



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:01 PM UTC

PDB ID : 8SGX / pdb_00008sgx
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:

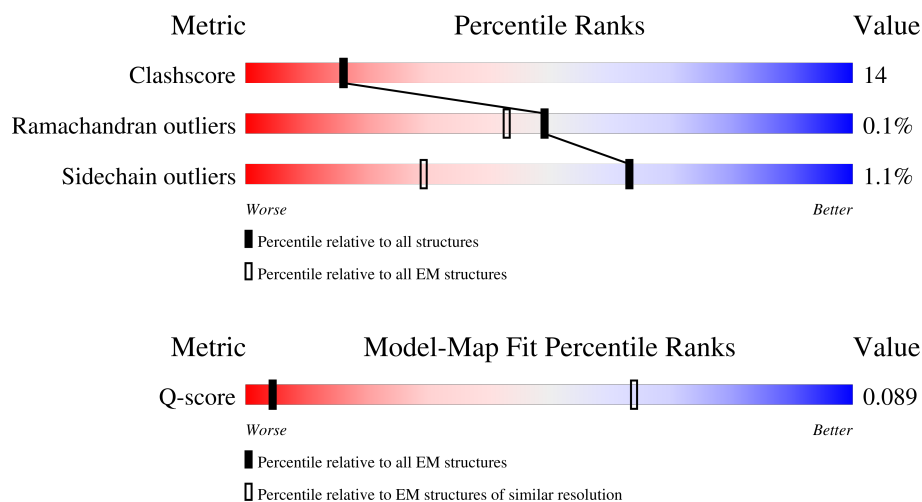
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	116 (9.80 - 10.80)

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

Mol	Chain	Length	Quality of chain
1	C	489	50% 81% 19%
1	D	489	69% 82% 18%
1	E	489	48% 81% 19%
1	F	489	54% 81% 18%

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Mol	Chain	Length	Quality of chain
1	G	489	
1	H	489	
2	S	657	
2	V	657	
2	X	657	
2	Z	657	

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.

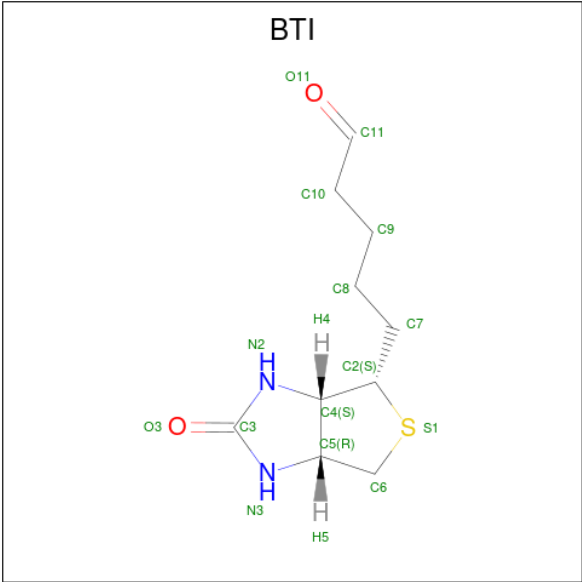
- Molecule 1 is a protein called Propionyl-coa carboxylase beta chain, putative.

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 (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S) (labeled as "Ligand of Interest" by depositor).

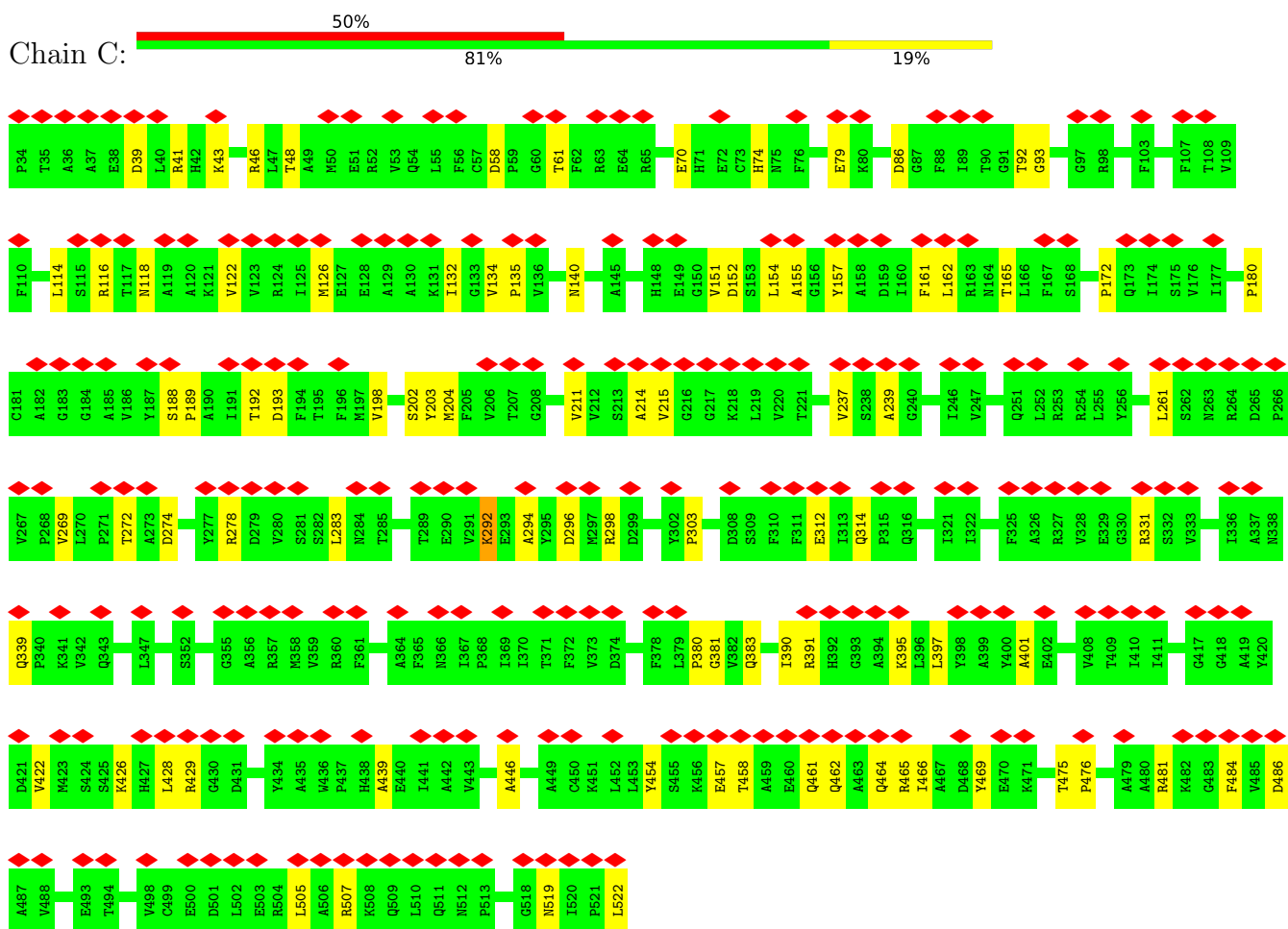


Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	E	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	F	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	G	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	H	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	V	1	Total	C	N	O	S	0
			15	10	2	2	1	

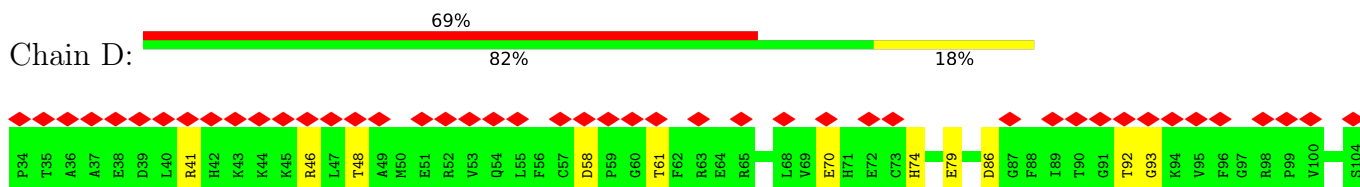
3 Residue-property plots

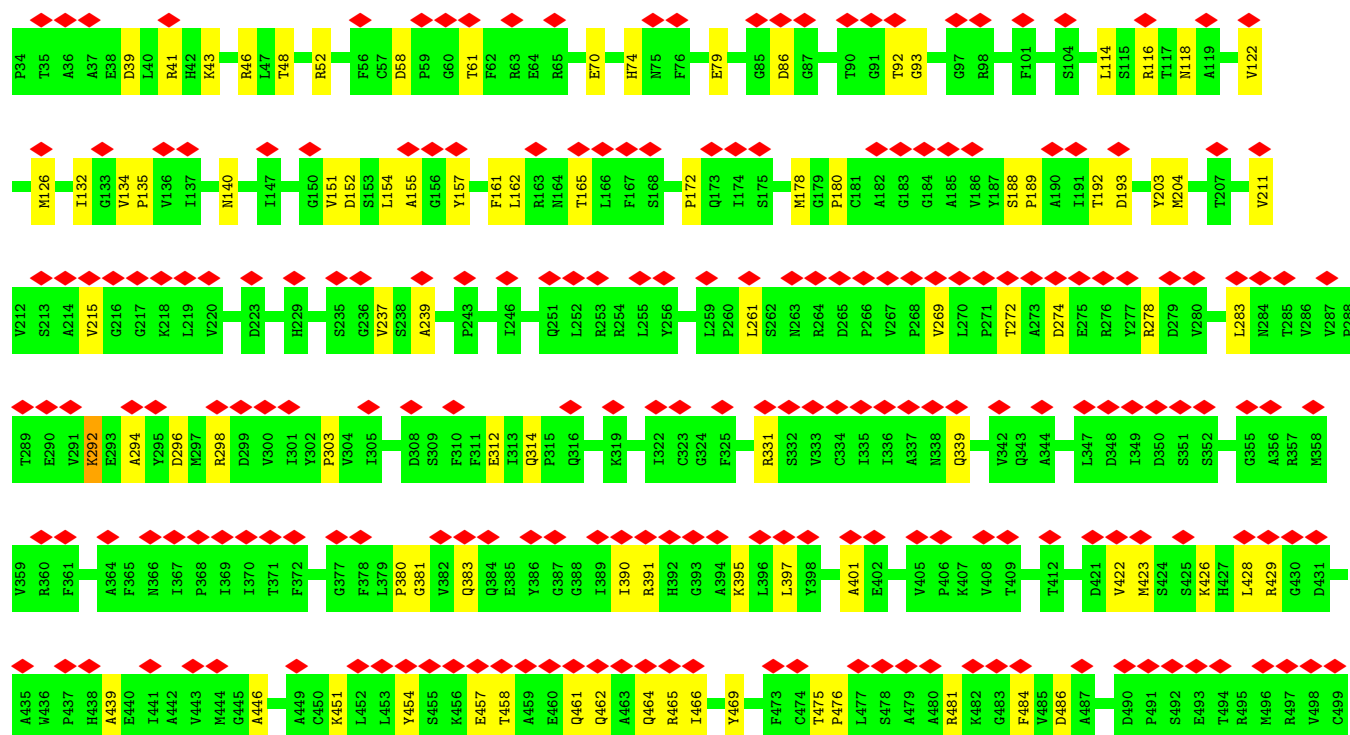
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

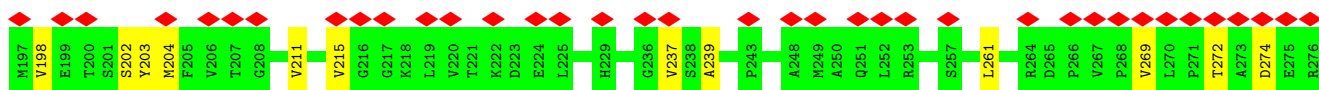
- Molecule 1: Propionyl-coa carboxylase beta chain, putative

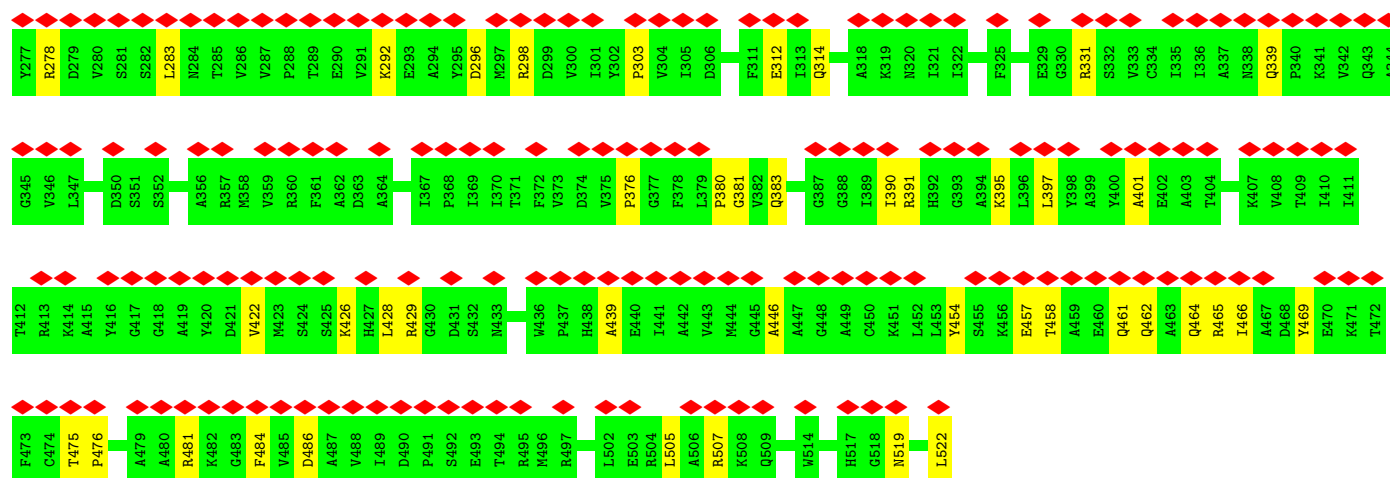


- Molecule 1: Propionyl-coa carboxylase beta chain, putative

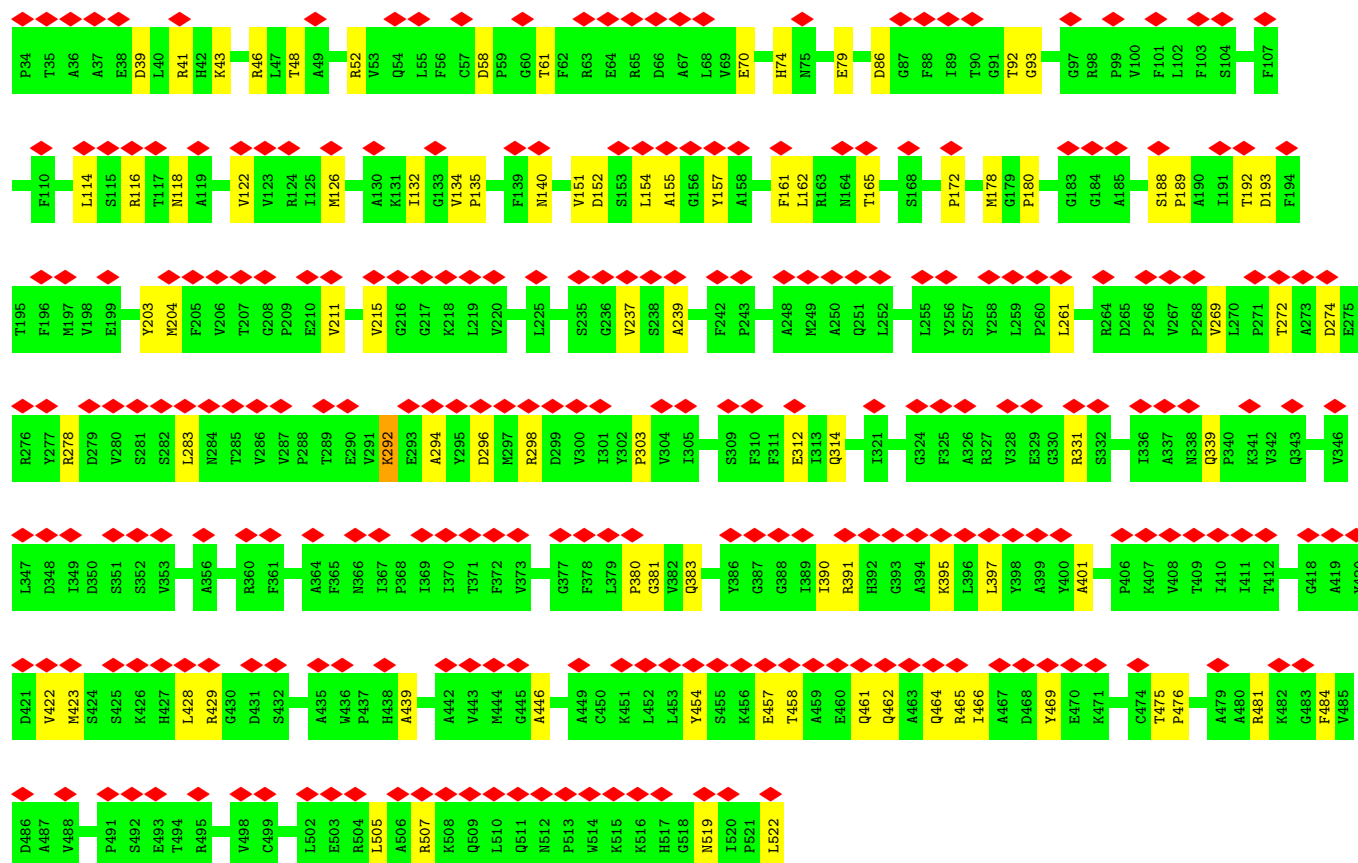
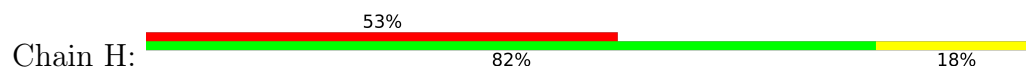






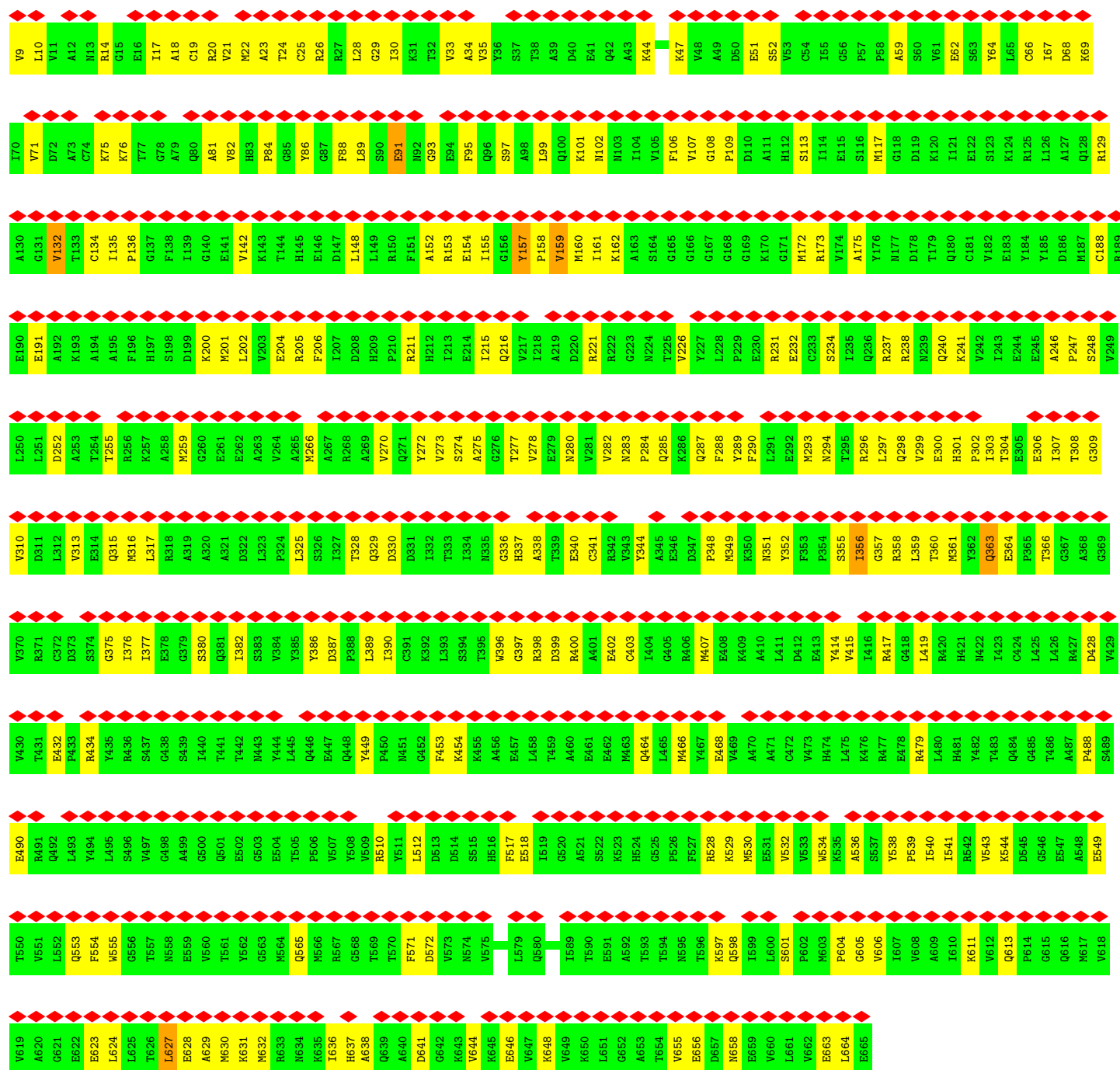


- Molecule 1: Propionyl-coa carboxylase beta chain, putative



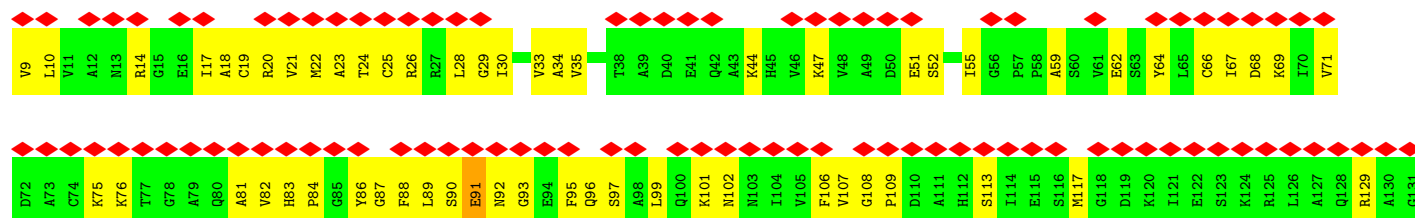
- Molecule 2: propionyl-CoA carboxylase

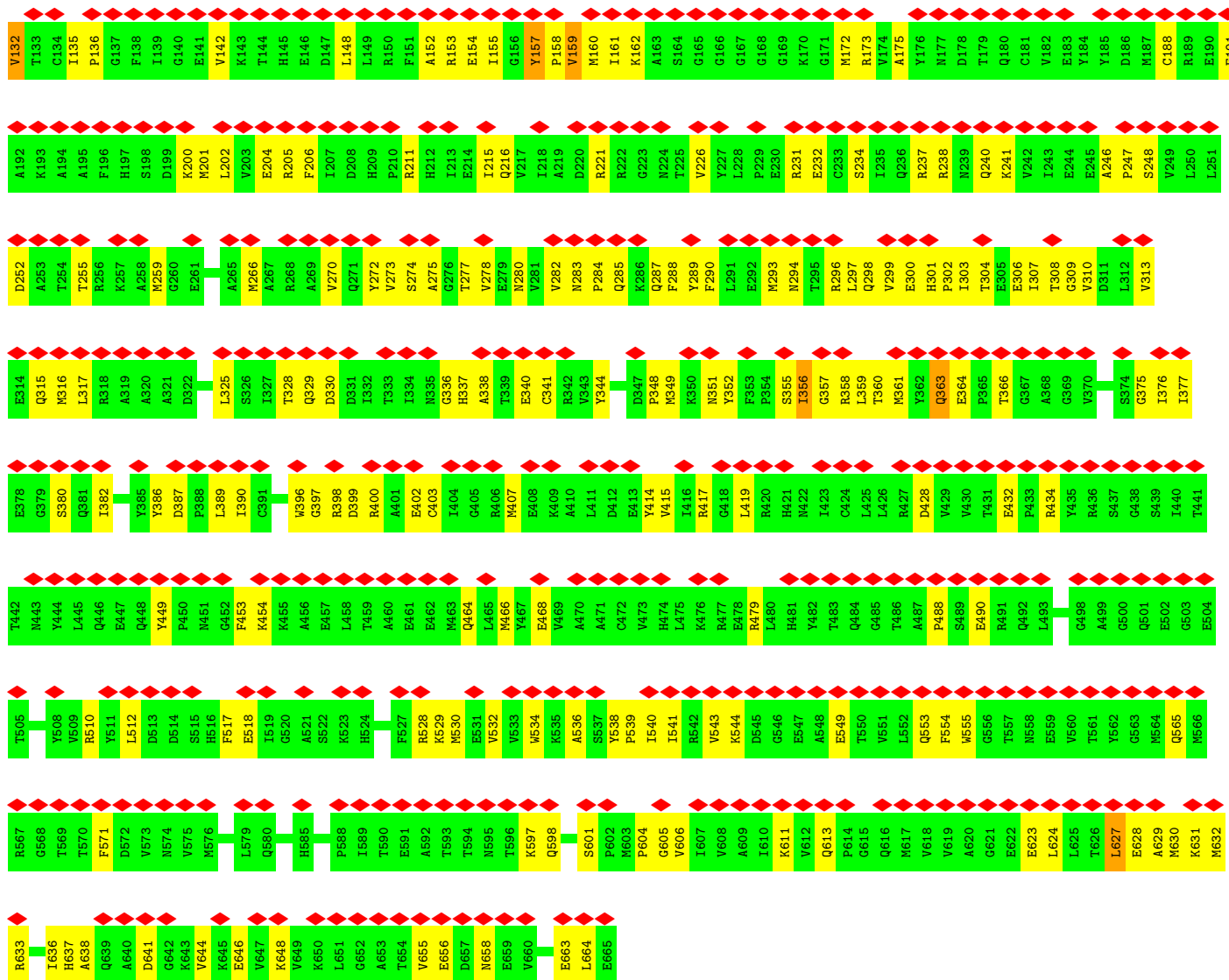




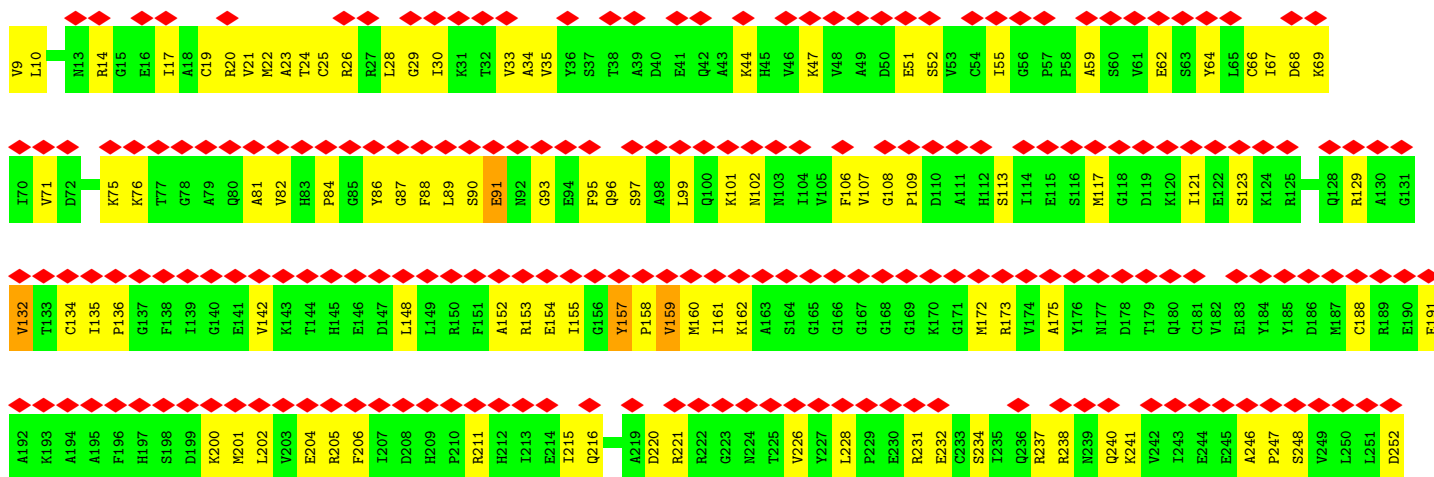
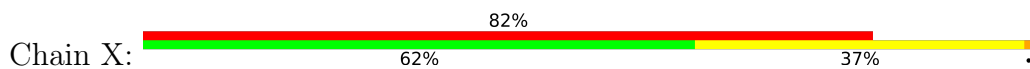
• Molecule 2: propionyl-CoA carboxylase

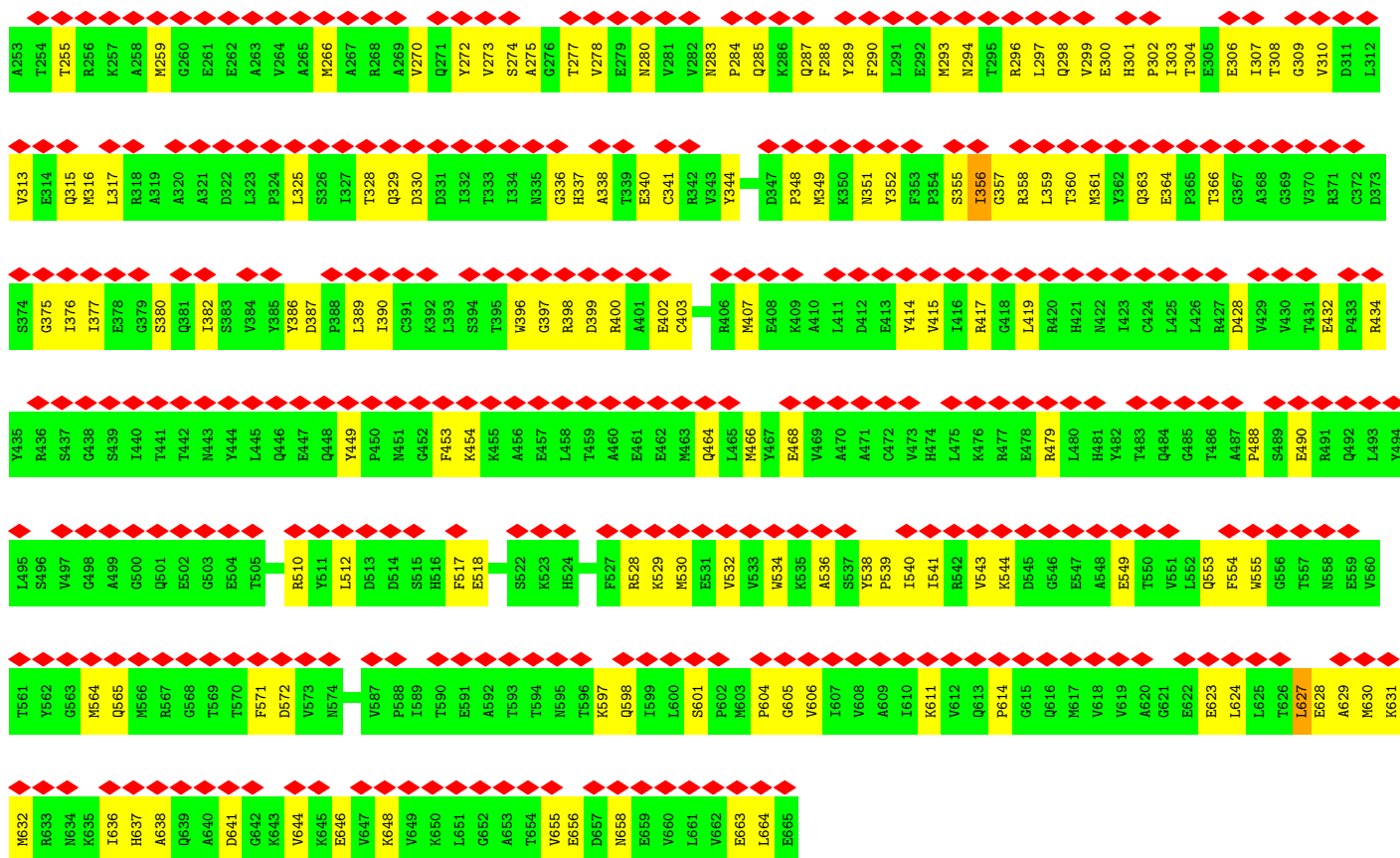
Chain V: 75% 62% 37%



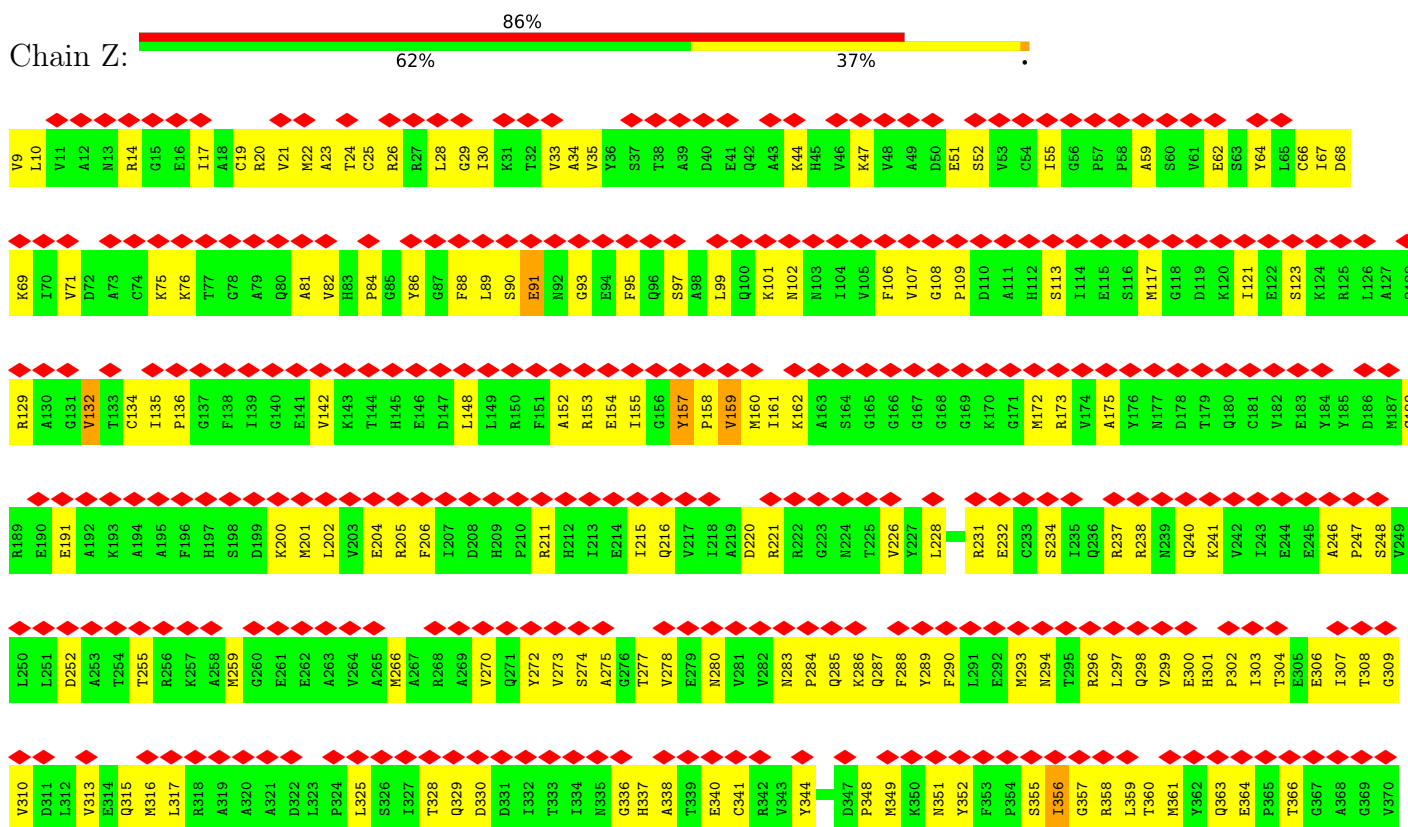


• Molecule 2: propionyl-CoA carboxylase





• Molecule 2: propionyl-CoA carboxylase



Q616	M617	V618	V619	A620	G621	E622	E623	L624	L625	T626	L627	E628	A629	M630	K631	M632	R633	M634	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	E663	L664	E665											
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		
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	
T431	E432	P433	R434	Y435	R436	S437	G438	S439	I440	T441	T442	M443	Q446	E447	Q448	Y449	P450	M451	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	
R371	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	C404	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

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	0.20	0/3851	0.36	0/5217
1	D	0.20	0/3851	0.36	0/5217
1	E	0.20	0/3851	0.36	0/5217
1	F	0.20	0/3851	0.36	0/5217
1	G	0.20	0/3851	0.36	0/5217
1	H	0.20	0/3851	0.36	0/5217
2	S	0.26	0/5213	0.55	1/7048 (0.0%)
2	V	0.26	0/5213	0.55	1/7048 (0.0%)
2	X	0.26	0/5213	0.55	1/7048 (0.0%)
2	Z	0.26	0/5213	0.55	1/7048 (0.0%)
All	All	0.23	0/43958	0.46	4/59494 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	309	GLY	N-CA-C	-5.68	107.35	115.64
2	X	309	GLY	N-CA-C	-5.65	107.40	115.64
2	S	309	GLY	N-CA-C	-5.64	107.40	115.64
2	Z	309	GLY	N-CA-C	-5.64	107.41	115.64

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	77	0
1	D	3766	0	3762	73	0
1	E	3766	0	3762	75	0
1	F	3766	0	3762	81	0
1	G	3766	0	3762	72	0
1	H	3766	0	3762	76	0
2	S	5124	0	5108	215	0
2	V	5124	0	5108	221	0
2	X	5124	0	5108	220	0
2	Z	5124	0	5108	219	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	1233	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1233) 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:X:160:MET:HE2	2:X:206:PHE:HA	1.51	0.91
2:V:160:MET:HE2	2:V:206:PHE:HA	1.51	0.91
2:Z:160:MET:HE2	2:Z:206:PHE:HA	1.51	0.90
2:S:160:MET:HE2	2:S:206:PHE:HA	1.51	0.89
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:S:528:ARG:HH12	2:S:530:MET:HE3	1.55	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:V:528:ARG:HH12	2:V:530:MET:HE3	1.55	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
2:Z:528:ARG:HH12	2:Z:530:MET:HE3	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:528:ARG:HH12	2:X:530:MET:HE3	1.55	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:S:313:VAL:HA	2:S:316:MET:HE2	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
2:S:348:PRO:HA	2:S:352:TYR:HD1	1.55	0.70
2:V:313:VAL:HA	2:V:316:MET:HE2	1.74	0.69
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:X:313:VAL:HA	2:X:316:MET:HE2	1.74	0.68
2:V:135:ILE:HD12	2:V:136:PRO:HD2	1.75	0.68
2:Z:313:VAL:HA	2:Z:316:MET:HE2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:V:298:GLN:OE1	2:V:300:GLU:CD	2.42	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:X:298:GLN:OE1	2:X:300:GLU:CD	2.42	0.62
2:Z:298:GLN:OE1	2:Z:300:GLU:CD	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:298:GLN:OE1	2:S:300:GLU:CD	2.42	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:X:466:MET:HE1	2:X:571:PHE:HB2	1.81	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:V:466:MET:HE1	2:V:571:PHE:HB2	1.81	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:Z:466:MET:HE1	2:Z:571:PHE:HB2	1.81	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
2:V:337:HIS:NE2	2:V:400:ARG:HD2	2.16	0.61
2:S:466:MET:HE1	2:S:571:PHE:HB2	1.81	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:132:ILE:HD11	1:D:505:LEU:HD23	1.86	0.58
1:C:390:ILE:HD13	1:H:204:MET:HE2	1.85	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
1:D:390:ILE:HD13	1:F:204:MET:HE2	1.87	0.57
2:V:364:GLU:OE2	2:V:540:ILE:HD11	2.04	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: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: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
1:E:390:ILE:HD13	1:G:204:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:204:MET:HE2	1:F:390:ILE:HD13	1.88	0.56
1:E:204:MET:HE2	1:G:390:ILE:HD13	1.87	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
1:C:204:MET:HE2	1:H:390:ILE:HD13	1.88	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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:301:HIS:O	2:X:302:PRO:C	2.51	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:S:360:THR:O	2:S:361:MET:C	2.52	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
2:Z:159:VAL:CB	2:Z:175:ALA:HB3	2.39	0.53
2:Z:301:HIS:O	2:Z:302:PRO:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:294:ALA:HA	2:V:632:MET:HE3	1.92	0.52
1:E:294:ALA:HA	2:X:632:MET:HE3	1.92	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:V:360:THR:O	2:V:361:MET:C	2.52	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
2:S:109:PRO:HB3	2:S:272:TYR:HE1	1.73	0.52
2:V:301:HIS:O	2:V:302:PRO:C	2.51	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:294:ALA:HA	2:Z:632:MET:HE3	1.92	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:E:189:PRO:O	1:E:192:THR:OG1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:189:PRO:O	1:C:192:THR:OG1	2.26	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
1:G:189:PRO:O	1:G:192:THR:OG1	2.26	0.51
2:S:129:ARG:HD3	2:S:129:ARG:C	2.36	0.51
2:V:129:ARG:C	2:V:129:ARG:HD3	2.36	0.51
2:V:226:VAL:HA	2:V:329:GLN:NE2	2.26	0.51
2:X:428:ASP:OD2	2:X:449:TYR:OH	2.28	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:294:ALA:HA	2:S:632:MET:HE3	1.92	0.51
1:F:457:GLU:OE2	1:F:465:ARG:NH2	2.44	0.51
2:S:301:HIS:O	2:S:302:PRO:C	2.52	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:129:ARG:HD3	2:Z:129:ARG:C	2.36	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:X:360:THR:O	2:X:361:MET:C	2.52	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
2:Z:360:THR:O	2:Z:361:MET:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:426:LYS:NZ	1:C:486:ASP:OD1	2.44	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
2:X:129:ARG:HD3	2:X:129:ARG:C	2.36	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:426:LYS:NZ	1:G:486:ASP:OD1	2.44	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:266:MET:HE1	2:X:293:MET:HG3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:Z:266:MET:HE1	2:Z:293:MET:HG3	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
2:Z:259:MET:HE1	2:Z:288:PHE:CD1	2.48	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:V:259:MET:HE1	2:V:288:PHE:CD1	2.48	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:V:117:MET:HE1	2:V:272:TYR:CG	2.49	0.48
2:X:259:MET:HE1	2:X:288:PHE:CD1	2.49	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:V:266:MET:HE1	2:V:293:MET:HG3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:158:PRO:O	2:X:159:VAL:HG12	2.12	0.48
1:D:519:ASN:ND2	1:F:193:ASP:OD1	2.47	0.48
2:S:259:MET:HE1	2:S:288:PHE:CD1	2.48	0.48
2:S:308:THR:HB	2:S:310:VAL:HG23	1.96	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:Z:59:ALA:HB3	2:Z:62:GLU:OE2	2.13	0.48
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:117:MET:HE1	2:S:272:TYR:CG	2.49	0.47
2:S:266:MET:HE1	2:S:293:MET:HG3	1.95	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
1:E:426:LYS:NZ	1:E:486:ASP:OD1	2.44	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
2:Z:117:MET:HE1	2:Z:272:TYR:CG	2.49	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: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: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:117:MET:HE1	2:X:272:TYR:CG	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:113:SER:HB2	2:X:117:MET:HE2	1.97	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:113:SER:HB2	2:Z:117:MET:HE2	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:33:VAL:HG22	2:Z:51:GLU:HB2	1.96	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
2:S:153:ARG:O	2:S:154:GLU:C	2.57	0.47
2:V:113:SER:HB2	2:V:117:MET:HE2	1.97	0.47
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:428:LEU:HA	1:H:162:LEU:HD12	1.96	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:211:ARG:NH2	2:V:248:SER:HB3	2.29	0.46
2:Z:153:ARG:O	2:Z:154:GLU:C	2.57	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:X:153:ARG:O	2:X:154:GLU:C	2.57	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:113:SER:HB2	2:S:117:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:V:301:HIS:N	2:V:302:PRO:HD2	2.31	0.46
2:S:252:ASP:OD1	2:S:252:ASP:N	2.43	0.46
1:D:198:VAL:O	1:D:202:SER:OG	2.33	0.45
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
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:V:153:ARG:O	2:V:154:GLU:C	2.57	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:S:623:GLU:CD	2:S:623:GLU:H	2.25	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:S:300:GLU:C	2:S:302:PRO:HD2	2.42	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
2:V:300:GLU:C	2:V:302:PRO:HD2	2.42	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:X:252:ASP:OD1	2:X:255:THR:OG1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:99:LEU:HD21	2:Z:106:PHE:CD1	2.51	0.45
2:Z:623:GLU:CD	2:Z:623:GLU:H	2.25	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:C:198:VAL:O	1:C:202:SER:OG	2.33	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
2:X:623:GLU:CD	2:X:623:GLU:H	2.25	0.44
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:X:300:GLU:C	2:X:302:PRO:HD2	2.42	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:93:GLY:C	2:V:95:PHE:N	2.73	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:159:VAL:O	2:Z:160:MET:C	2.61	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:V:623:GLU:H	2:V:623:GLU:CD	2.25	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:OD1	2:Z:252:ASP:N	2.43	0.44
2:Z:300:GLU:C	2:Z:302:PRO:HD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:93:GLY:C	2:S:95:PHE:N	2.73	0.44
2:X:159:VAL:O	2:X:160:MET:C	2.61	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:93:GLY:C	2:X:95:PHE:N	2.73	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:157:TYR:C	2:X:159:VAL:H	2.26	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:157:TYR:C	2:Z:159:VAL:H	2.26	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
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:S:349:MET:HE1	2:S:454:LYS:HA	2.00	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:S:21:VAL:C	2:S:23:ALA:H	2.27	0.43
2:V:44:LYS:HD2	2:V:377:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:MET:HE1	2:X:454:LYS:HA	2.00	0.43
2:X:544:LYS:HG3	2:X:549:GLU:HG2	2.00	0.43
2:Z:93:GLY:C	2:Z:95:PHE:N	2.73	0.43
2:Z:160:MET:O	2:Z:160:MET:HG3	2.19	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:S:629:ALA:O	2:S:630:MET:C	2.60	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
1:G:122:VAL:HG12	1:G:126:MET:HE2	2.01	0.43
1:H:423:MET:HE3	1:H:423:MET:HB3	1.96	0.43
2:S:160:MET:O	2:S:160:MET:HG3	2.19	0.43
2:V:349:MET:HE1	2:V:454:LYS:HA	2.00	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:349:MET:HE1	2:Z:454:LYS:HA	2.00	0.43
2:Z:532:VAL:HG22	2:Z:543:VAL:CG2	2.44	0.43
2:Z:629:ALA:O	2:Z:630:MET:C	2.60	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:252:ASP:OD1	2:V:255:THR:OG1	2.32	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:C:122:VAL:HG12	1:C:126:MET:HE2	2.01	0.43
1:D:454:TYR:HB3	1:D:457:GLU:HB2	2.00	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:629:ALA:O	2:X:630:MET:C	2.60	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
1:E:122:VAL:HG12	1:E:126:MET:HE2	2.01	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
1:H:122:VAL:HG12	1:H:126:MET:HE2	2.01	0.42
2:S:157:TYR:C	2:S:159:VAL:H	2.26	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:231:ARG:NH2	2:X:300:GLU:HB2	2.34	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:134:CYS:O	2:S:135:ILE:C	2.62	0.42
2:Z:231:ARG:NH2	2:Z:300:GLU:HB2	2.34	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
1:F:198:VAL:O	1:F:202:SER:OG	2.33	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:200:LYS:O	2:X:201:MET:HE2	2.20	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:200:LYS:O	2:Z:201:MET:HE2	2.20	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:S:117:MET:HE1	2:S:272:TYR:CD2	2.55	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:564:MET:HE2	2:Z:564:MET:HB3	1.81	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:S:613:GLN:C	2:S:648:LYS:HZ3	2.27	0.42
2:V:629:ALA:O	2:V:630:MET:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:157:TYR:C	2:V:159:VAL:H	2.26	0.42
2:V:159:VAL:O	2:V:160:MET:C	2.61	0.42
2:V:283:ASN:OD1	2:V:284:PRO:HD2	2.18	0.42
2:V:349:MET:HE2	2:V:453:PHE:CE2	2.55	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
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:E:423:MET:HE3	1:E:423:MET:HB3	1.96	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: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:349:MET:HE2	2:X:453:PHE:CE2	2.55	0.42
2:X:397:GLY:HA3	2:X:403:CYS:HB2	2.00	0.42
2:Z:293:MET:HE3	2:Z:293:MET:HB3	1.97	0.42
1:E:278:ARG:NH1	1:E:303:PRO:O	2.40	0.42
1:F:122:VAL:HG12	1:F:126:MET:HE2	2.01	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:21:VAL:C	2:V:23:ALA:H	2.27	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:21:VAL:C	2:X:23:ALA:H	2.27	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
1:D:122:VAL:HG12	1:D:126:MET:HE2	2.01	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:66:CYS:O	2:S:67:ILE:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:200:LYS:O	2:V:201:MET:HE2	2.20	0.42
2:V:604:PRO:HA	2:V:656:GLU:HB3	2.02	0.42
2:V:613:GLN:C	2:V:648:LYS:HZ3	2.27	0.42
2:X:231:ARG:HG2	2:X:246:ALA:HA	2.02	0.42
2:Z:349:MET:HE2	2:Z:453:PHE:CE2	2.55	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:117:MET:HE1	2:X:272:TYR:CD2	2.55	0.41
2:X:344:TYR:CE1	2:X:389:LEU:HG	2.55	0.41
2:Z:21:VAL:C	2:Z:23:ALA:H	2.27	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
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:66:CYS:O	2:V:67:ILE:C	2.63	0.41
2:V:109:PRO:HB3	2:V:272:TYR:CE1	2.55	0.41
2:Z:44:LYS:HD3	2:Z:375:GLY:HA2	2.02	0.41
2:Z:134:CYS:O	2:Z:135:ILE:C	2.63	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:S:200:LYS:O	2:S:201:MET:HE2	2.20	0.41
2:X:17:ILE:HG21	2:X:86:TYR:HD1	1.85	0.41
2:X:134:CYS:O	2:X:135:ILE:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:MET:HE1	2:V:272:TYR:CD2	2.55	0.41
2:V:162:LYS:O	2:V:202:LEU:HG	2.20	0.41
2:X:572:ASP:OD1	2:X:572:ASP:N	2.53	0.41
2:X:614:PRO:HA	2:X:648:LYS:HZ3	1.84	0.41
2:Z:117:MET:HE1	2:Z:272:TYR:CD2	2.55	0.41
2:Z:344:TYR:CE1	2:Z:389:LEU:HG	2.55	0.41
1:D:254:ARG:O	1:D:257:SER:OG	2.37	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
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:341:CYS:SG	2:X:407:MET:HE2	2.61	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
2:V:341:CYS:SG	2:V:407:MET:HE2	2.61	0.41
3:V:801:BTI:HN2	3:V:801:BTI:H72	1.73	0.41
2:X:66:CYS:O	2:X:67:ILE:C	2.63	0.41
2:X:296:ARG:HE	2:X:296:ARG:HB3	1.75	0.41
2:Z:341:CYS:SG	2:Z:407:MET:HE2	2.61	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:159:VAL:O	2:S:160:MET:C	2.61	0.41
2:S:349:MET:HE2	2:S:453:PHE:CE2	2.55	0.41
2:S:359:LEU:HA	2:S:380:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:CYS:O	2:Z:67:ILE:C	2.63	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
2:Z:284:PRO:O	2:Z:286:LYS:NZ	2.36	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:293:MET:HE3	2:V:293:MET:HB3	1.97	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
2:X:283:ASN:CG	2:X:284:PRO:HD2	2.46	0.41
2:X:293:MET:HE3	2:X:293:MET:HB3	1.97	0.41
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:283:ASN:CG	2:Z:284:PRO:HD2	2.46	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
1:E:52:ARG:HD2	1:E:178:MET:HE3	2.03	0.41
2:S:283:ASN:CG	2:S:284:PRO:HD2	2.46	0.41
2:S:341:CYS:SG	2:S:407:MET:HE2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:564:MET:HE2	2:X:564:MET:HB3	1.81	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:572:ASP:OD1	2:S:572:ASP:N	2.53	0.40
2:V:55:ILE:CG2	2:V:69:LYS:HD3	2.51	0.40
2:V:87:GLY:O	2:V:88:PHE:C	2.64	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
2:Z:613:GLN:C	2:Z:648:LYS:HZ3	2.29	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
1:G:198:VAL:O	1:G:202:SER:OG	2.33	0.40
2:S:159:VAL:CG1	2:S:175:ALA:H	2.35	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:121:ILE:C	2:X:123:SER:H	2.29	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:75:LYS:HB2	2:S:76:LYS:HZ2	1.86	0.40
2:S:109:PRO:HB3	2:S:272:TYR:CE1	2.55	0.40
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:V:283:ASN:CG	2:V:284:PRO:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:90:SER:O	2:X:91:GLU:C	2.64	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
2:Z:614:PRO:HA	2:Z:648:LYS:HZ3	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: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:87:GLY:O	2:X:88:PHE:C	2.65	0.40
2:X:132:VAL:HG11	2:X:290:PHE:HD2	1.85	0.40
2:Z:90:SER:O	2:Z:91:GLU:C	2.64	0.40
2:Z:121:ILE:C	2:Z:123:SER:H	2.30	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
1:H:52:ARG:HD2	1:H:178:MET:HE3	2.03	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:90:SER:O	2:V:91:GLU:C	2.65	0.40
2:V:296:ARG:HD2	2:V:297:LEU:N	2.35	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%)	43	78
2	V	655/657 (100%)	588 (90%)	66 (10%)	1 (0%)	43	78
2	X	655/657 (100%)	588 (90%)	66 (10%)	1 (0%)	43	78
2	Z	655/657 (100%)	588 (90%)	66 (10%)	1 (0%)	43	78
All	All	5542/5562 (100%)	5165 (93%)	373 (7%)	4 (0%)	49	83

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%)	399 (100%)	1 (0%)	86	86
1	D	400/400 (100%)	399 (100%)	1 (0%)	86	86
1	E	400/400 (100%)	399 (100%)	1 (0%)	86	86
1	F	400/400 (100%)	399 (100%)	1 (0%)	86	86
1	G	400/400 (100%)	399 (100%)	1 (0%)	86	86
1	H	400/400 (100%)	399 (100%)	1 (0%)	86	86
2	S	553/553 (100%)	542 (98%)	11 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	553/553 (100%)	542 (98%)	11 (2%)	48	66
2	X	553/553 (100%)	542 (98%)	11 (2%)	48	66
2	Z	553/553 (100%)	542 (98%)	11 (2%)	48	66
All	All	4612/4612 (100%)	4562 (99%)	50 (1%)	63	76

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	292	LYS
1	D	292	LYS
1	E	292	LYS
1	F	292	LYS
1	G	292	LYS
1	H	292	LYS
2	S	91	GLU
2	S	132	VAL
2	S	157	TYR
2	S	159	VAL
2	S	299	VAL
2	S	351	ASN
2	S	356	ILE
2	S	363	GLN
2	S	627	LEU
2	S	628	GLU
2	S	636	ILE
2	V	91	GLU
2	V	132	VAL
2	V	157	TYR
2	V	159	VAL
2	V	299	VAL
2	V	351	ASN
2	V	356	ILE
2	V	363	GLN
2	V	627	LEU
2	V	628	GLU
2	V	636	ILE
2	X	91	GLU
2	X	132	VAL
2	X	157	TYR
2	X	159	VAL
2	X	299	VAL

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Mol	Chain	Res	Type
2	X	351	ASN
2	X	356	ILE
2	X	363	GLN
2	X	627	LEU
2	X	628	GLU
2	X	636	ILE
2	Z	91	GLU
2	Z	132	VAL
2	Z	157	TYR
2	Z	159	VAL
2	Z	299	VAL
2	Z	351	ASN
2	Z	356	ILE
2	Z	363	GLN
2	Z	627	LEU
2	Z	628	GLU
2	Z	636	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	339	GLN
2	S	80	GLN
2	S	102	ASN
2	S	271	GLN
2	S	280	ASN
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	280	ASN
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	280	ASN
2	X	301	HIS
2	X	329	GLN

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Mol	Chain	Res	Type
2	X	634	ASN
2	Z	80	GLN
2	Z	102	ASN
2	Z	271	GLN
2	Z	280	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BTI	F	801	-	15,16,16	1.42	1 (6%)	20,21,21	1.56	4 (20%)
3	BTI	V	801	-	15,16,16	1.42	1 (6%)	20,21,21	1.56	4 (20%)
3	BTI	D	801	-	15,16,16	1.43	1 (6%)	20,21,21	1.57	4 (20%)
3	BTI	H	801	-	15,16,16	1.42	1 (6%)	20,21,21	1.57	4 (20%)
3	BTI	E	801	-	15,16,16	1.43	1 (6%)	20,21,21	1.57	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BTI	G	801	-	15,16,16	1.42	1 (6%)	20,21,21	1.56	4 (20%)

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	F	801	-	-	2/6/27/27	0/2/2/2
3	BTI	V	801	-	-	2/6/27/27	0/2/2/2
3	BTI	D	801	-	-	2/6/27/27	0/2/2/2
3	BTI	H	801	-	-	2/6/27/27	0/2/2/2
3	BTI	E	801	-	-	2/6/27/27	0/2/2/2
3	BTI	G	801	-	-	2/6/27/27	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	801	BTI	C2-S1	-4.06	1.76	1.82
3	D	801	BTI	C2-S1	-4.06	1.76	1.82
3	V	801	BTI	C2-S1	-4.04	1.76	1.82
3	E	801	BTI	C2-S1	-4.04	1.76	1.82
3	G	801	BTI	C2-S1	-4.01	1.76	1.82
3	F	801	BTI	C2-S1	-3.98	1.76	1.82

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	801	BTI	C4-C2-S1	3.31	108.79	105.03
3	V	801	BTI	C4-C2-S1	3.31	108.79	105.03
3	E	801	BTI	C4-C2-S1	3.31	108.79	105.03
3	H	801	BTI	C4-C2-S1	3.30	108.78	105.03
3	G	801	BTI	C4-C2-S1	3.28	108.76	105.03
3	F	801	BTI	C4-C2-S1	3.28	108.75	105.03
3	H	801	BTI	C6-S1-C2	2.70	95.60	89.98
3	G	801	BTI	C6-S1-C2	2.69	95.58	89.98
3	E	801	BTI	C6-S1-C2	2.69	95.58	89.98
3	V	801	BTI	C6-S1-C2	2.69	95.58	89.98
3	D	801	BTI	C6-S1-C2	2.69	95.57	89.98
3	F	801	BTI	C6-S1-C2	2.68	95.57	89.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	801	BTI	C2-C4-N2	-2.23	110.98	113.34
3	F	801	BTI	C2-C4-C5	2.23	111.62	108.89
3	F	801	BTI	C2-C4-N2	-2.22	110.99	113.34
3	E	801	BTI	C2-C4-N2	-2.22	110.99	113.34
3	G	801	BTI	C2-C4-N2	-2.22	110.99	113.34
3	V	801	BTI	C2-C4-C5	2.21	111.60	108.89
3	V	801	BTI	C2-C4-N2	-2.21	111.00	113.34
3	D	801	BTI	C2-C4-N2	-2.21	111.00	113.34
3	G	801	BTI	C2-C4-C5	2.20	111.59	108.89
3	D	801	BTI	C2-C4-C5	2.18	111.56	108.89
3	H	801	BTI	C2-C4-C5	2.17	111.55	108.89
3	E	801	BTI	C2-C4-C5	2.15	111.53	108.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

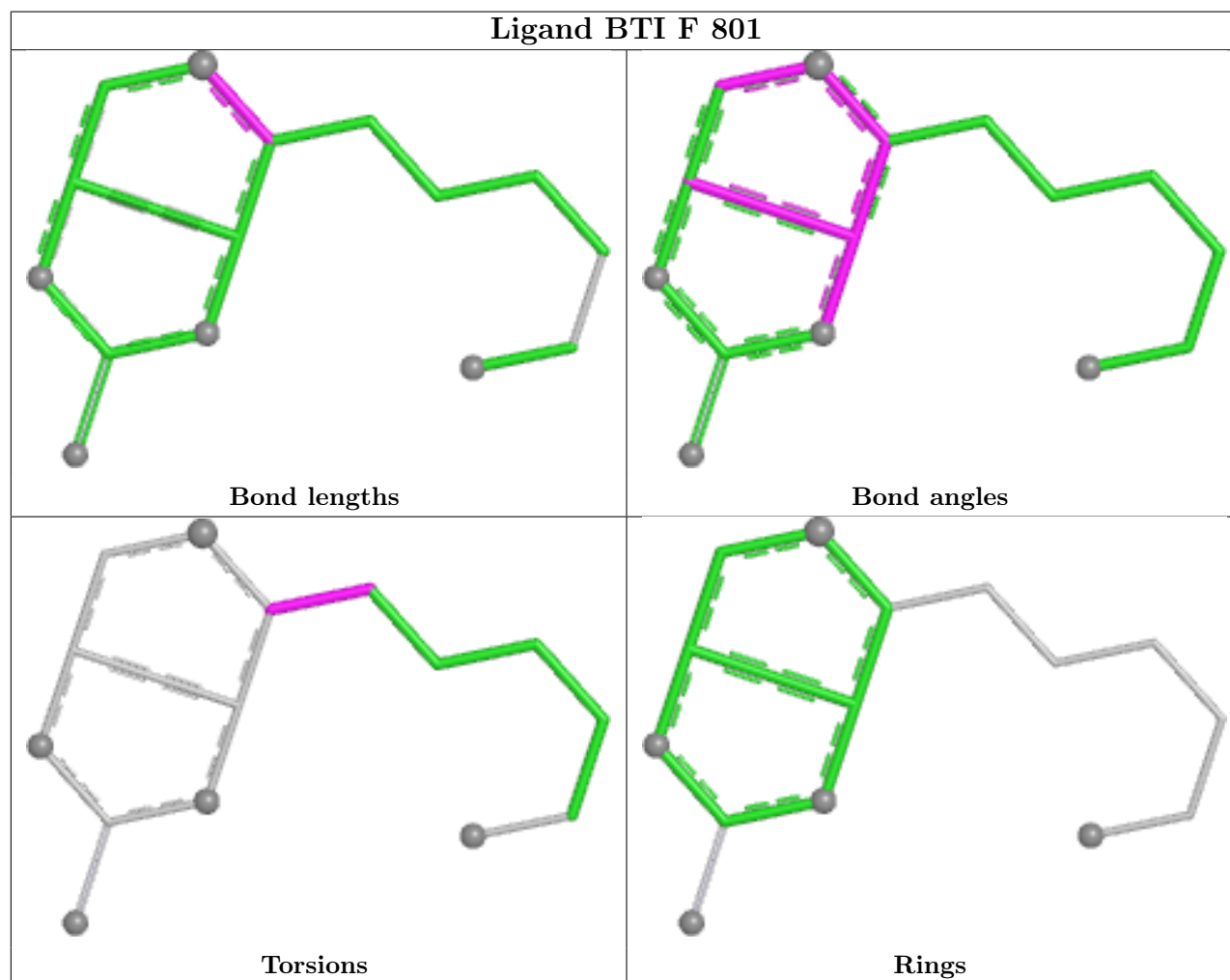
Mol	Chain	Res	Type	Atoms
3	D	801	BTI	S1-C2-C7-C8
3	D	801	BTI	C4-C2-C7-C8
3	E	801	BTI	S1-C2-C7-C8
3	E	801	BTI	C4-C2-C7-C8
3	F	801	BTI	S1-C2-C7-C8
3	F	801	BTI	C4-C2-C7-C8
3	G	801	BTI	S1-C2-C7-C8
3	G	801	BTI	C4-C2-C7-C8
3	H	801	BTI	S1-C2-C7-C8
3	H	801	BTI	C4-C2-C7-C8
3	V	801	BTI	S1-C2-C7-C8
3	V	801	BTI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

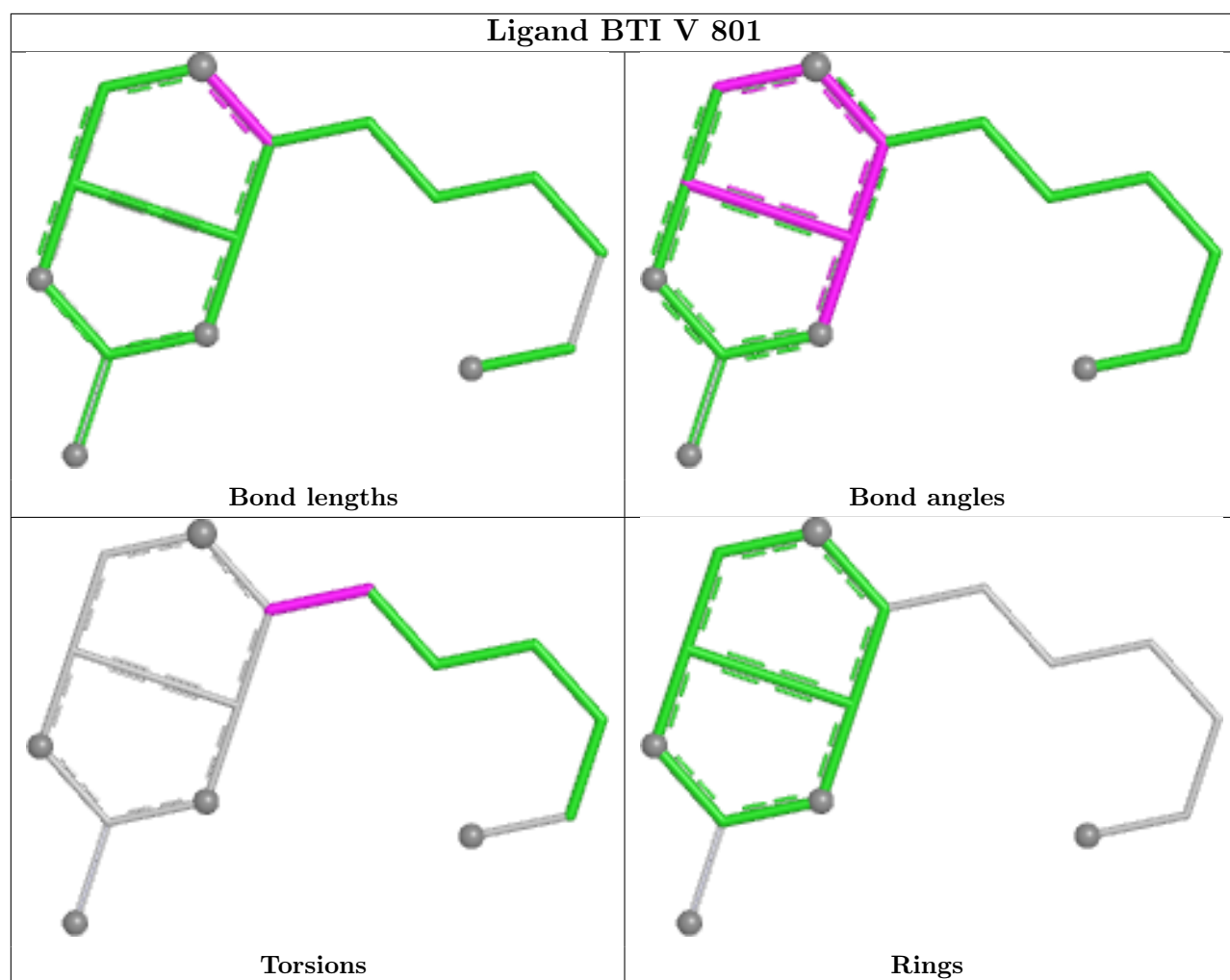
There are no ring outliers.

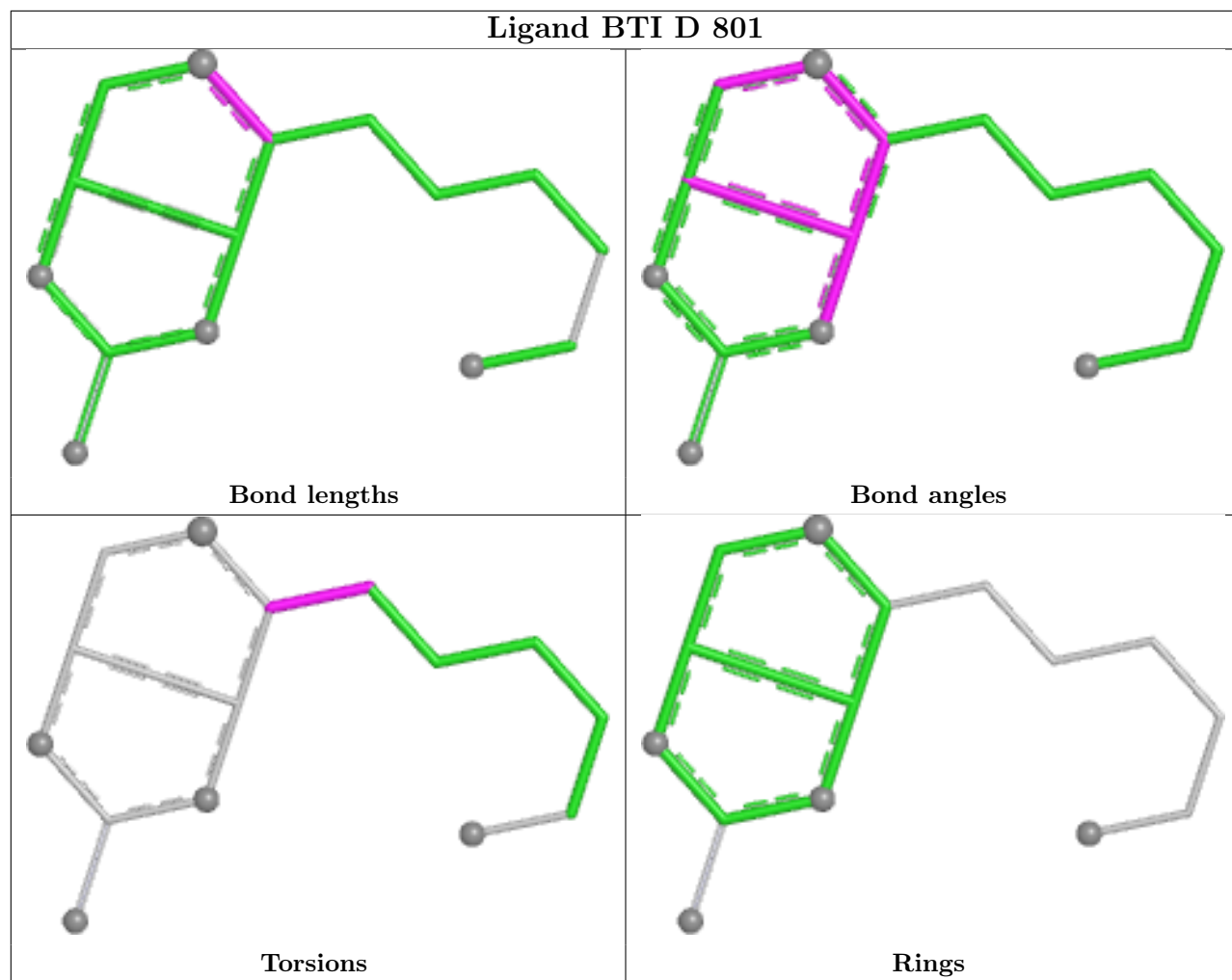
6 monomers are involved in 25 short contacts:

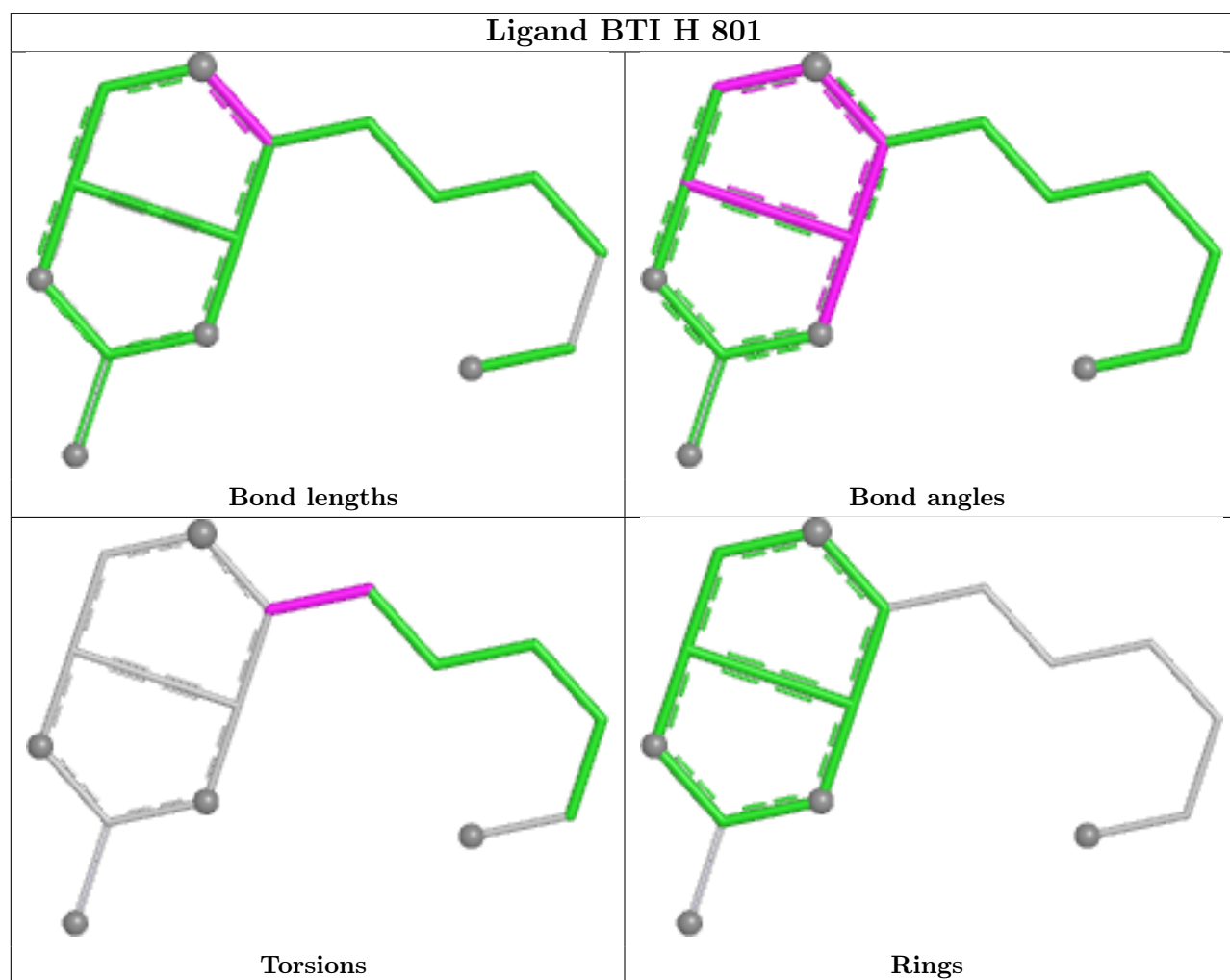
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	BTI	8	0
3	V	801	BTI	2	0
3	D	801	BTI	5	0
3	H	801	BTI	6	0
3	E	801	BTI	1	0
3	G	801	BTI	3	0

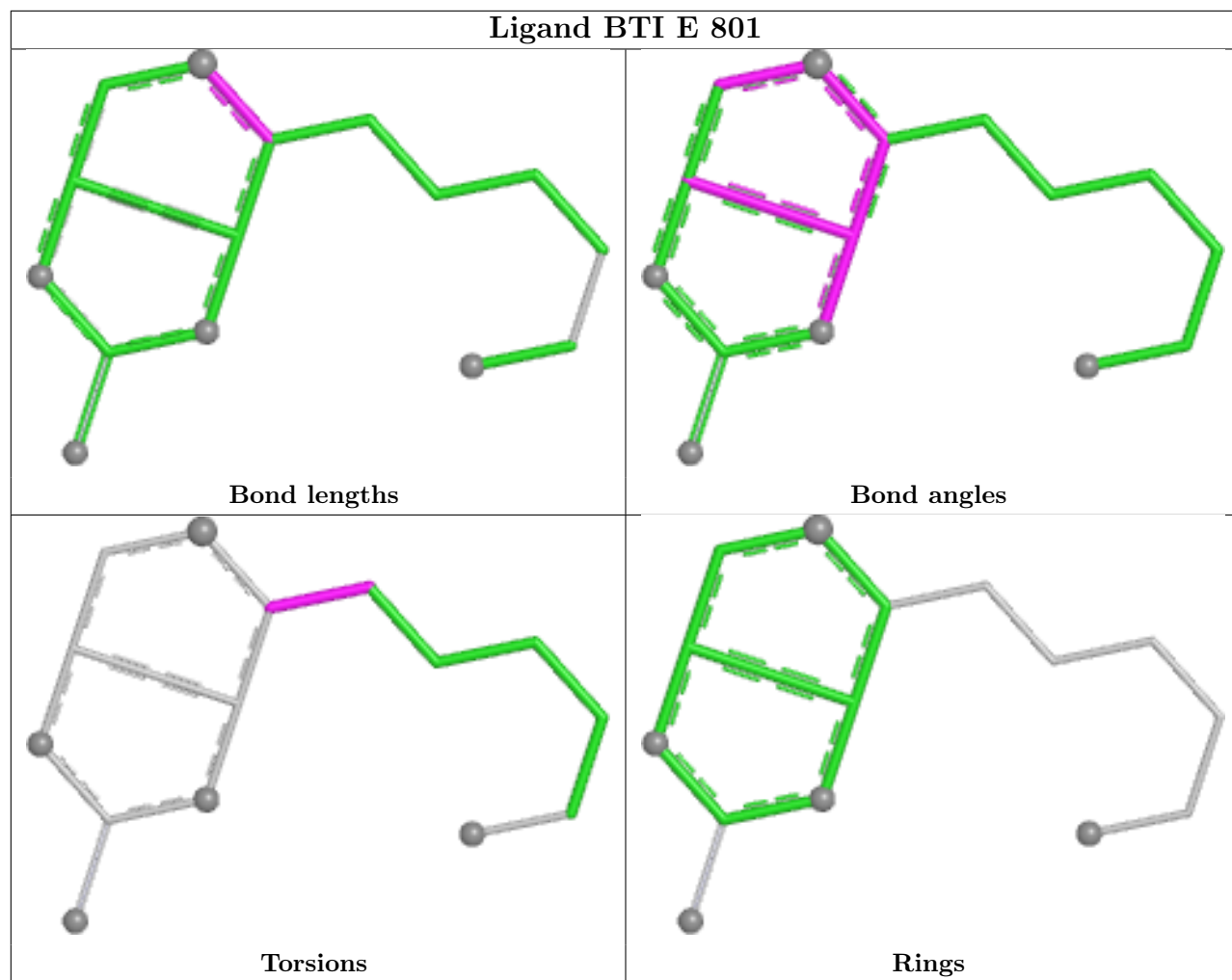
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

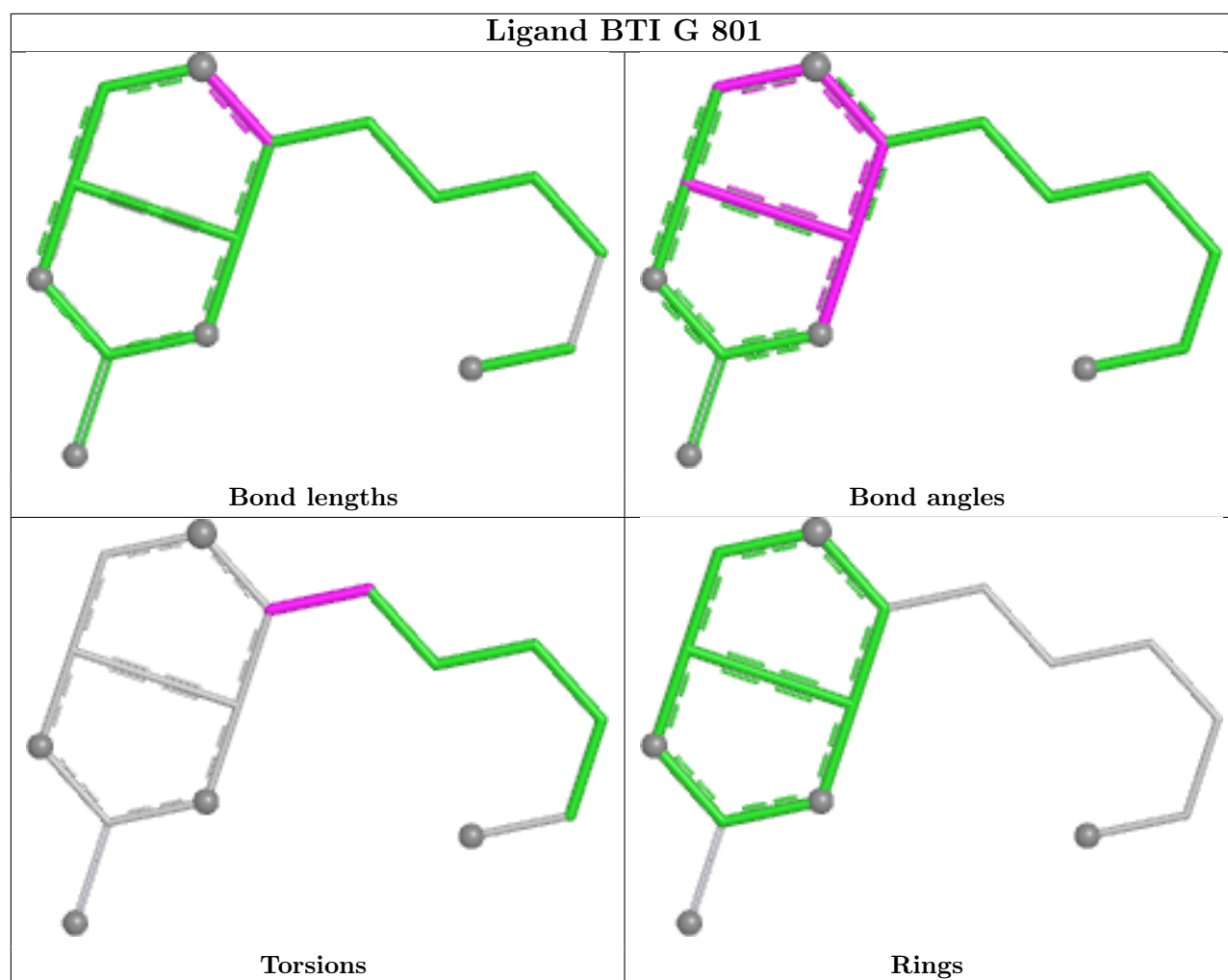












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

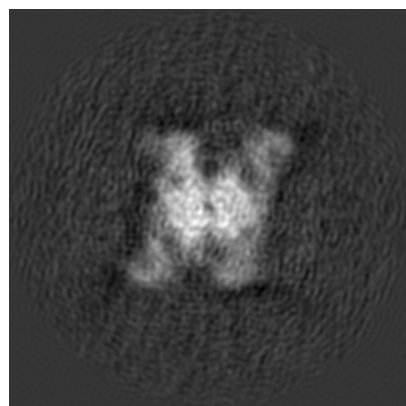
6 Map visualisation [i](#)

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.

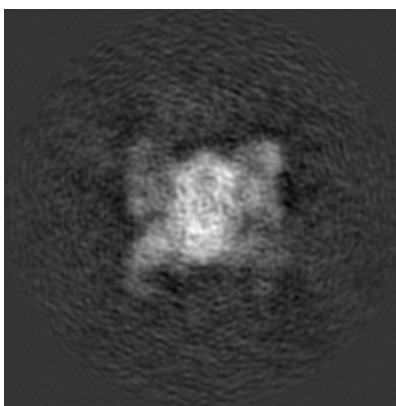
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

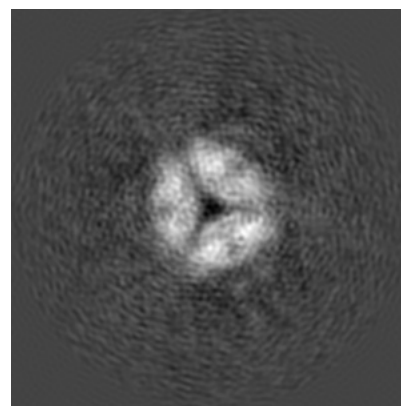
6.1.1 Primary map



X

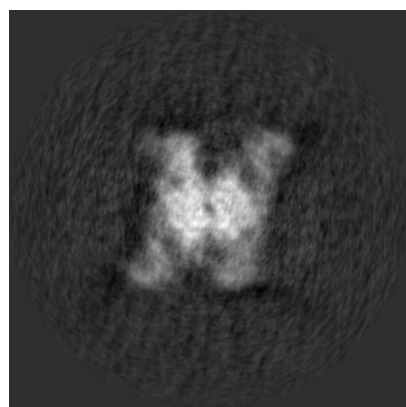


Y

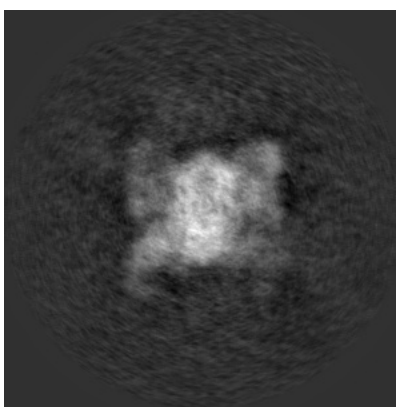


Z

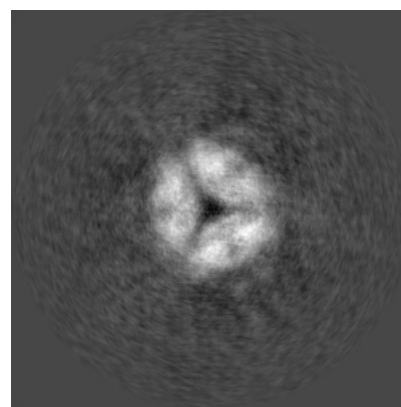
6.1.2 Raw map



X



Y

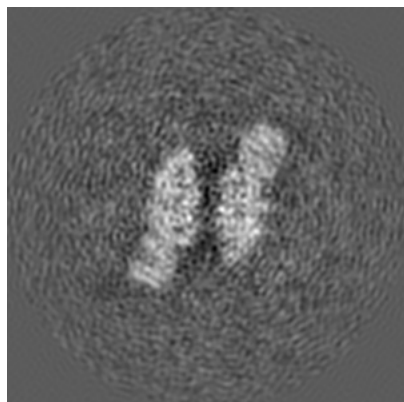


Z

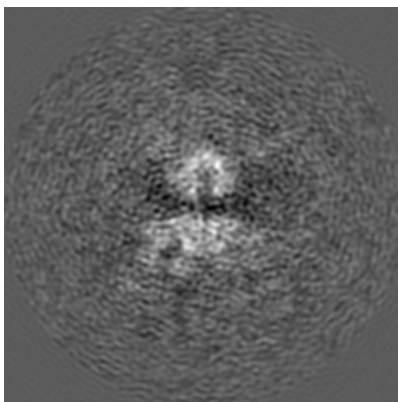
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

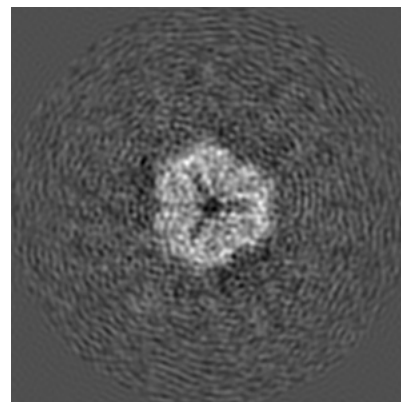
6.2.1 Primary map



X Index: 192

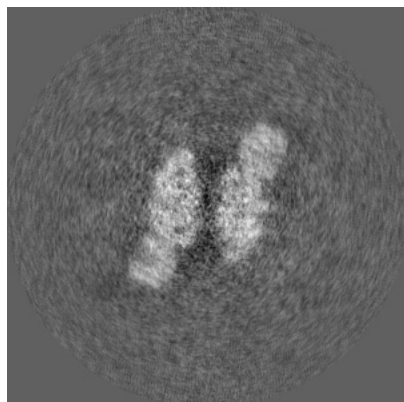


Y Index: 192

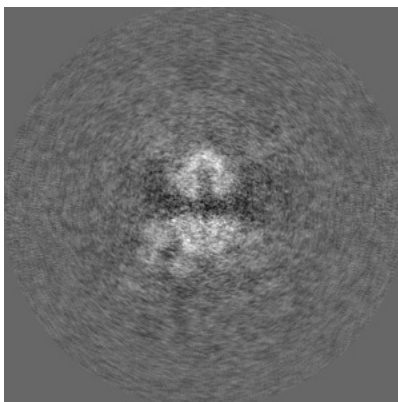


Z Index: 192

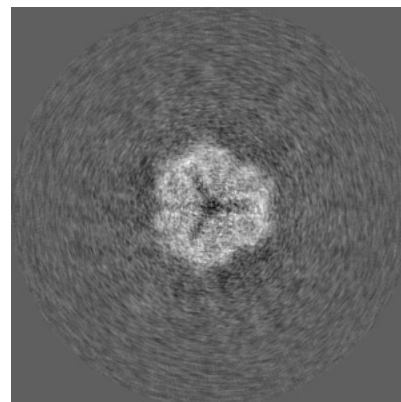
6.2.2 Raw map



X Index: 192



Y Index: 192

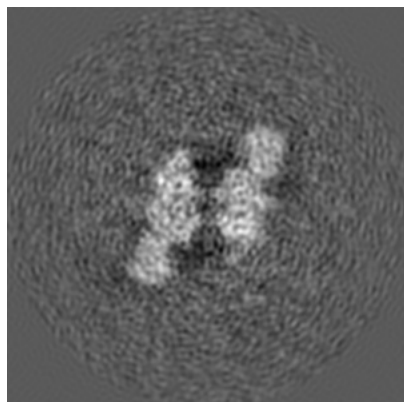


Z Index: 192

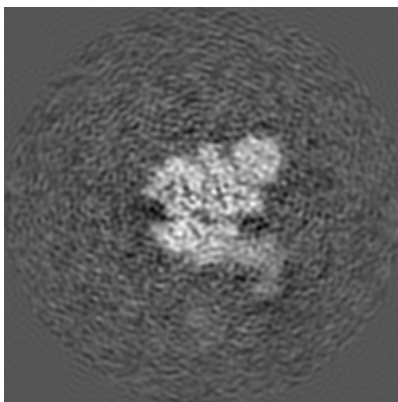
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

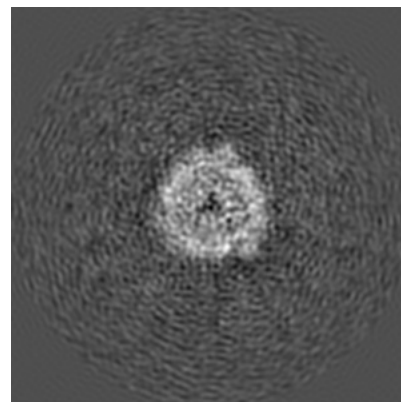
6.3.1 Primary map



X Index: 187

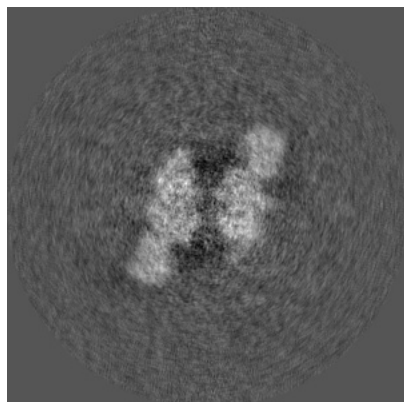


Y Index: 173

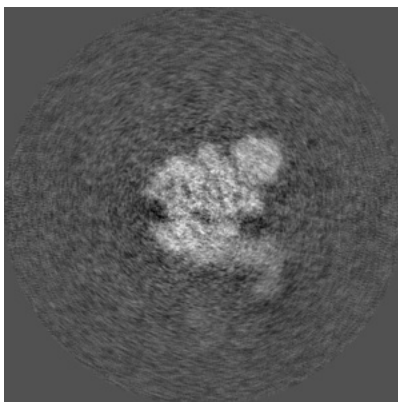


Z Index: 204

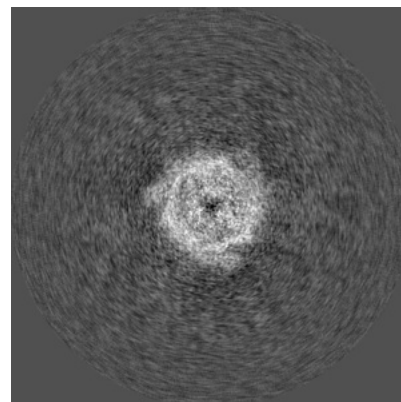
6.3.2 Raw map



X Index: 187



Y Index: 173

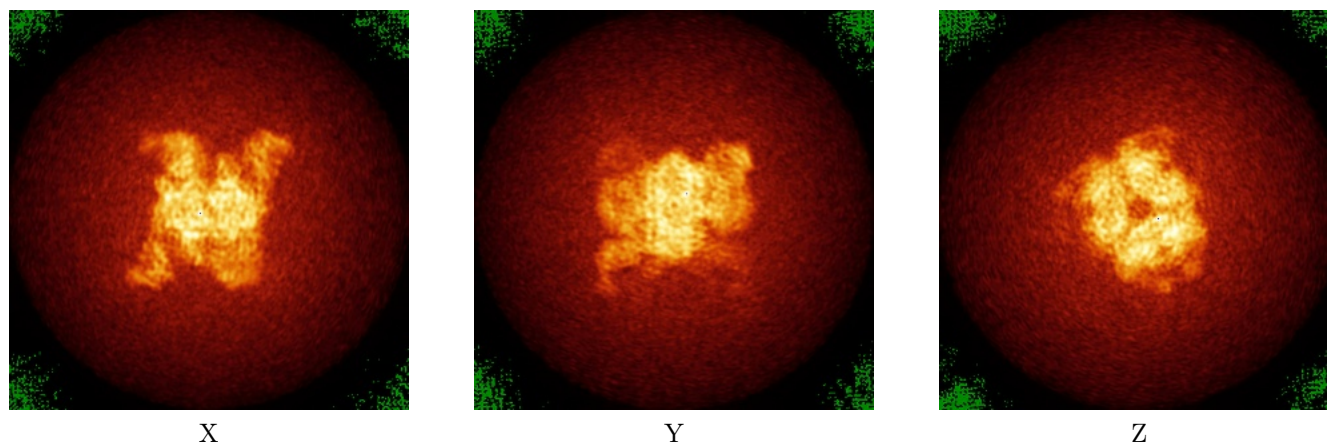


Z Index: 179

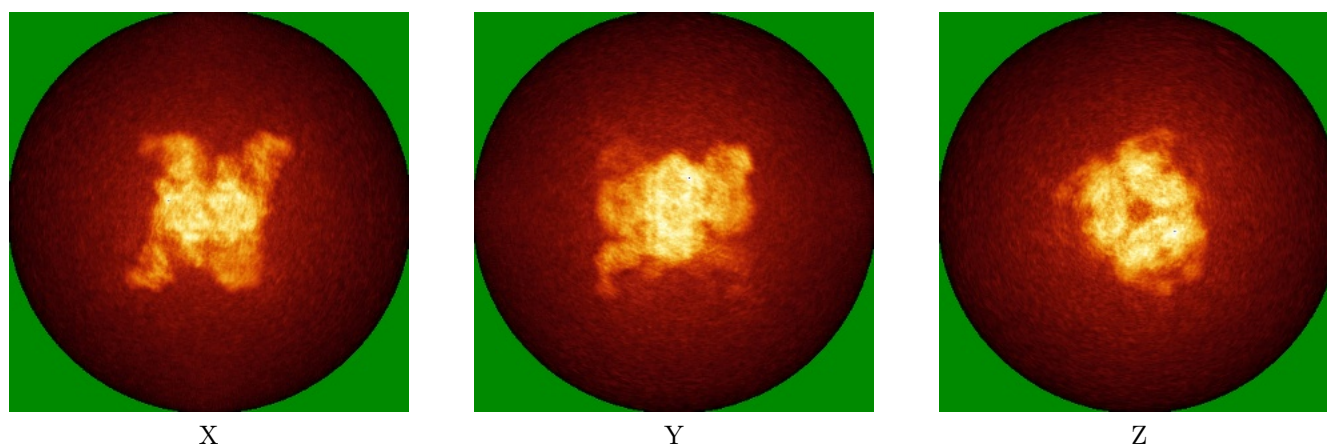
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

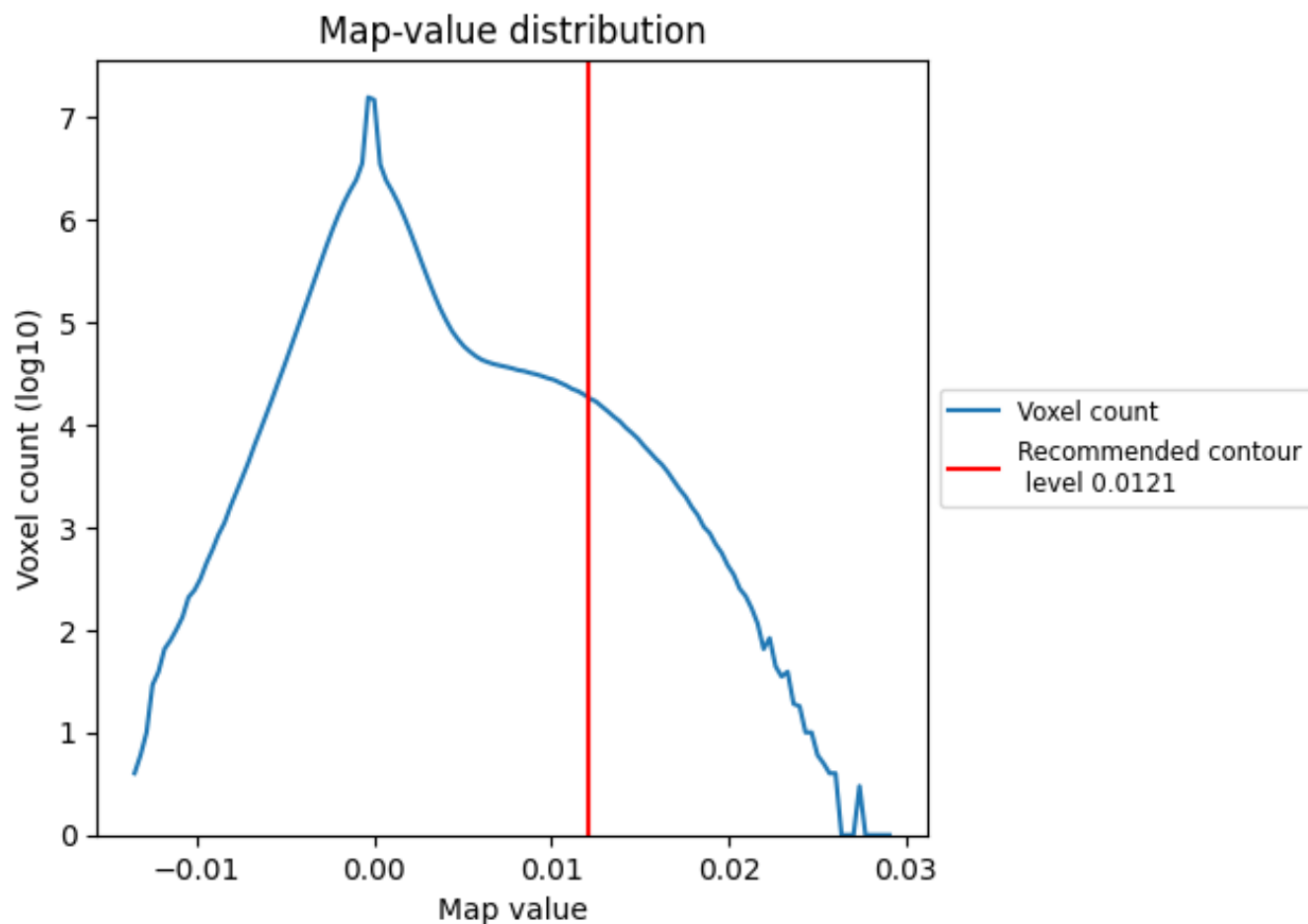
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

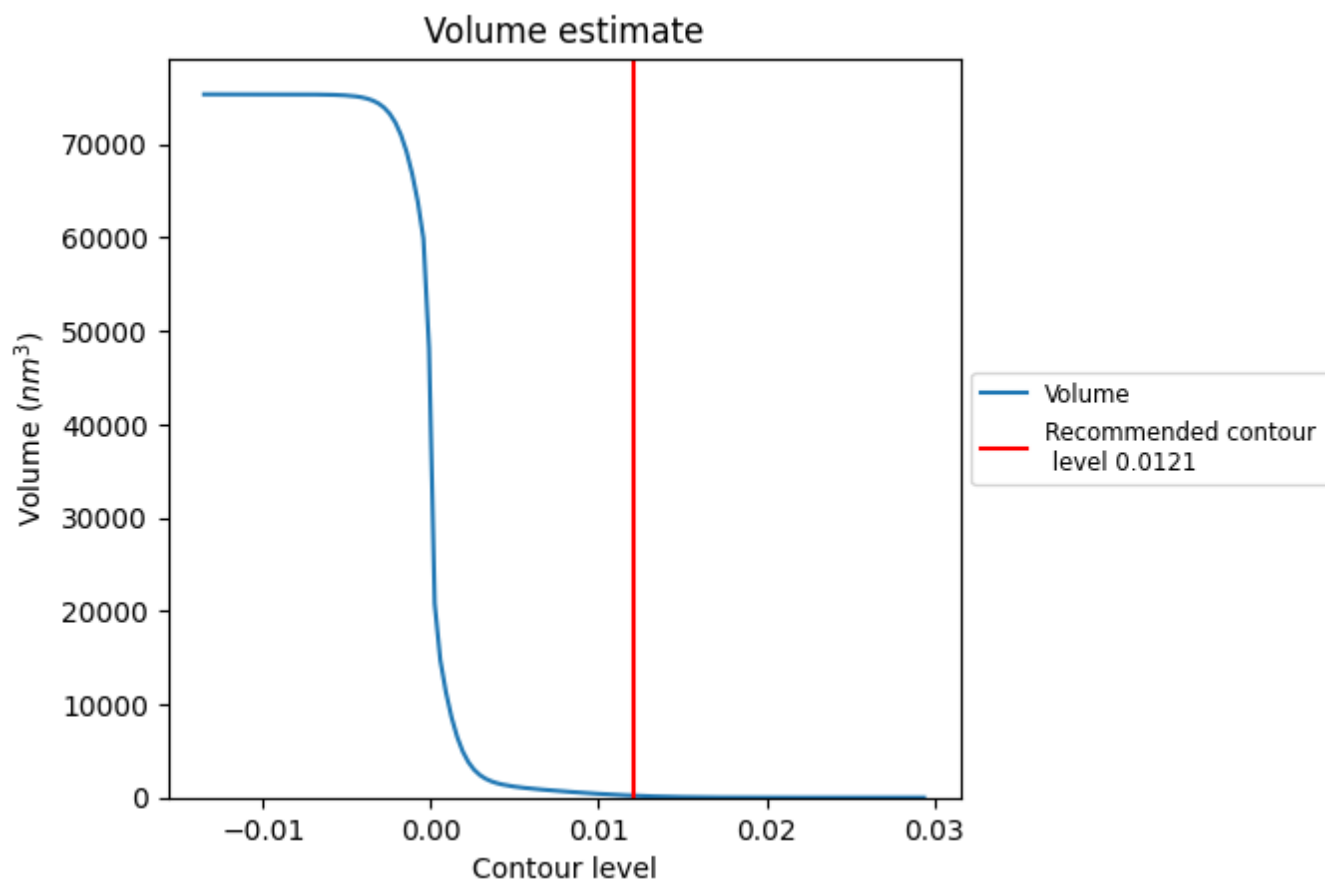
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

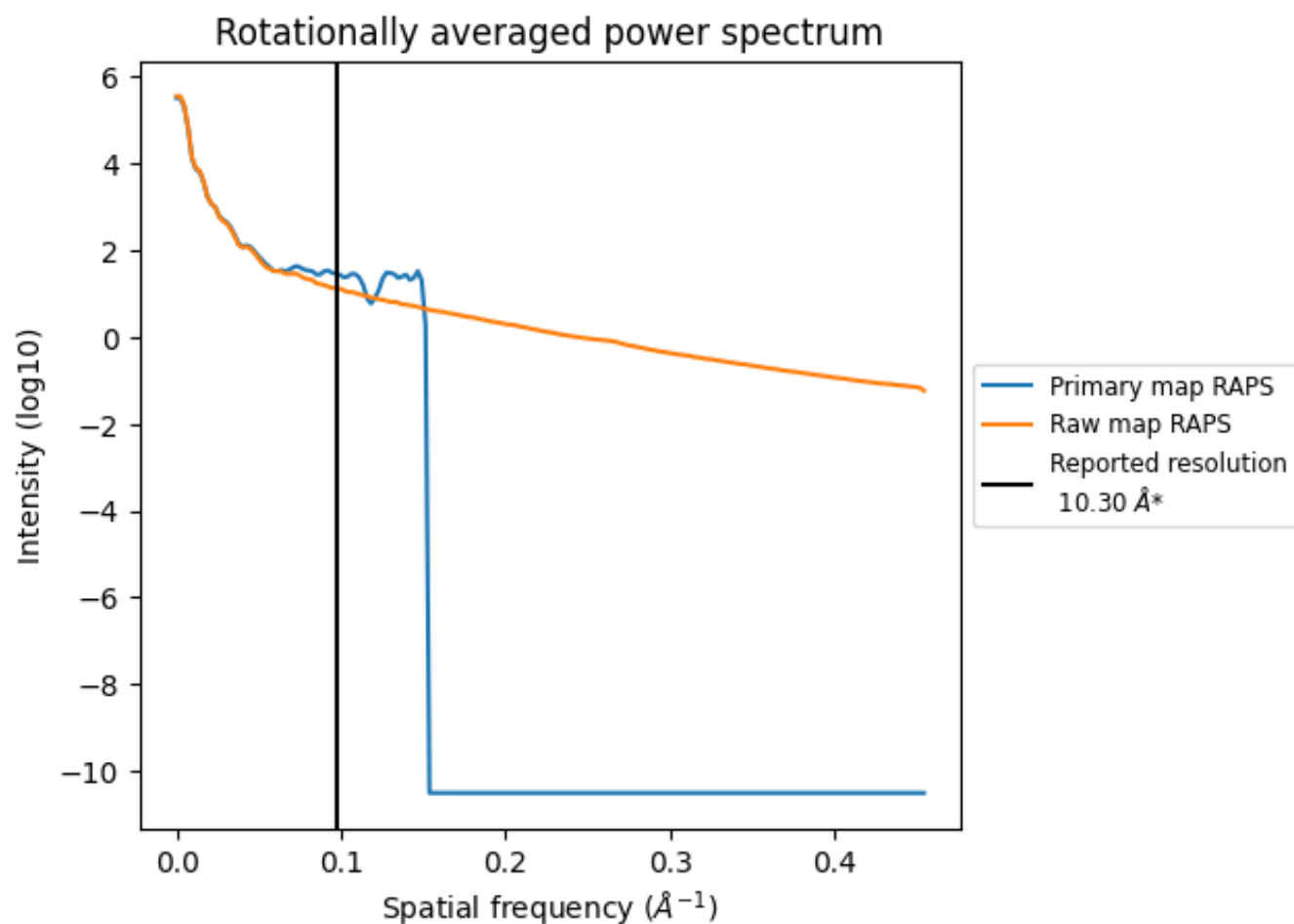
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm³; 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 ⓘ

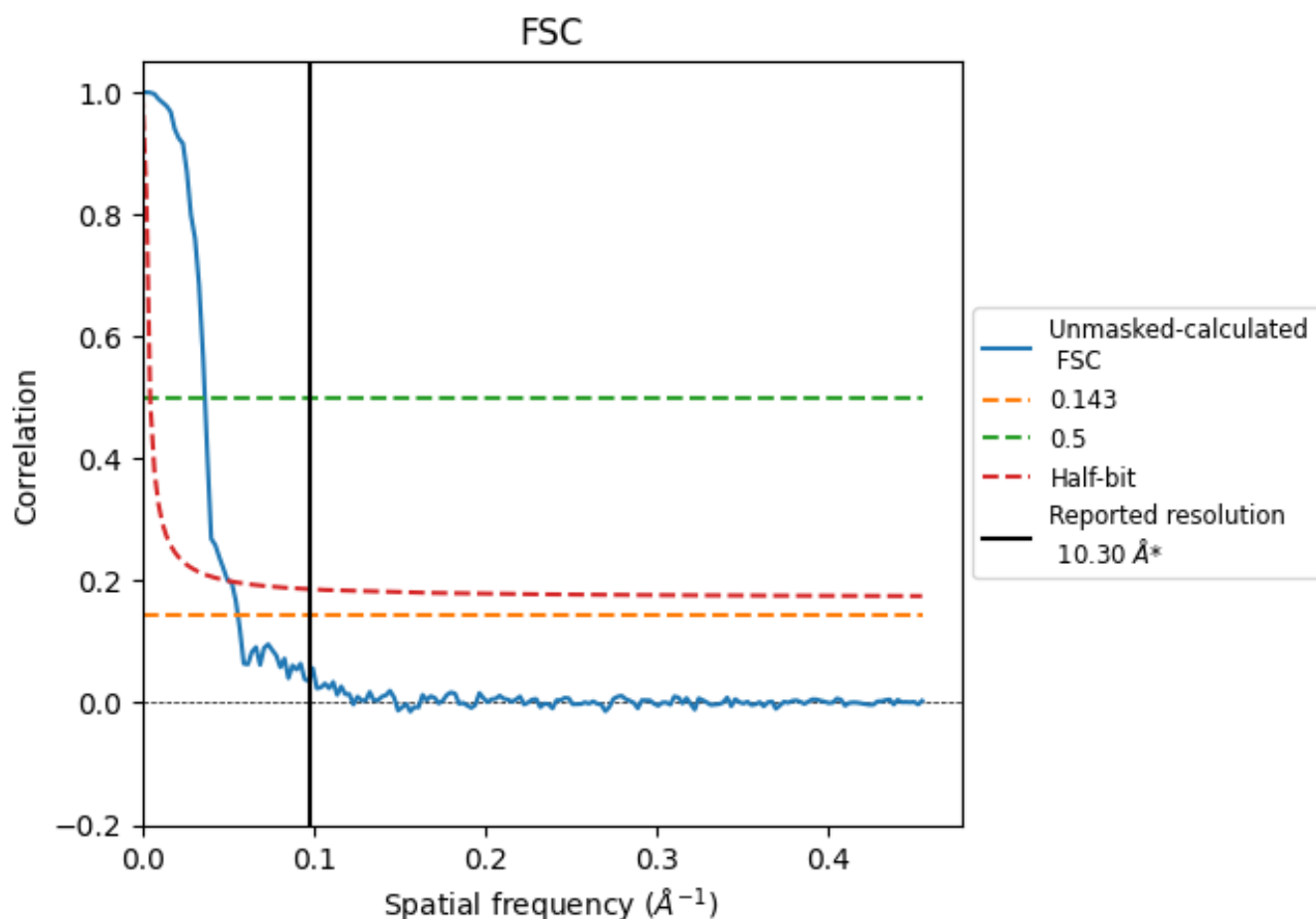


*Reported resolution corresponds to spatial frequency of 0.097 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.097 Å⁻¹

8.2 Resolution estimates [i](#)

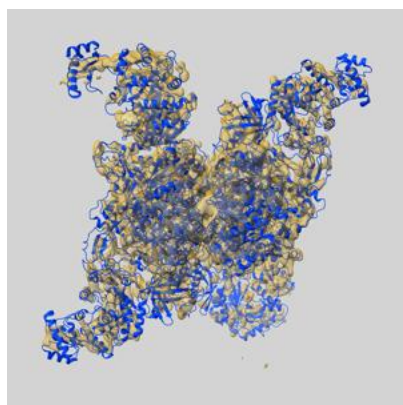
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	17.95	27.40	19.72

*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 %

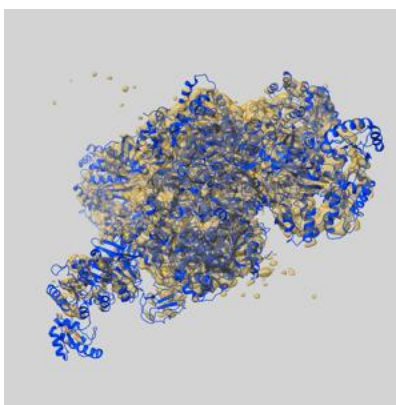
9 Map-model fit [i](#)

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.

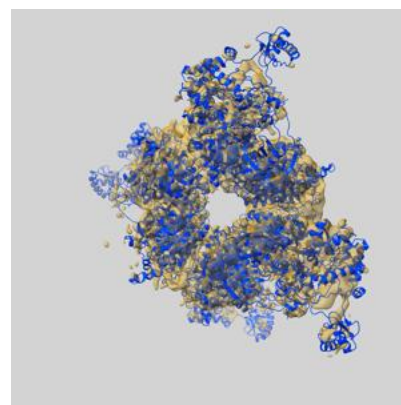
9.1 Map-model overlay [i](#)



X



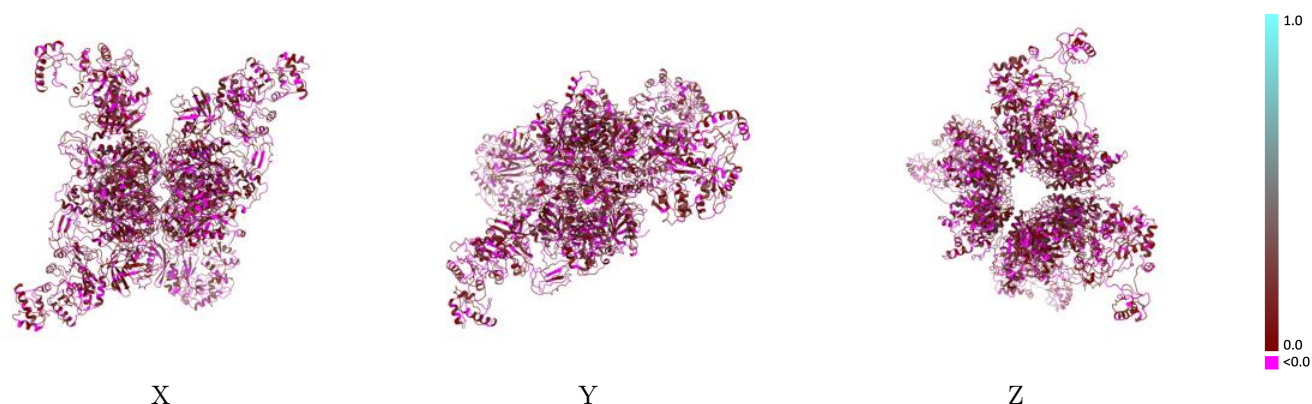
Y



Z

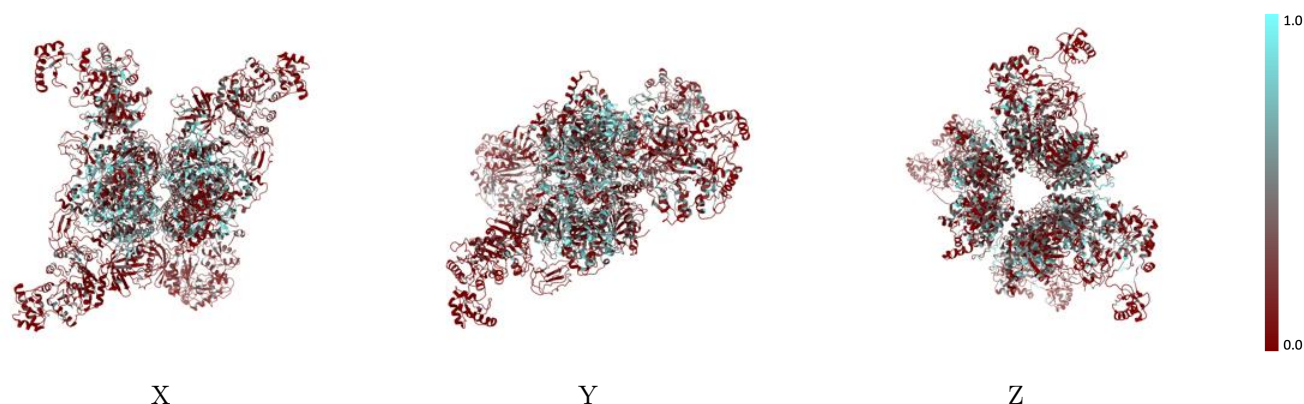
The images above show the 3D surface view of the map at the recommended contour level 0.0121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



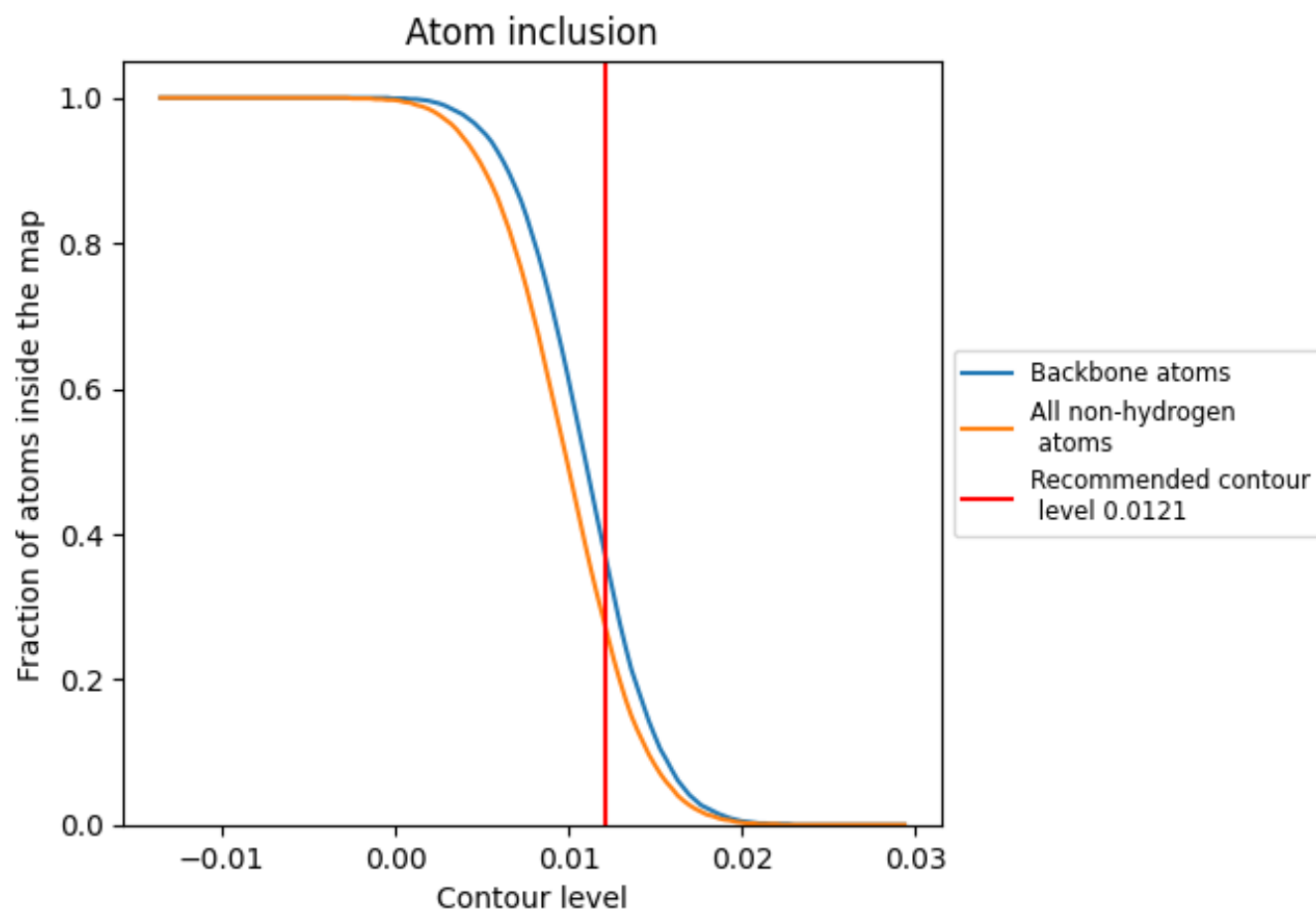
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	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	0.0780
V	0.2320	0.0830
X	0.1800	0.0860
Z	0.1380	0.0850

1.0

0.0

<0.0