661	S601	S637	K476	V415
V662	P602	Y638	R477	I416
E663	M603	P539	E478	R417
L664	P604	I540	R479	G418
E665	G605	I541	L480	L419
	V606	R542	L480	R420
	I607	V543	H481	H421
	V608	K544	Y482	N422
	A609	D545	T483	I423
	I610	G546	Q484	C424
	K611	E547	G485	L425
	V612	A548	T486	L426
	Q613	E549	A487	R427
	P614	T550	P488	D428
	G615	V551	S489	V429
	Q616	L552	E490	V430
		Q553	R491	T431

## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 ( $\text{\AA}$ )	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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 ⓘ

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 [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	H	801	-	16,16,16	1.41	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	V	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%)
3	BTI	D	801	-	16,16,16	1.42	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%)

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	H	801	-	-	2/5/27/27	0/2/2/2
3	BTI	E	801	-	-	2/5/27/27	0/2/2/2
3	BTI	V	801	-	-	2/5/27/27	0/2/2/2
3	BTI	F	801	-	-	2/5/27/27	0/2/2/2
3	BTI	D	801	-	-	2/5/27/27	0/2/2/2
3	BTI	G	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(°)	Ideal(°)
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(°)	Ideal(°)
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

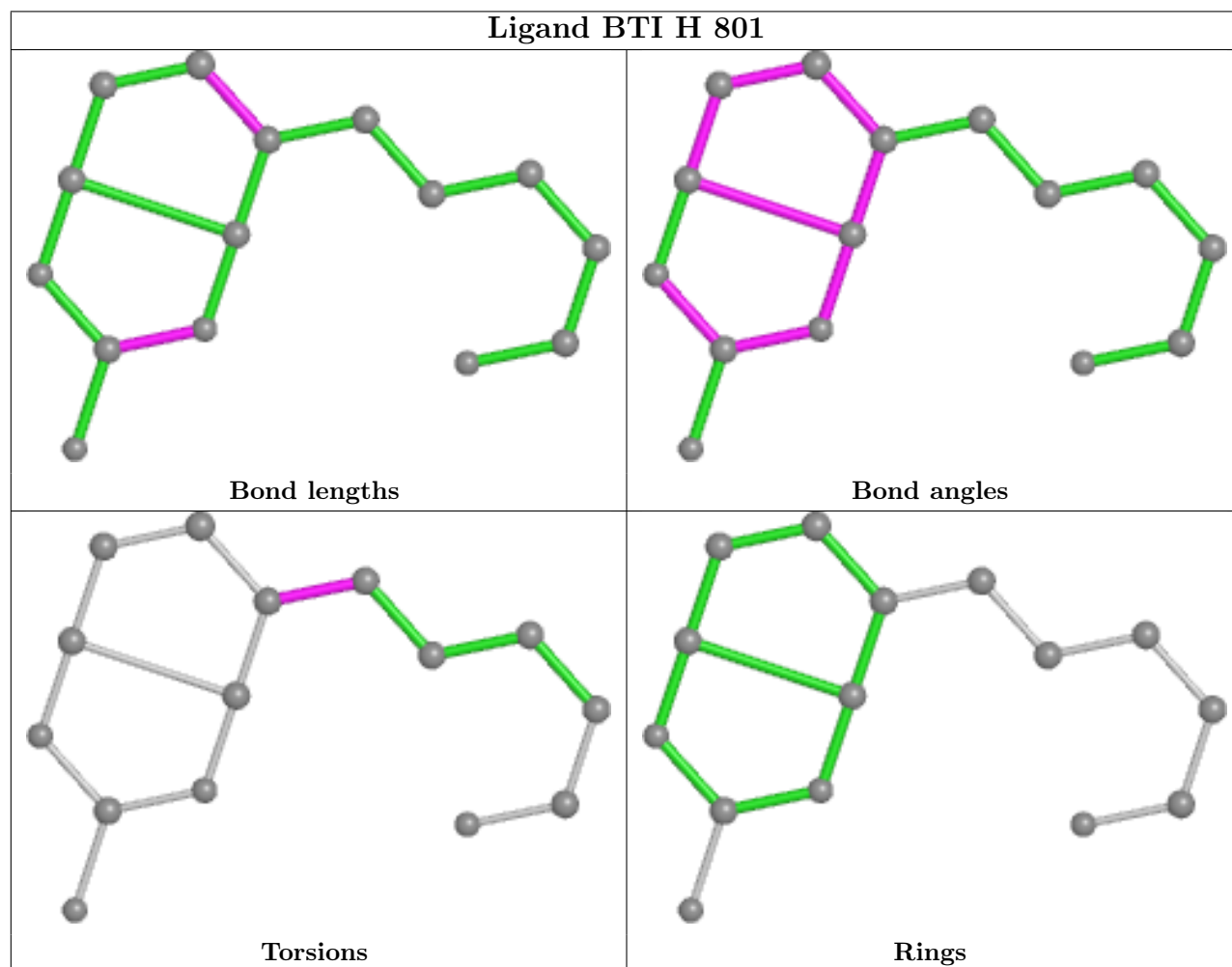
There are no ring outliers.

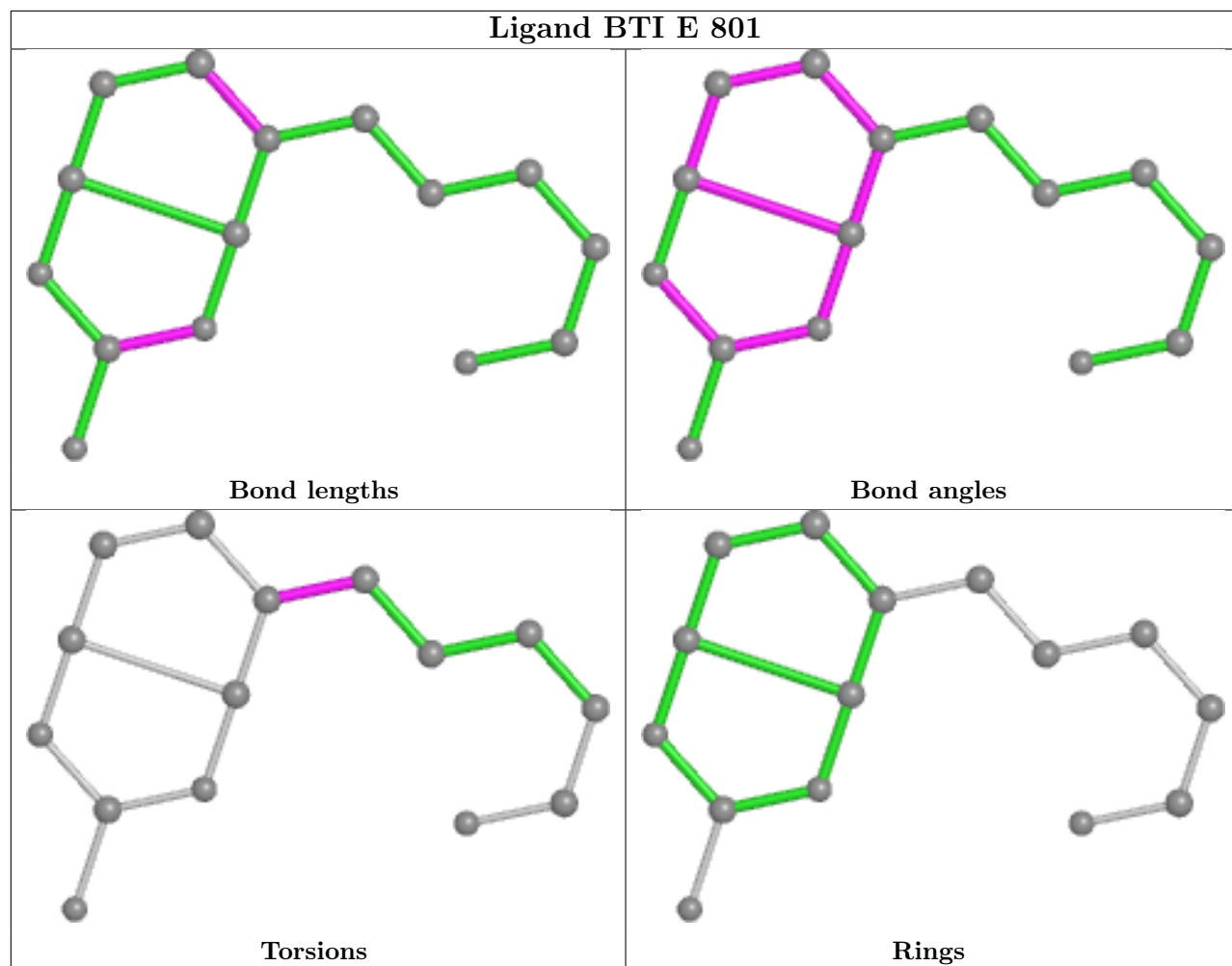
6 monomers are involved in 25 short contacts:

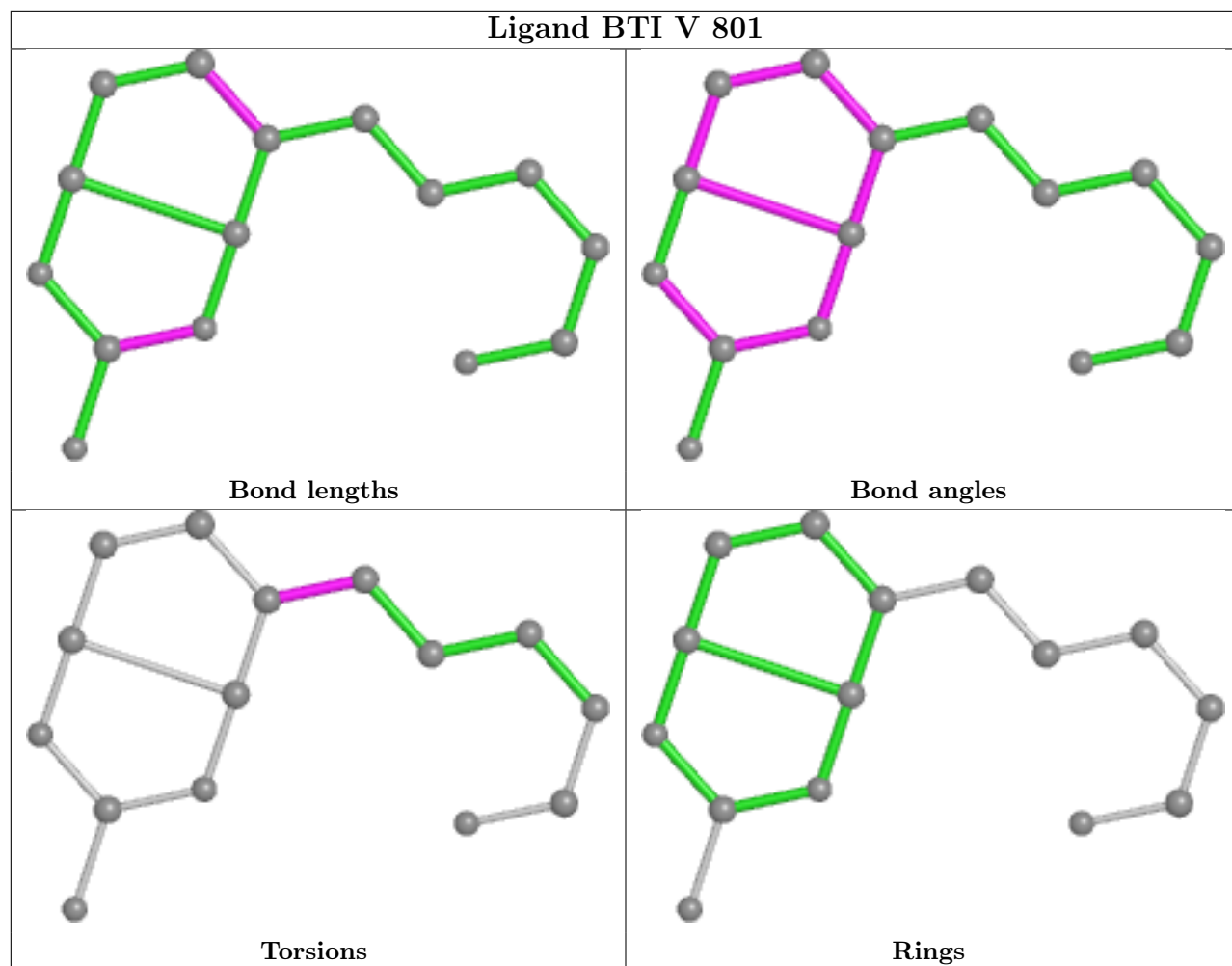
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	801	BTI	6	0
3	E	801	BTI	1	0
3	V	801	BTI	2	0
3	F	801	BTI	8	0
3	D	801	BTI	5	0
3	G	801	BTI	3	0

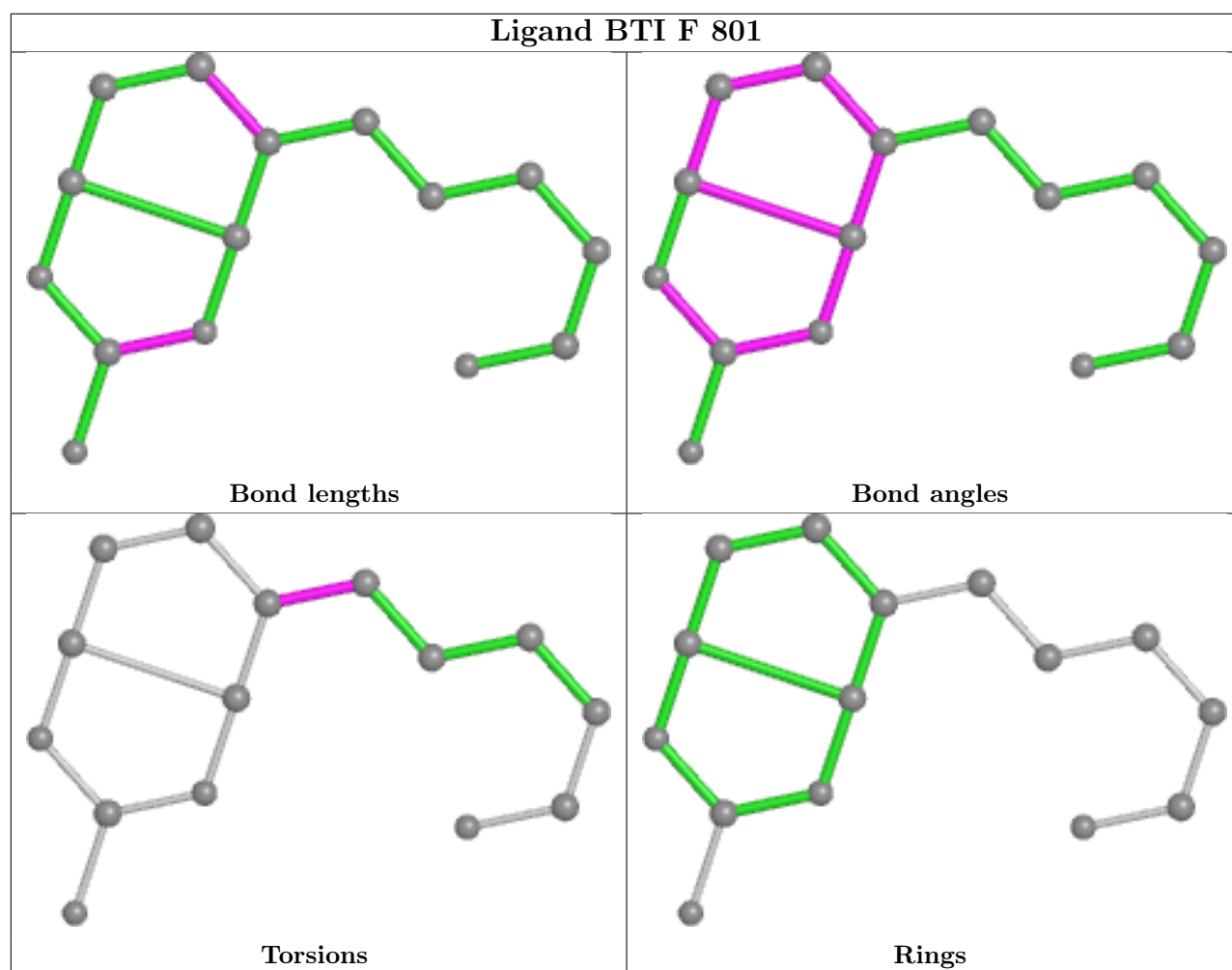
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

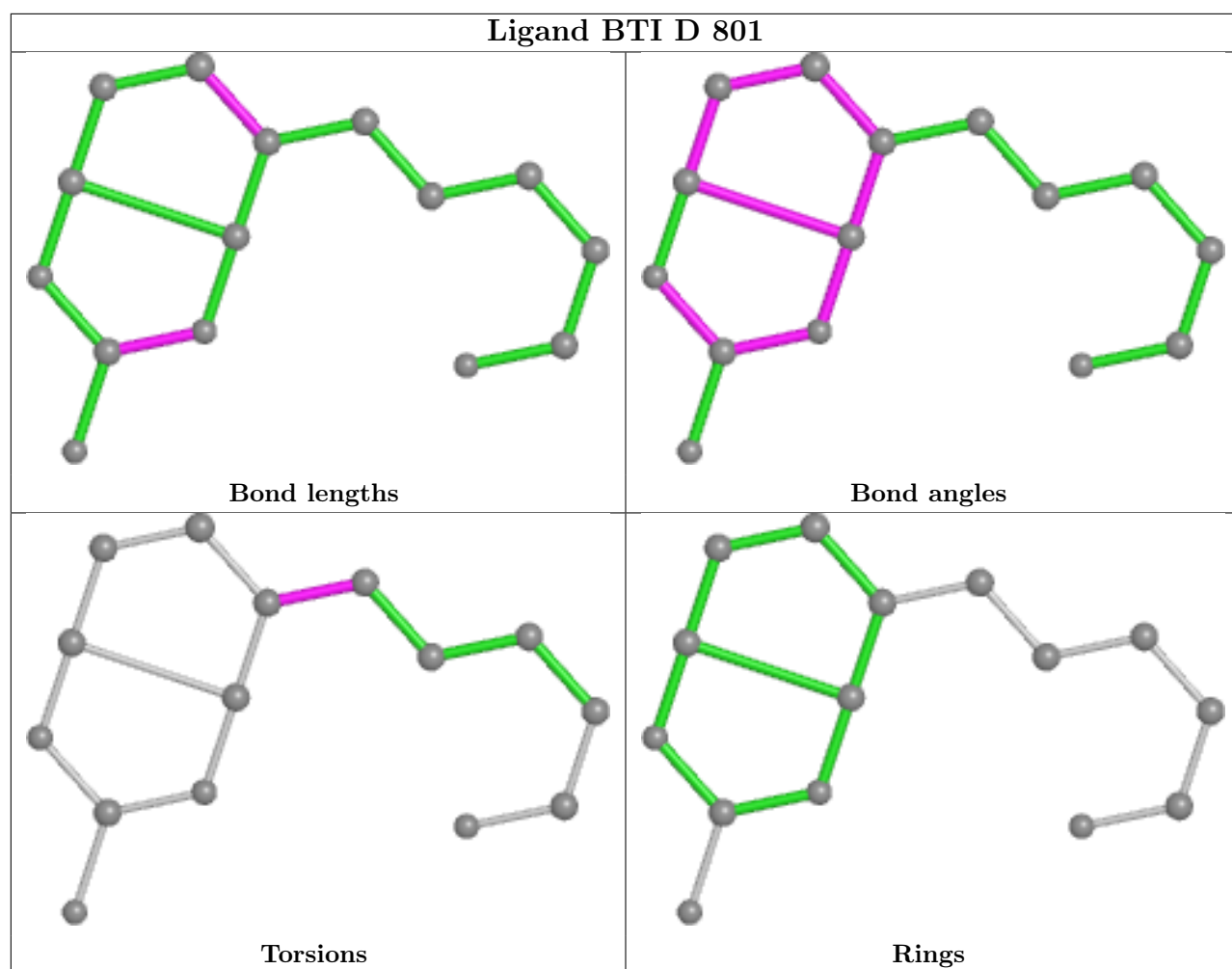
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

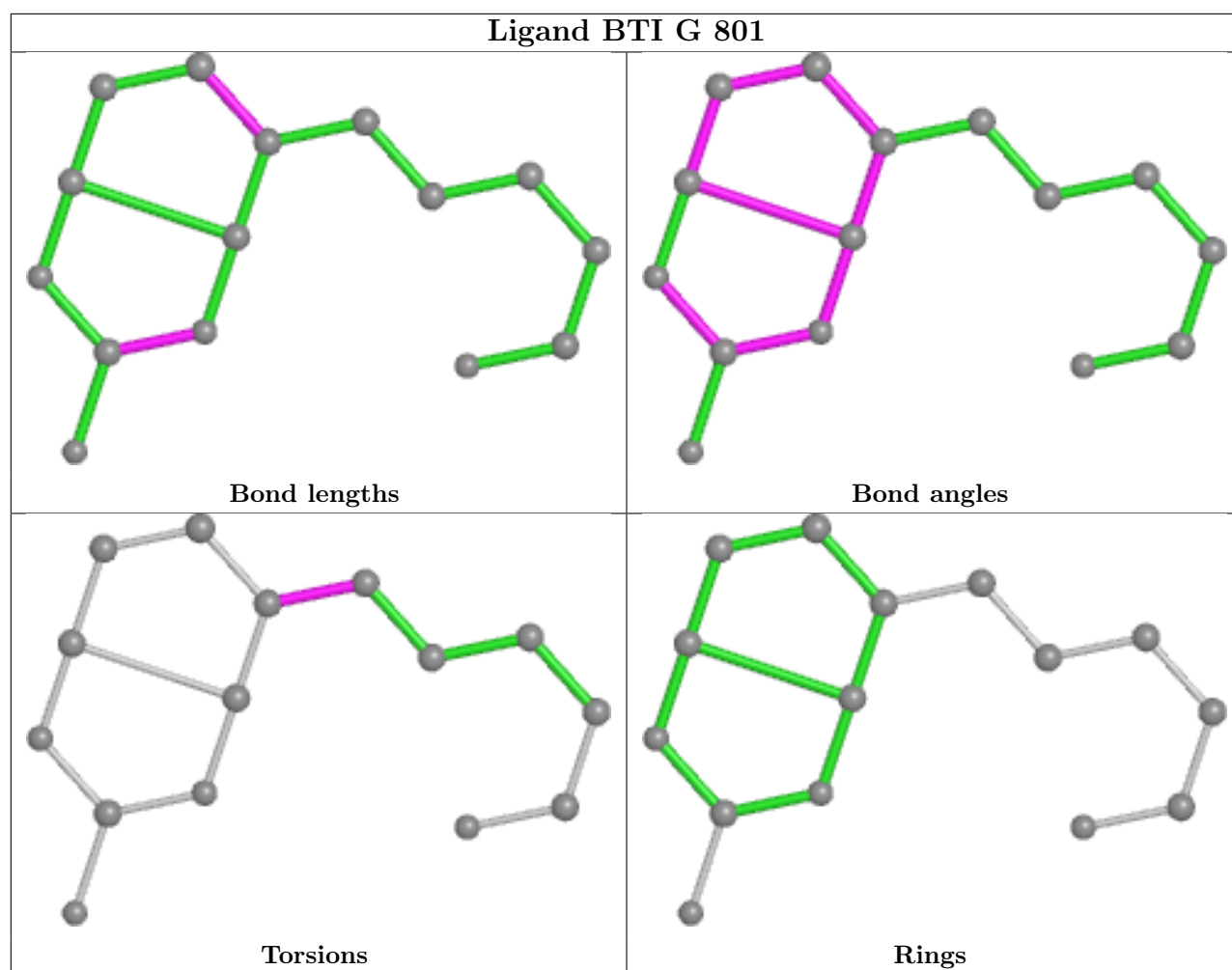












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

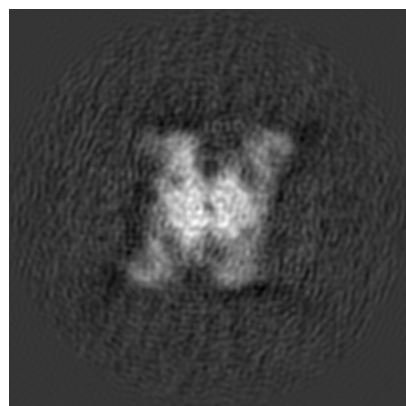
## 6 Map visualisation [i](#)

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

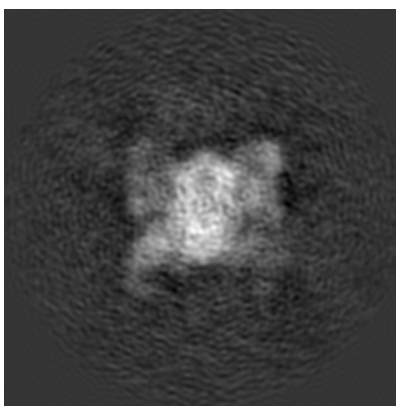
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

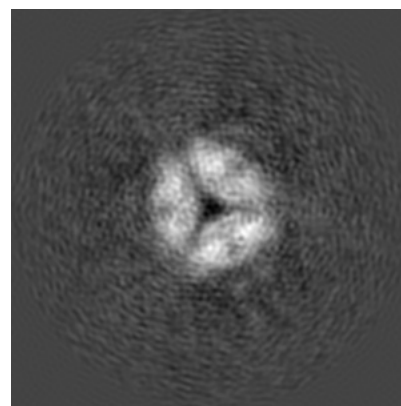
#### 6.1.1 Primary map



X

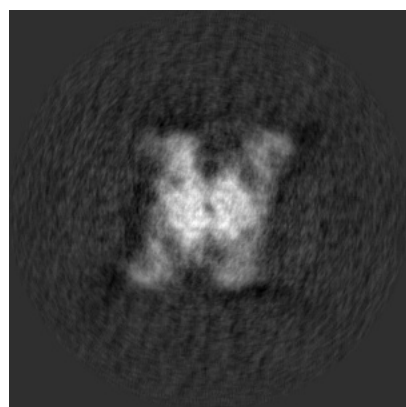


Y

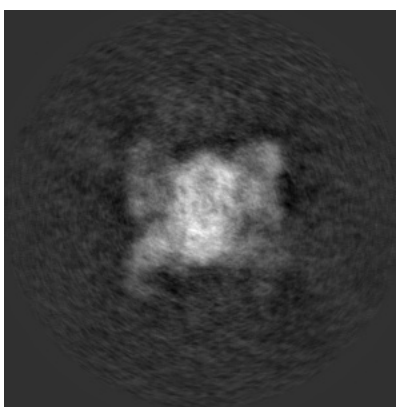


Z

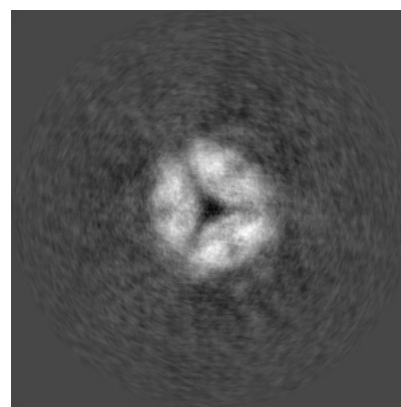
#### 6.1.2 Raw map



X



Y



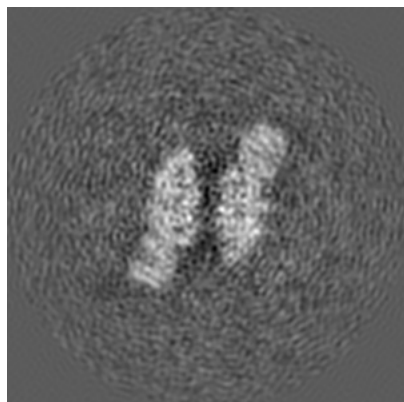
Z

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

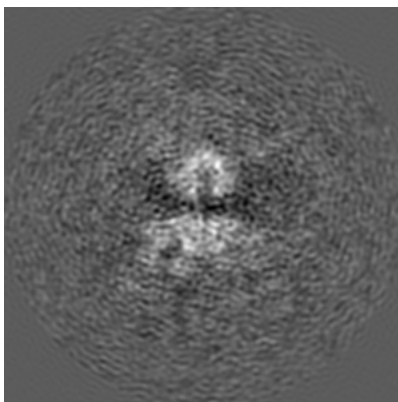


## 6.2 Central slices [i](#)

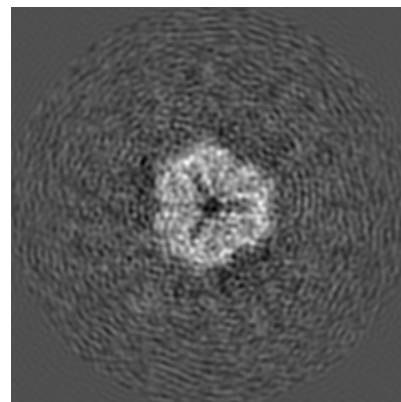
### 6.2.1 Primary map



X Index: 192

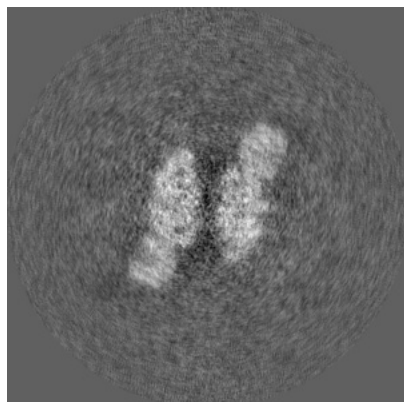


Y Index: 192

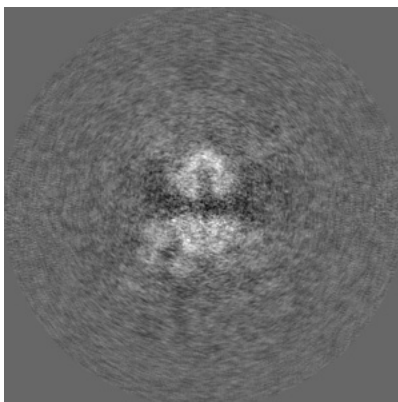


Z Index: 192

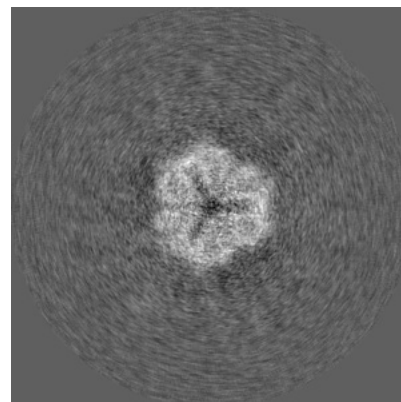
### 6.2.2 Raw map



X Index: 192



Y Index: 192

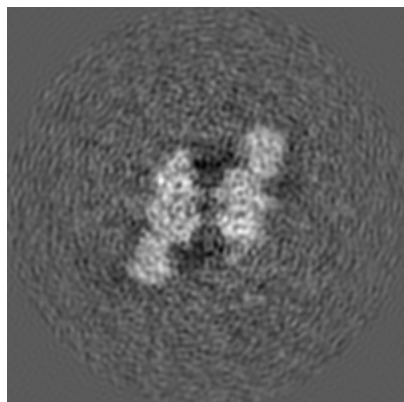


Z Index: 192

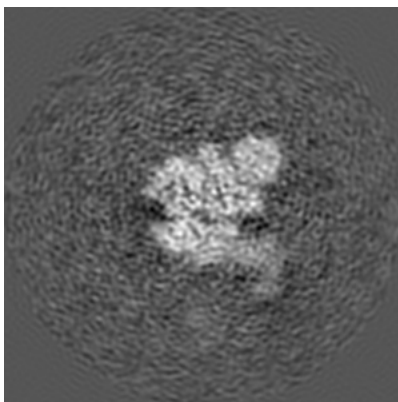
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

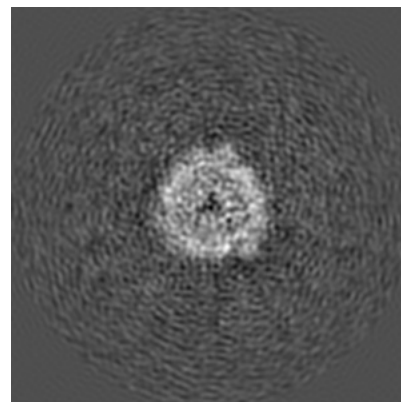
### 6.3.1 Primary map



X Index: 187

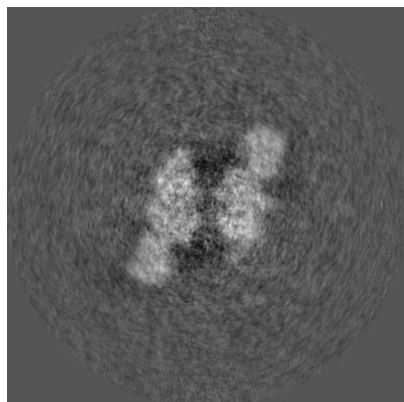


Y Index: 173

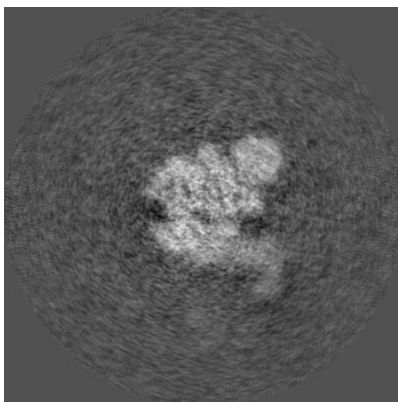


Z Index: 204

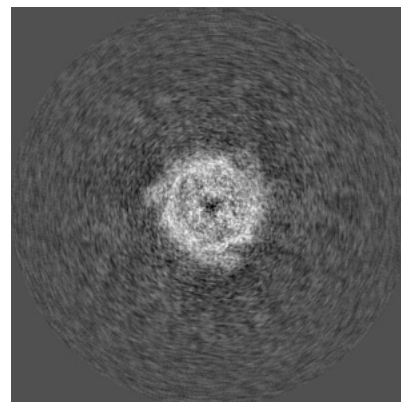
### 6.3.2 Raw map



X Index: 187



Y Index: 173

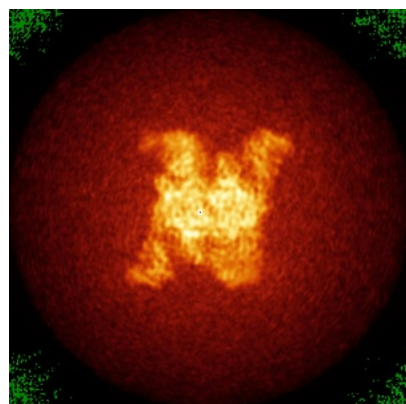


Z Index: 179

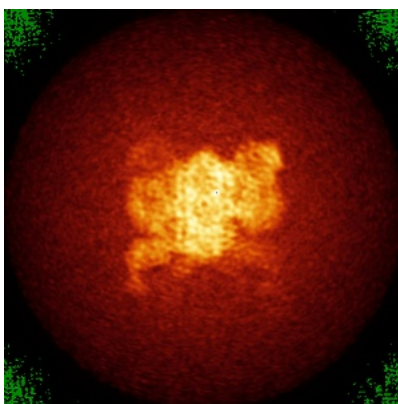
The images above show the largest variance slices of the map in three orthogonal directions.

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

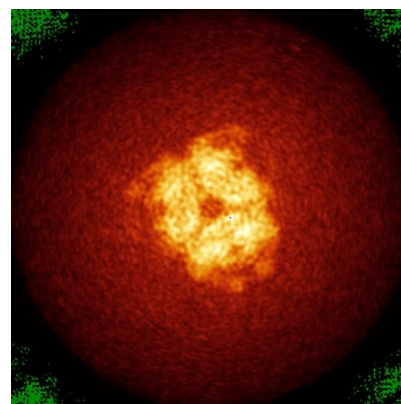
### 6.4.1 Primary map



X

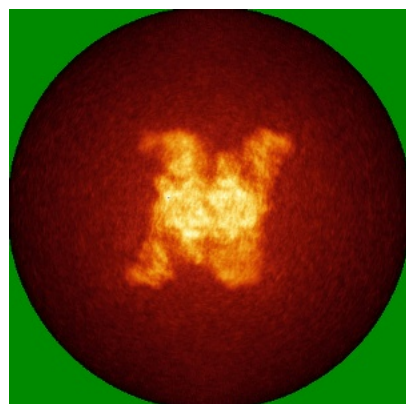


Y

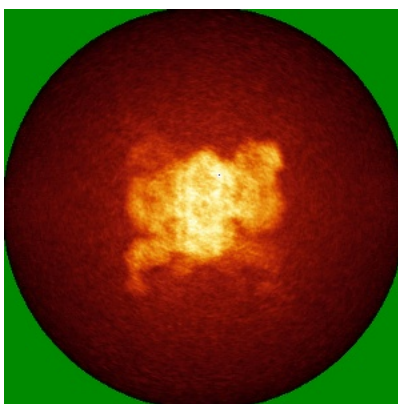


Z

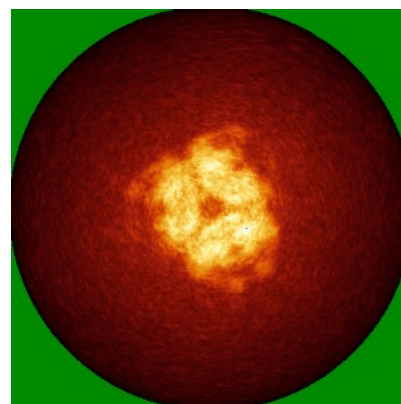
### 6.4.2 Raw map



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.

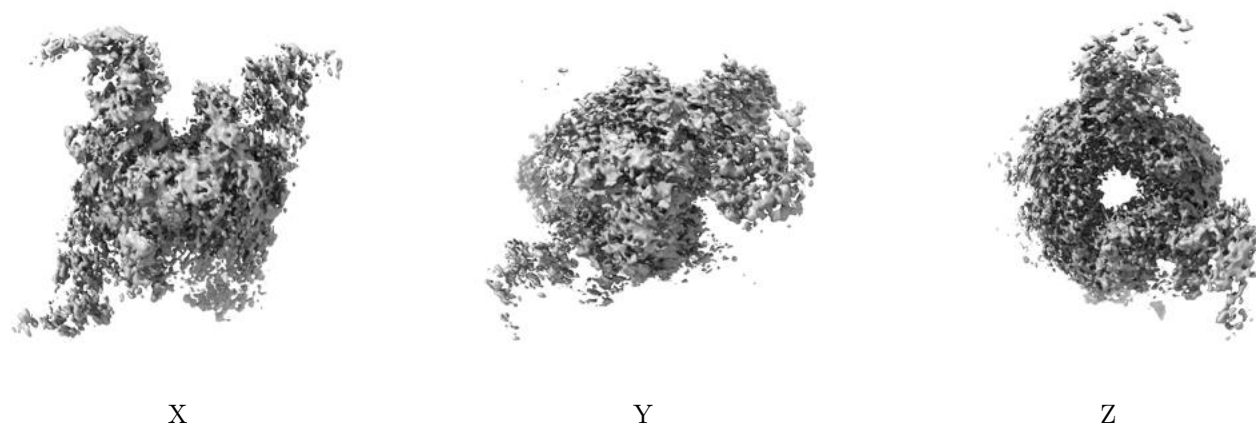
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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



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.

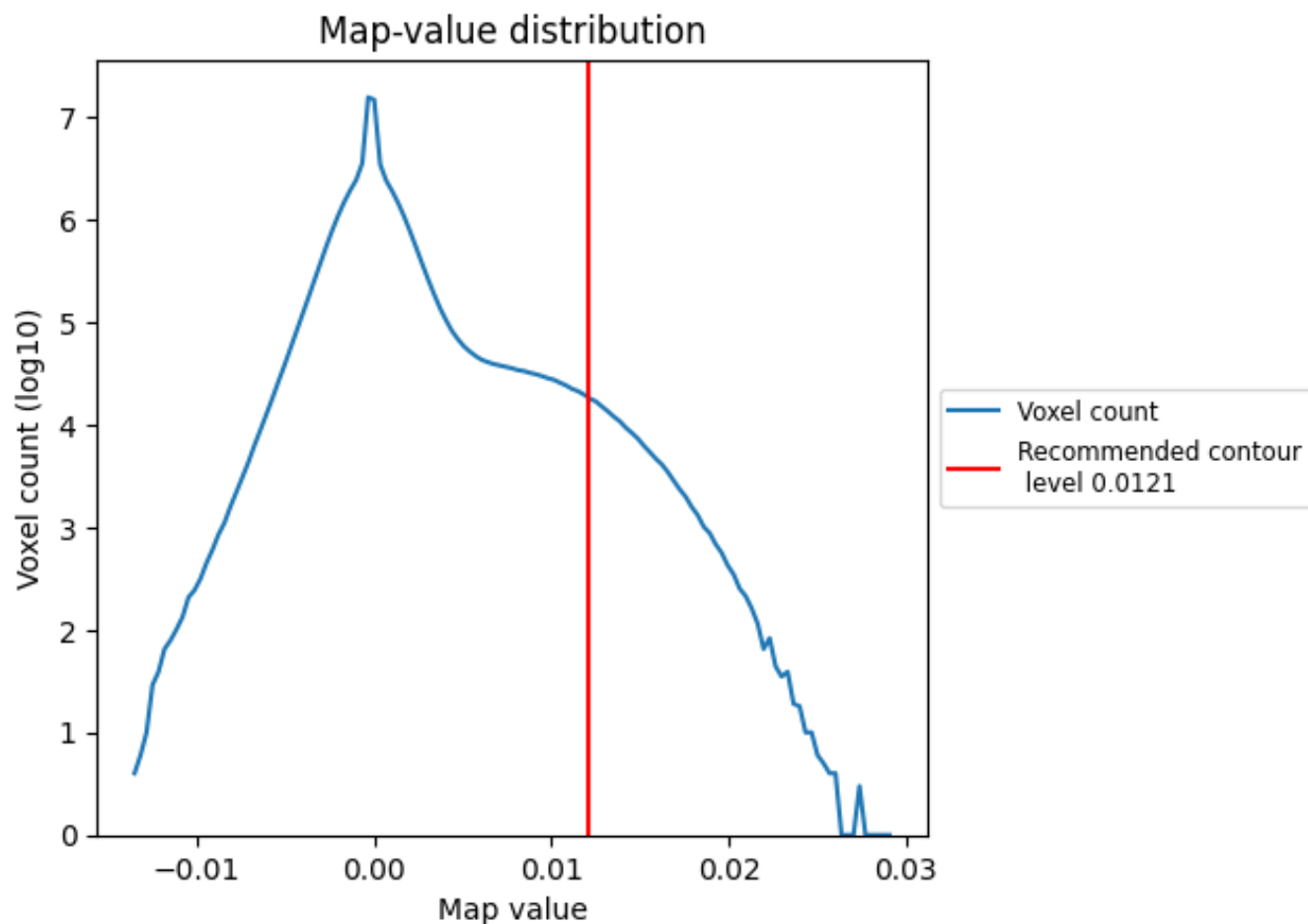
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

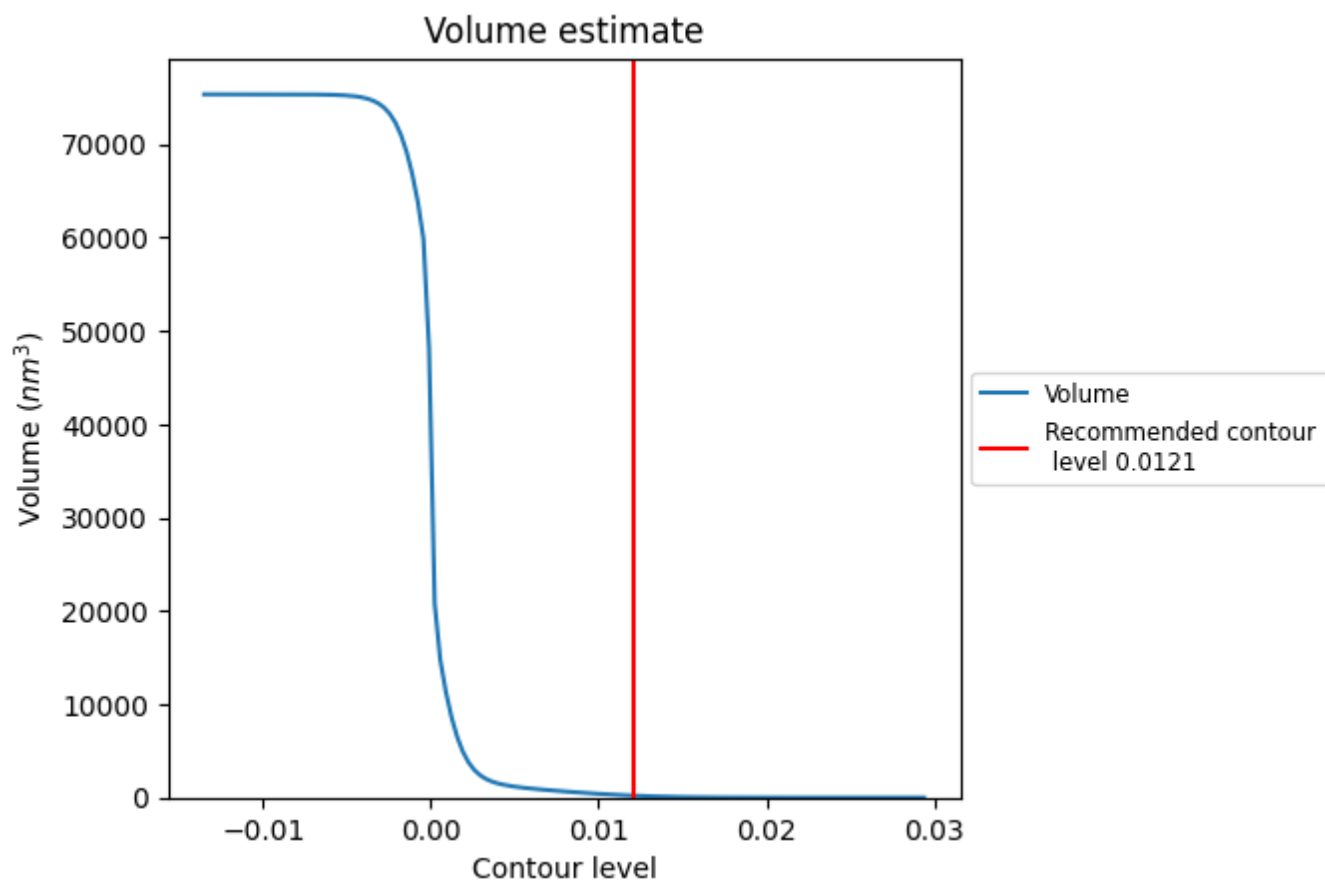
### 7.1 Map-value distribution [i](#)



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



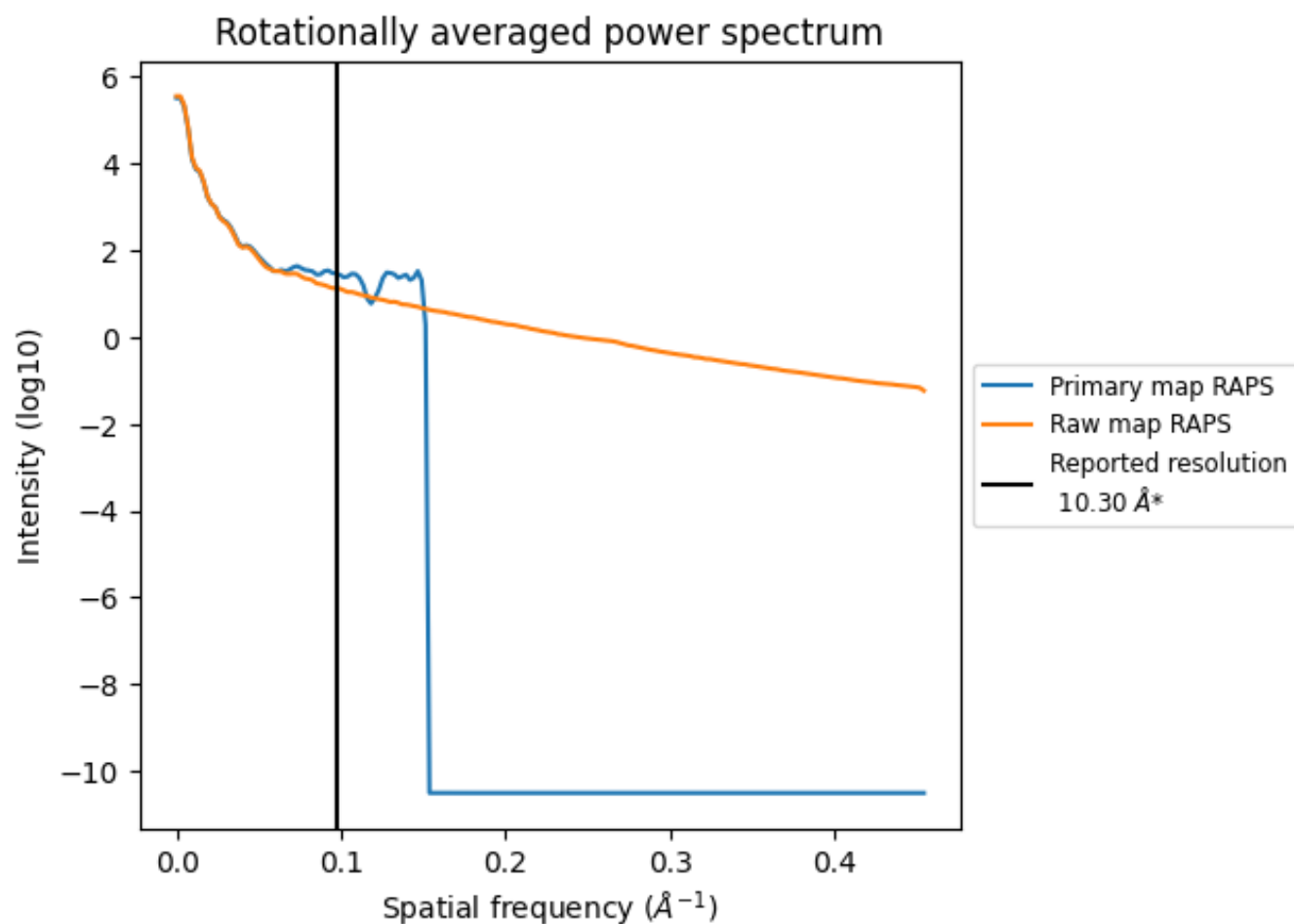
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm<sup>3</sup>; 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 ⓘ

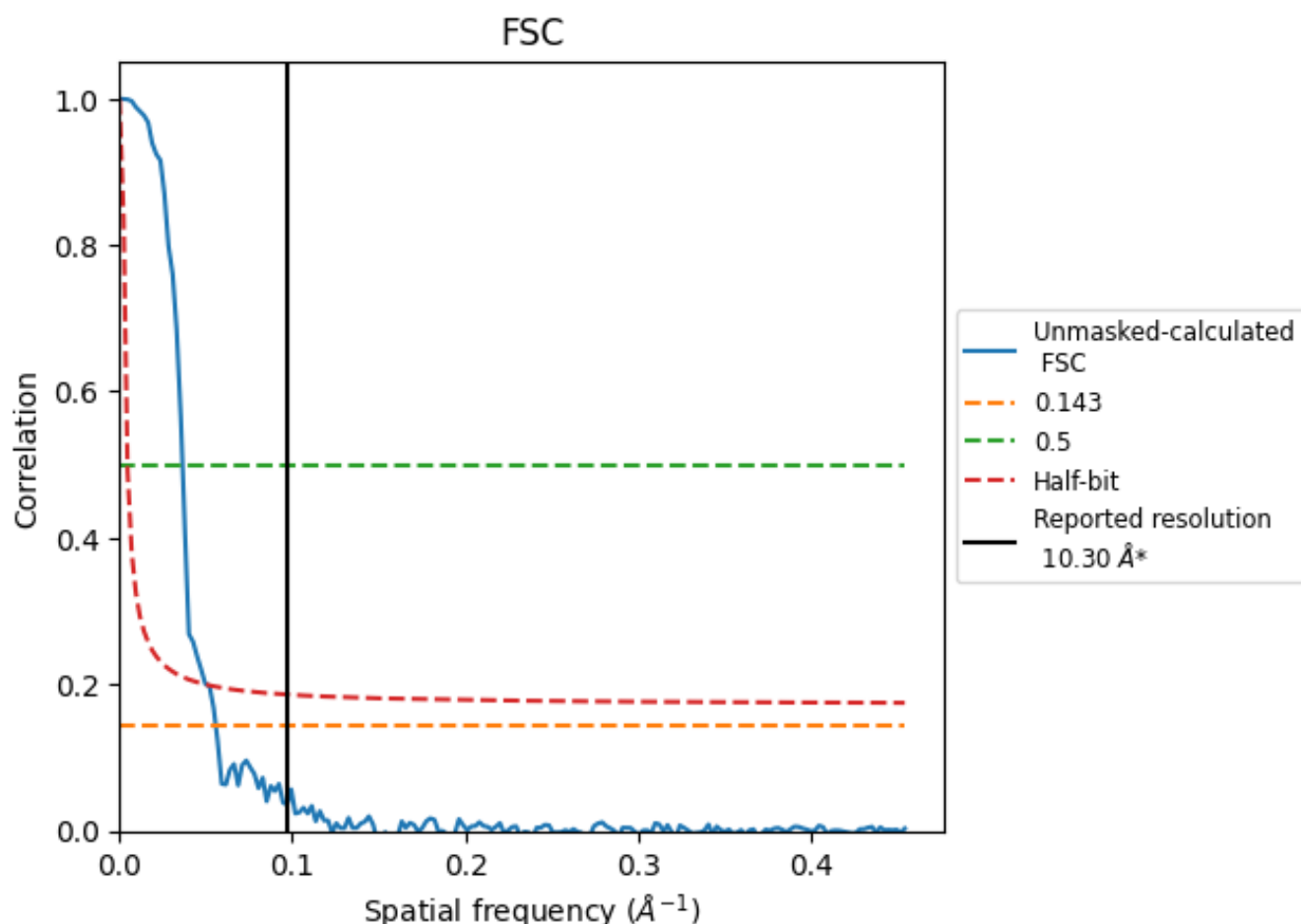


\*Reported resolution corresponds to spatial frequency of 0.097 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.097 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

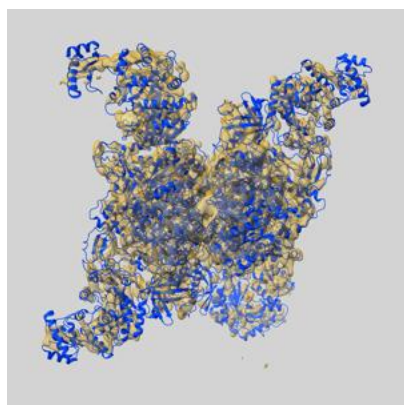
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	17.95	27.40	19.72

\*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 %

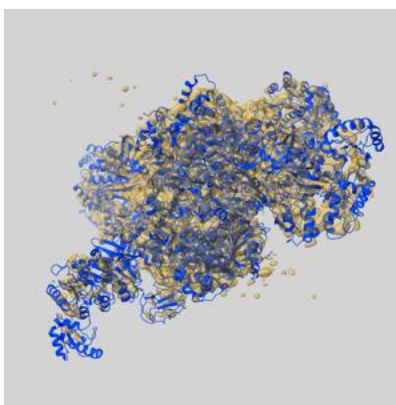
## 9 Map-model fit [i](#)

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.

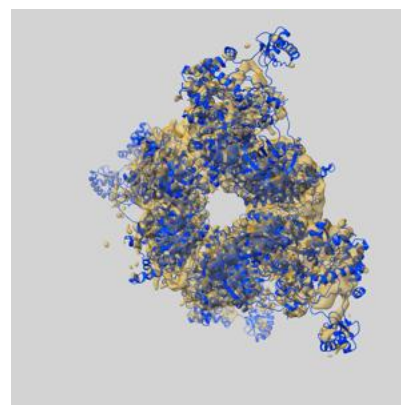
### 9.1 Map-model overlay [i](#)



X



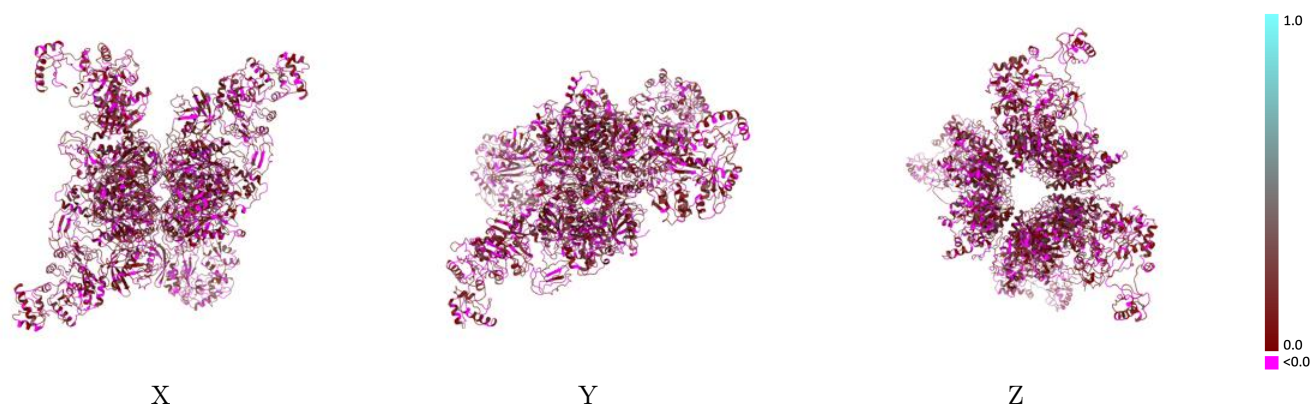
Y



Z

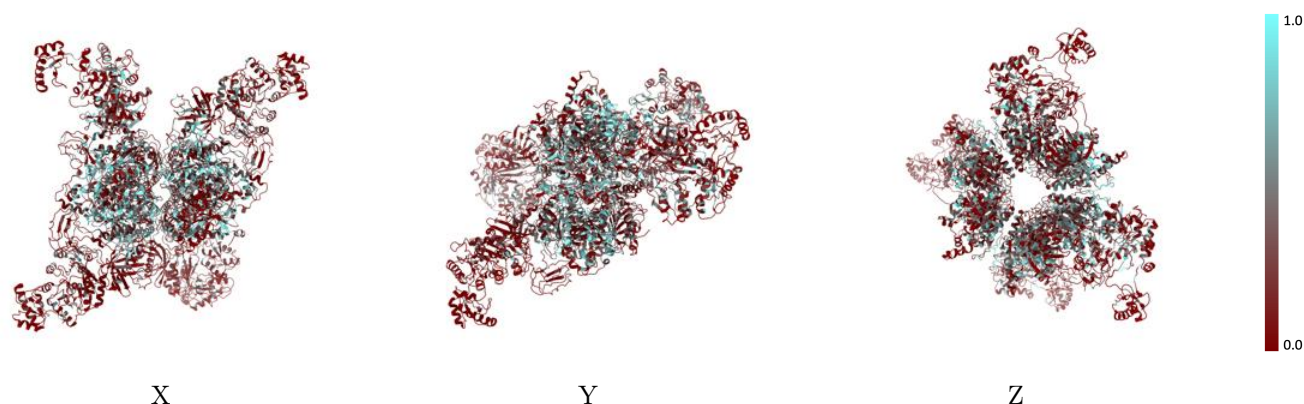
The images above show the 3D surface view of the map at the recommended contour level 0.0121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



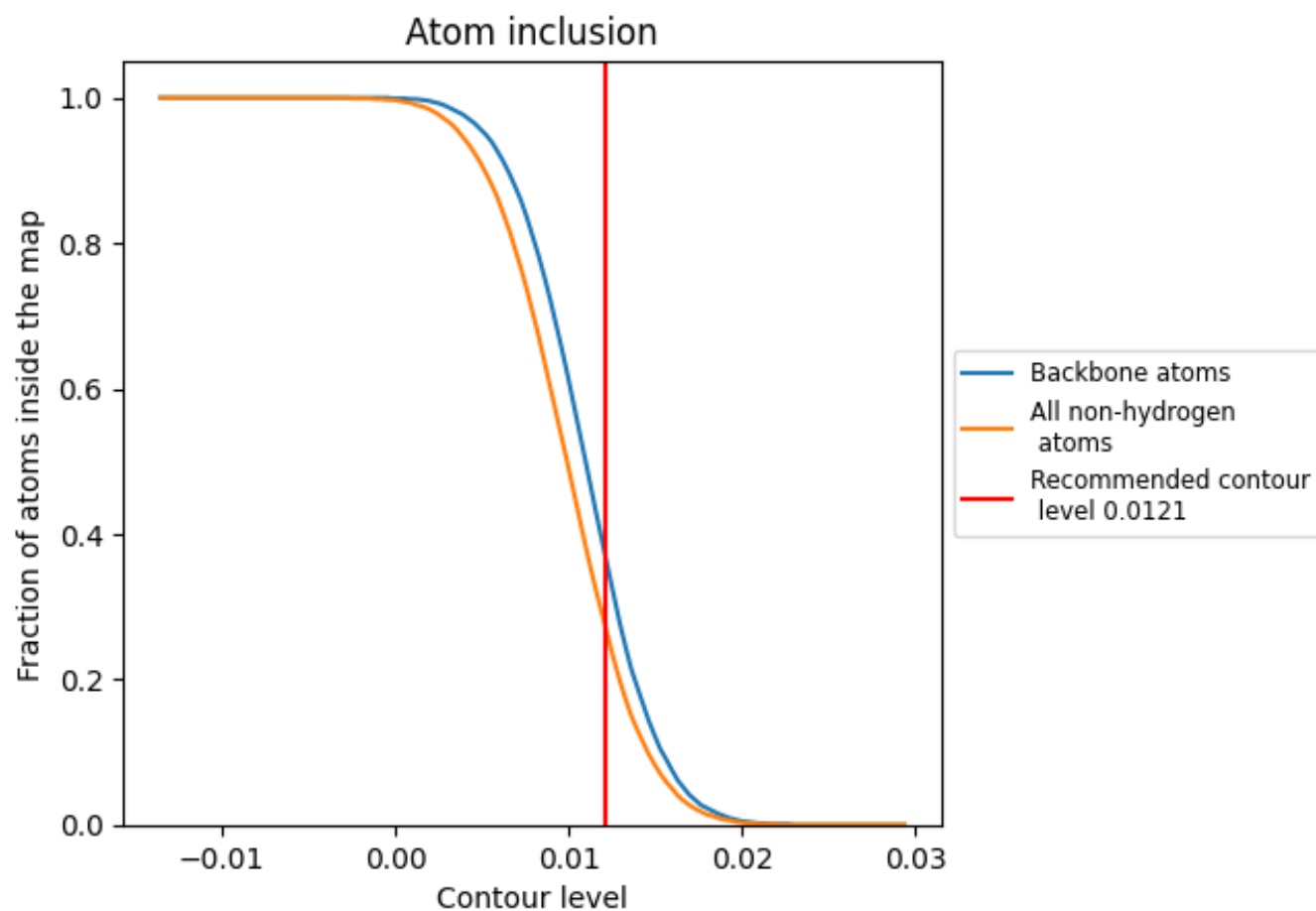
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0121).

## 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	<div></div> 0.2760	<div></div> 0.0890
C	<div></div> 0.4180	<div></div> 0.1080
D	<div></div> 0.2810	<div></div> 0.0790
E	<div></div> 0.4280	<div></div> 0.1100
F	<div></div> 0.3940	<div></div> 0.0980
G	<div></div> 0.3590	<div></div> 0.0810
H	<div></div> 0.4030	<div></div> 0.0970
S	<div></div> 0.0880	<div></div> 0.0780
V	<div></div> 0.2320	<div></div> 0.0830
X	<div></div> 0.1800	<div></div> 0.0860
Z	<div></div> 0.1380	<div></div> 0.0850

1.0

0.0

<0.0