



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 07:44 AM UTC

PDB ID : 7AKV / pdb_00007akv
EMDB ID : EMD-11814
Title : The cryo-EM structure of the Vag8-C1 inhibitor complex
Authors : Johnson, S.; Lea, S.M.; Deme, J.C.; Furlong, E.; Dhillon, A.
Deposited on : 2020-10-02
Resolution : 3.60 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
MolProbity : 4-5-2 with Phenix2.0
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

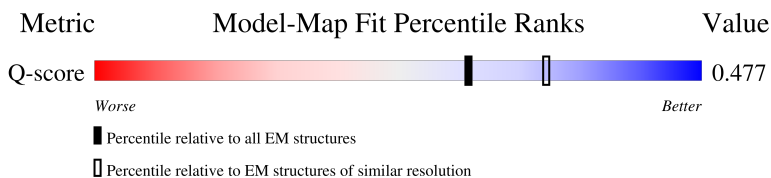
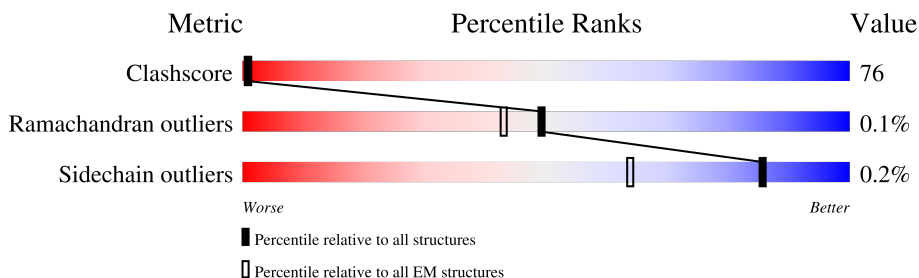
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	403	 24% 70% 6%
2	G	877	 11% 37% 52%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6201 atoms, of which 245 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 Plasma protease C1 inhibitor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	378	Total	C	N	O	S	0	0
			2979	1915	494	554	16		

- Molecule 2 is a protein called Vag8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	421	Total	C	H	N	O S	0	0
			3222	1806	245	558	609 4		

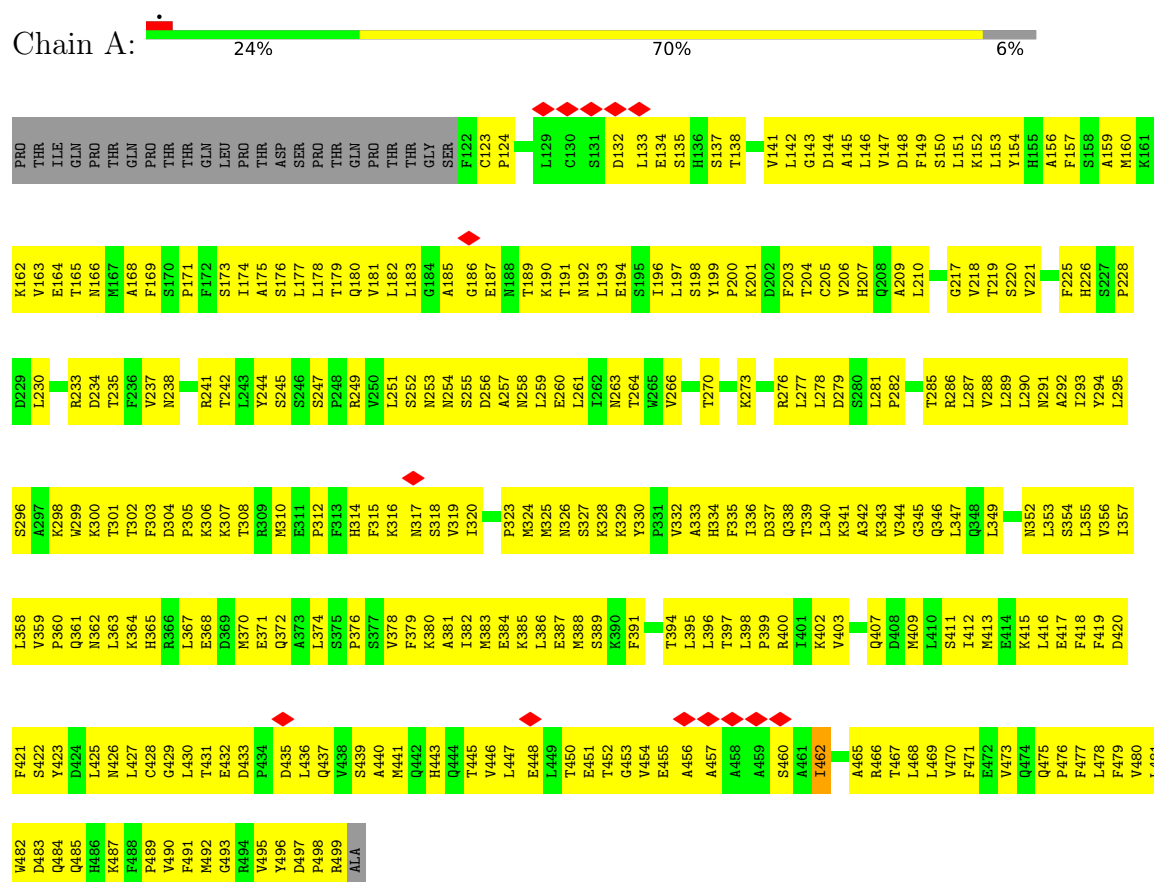
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	107	VAL	LEU	conflict	UNP O66044
G	108	VAL	GLY	conflict	UNP O66044

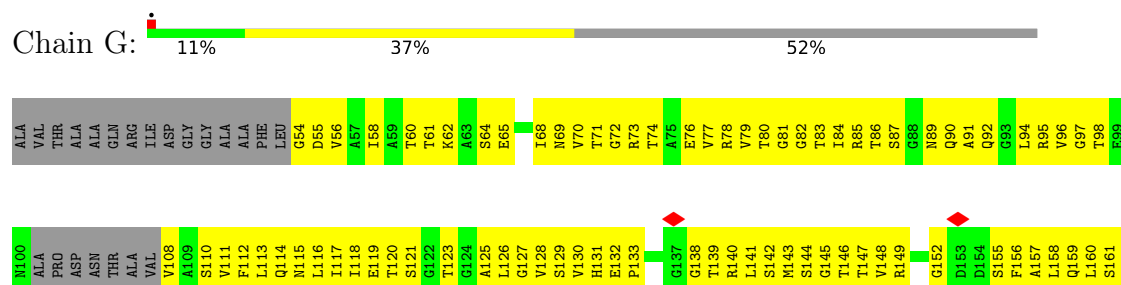
3 Residue-property plots

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: Plasma protease C1 inhibitor



• Molecule 2: Vag8



ALA	ARG	ARG	ALA	GLU	VAL	ILE	HIS	SER	ALA	ASP	R474	K418	T352	L287	L223	P163
PHE	GLU	THR	ALA	THR	PRO	ILE	SER	GLN	ARG	ARG	V475	D419	G352	A288	T224	A164
LEU	ALA	TRP	ALA	GLN	TRP	GLN	ALA	THR	GLN	THR	E476	R420	G355	G289	R225	S165
PRO	ALA	ALA	VAL	ARG	TRP	VAL	VAL	LEU	VAL	VAL	E477	A421	A356	G290	R226	A166
TRP	LEU	ALA	GLY	LEU	ALA	GLY	ASP	LEU	VAL	VAL	K478	Q422	A357	S291	G227	T167
THR	LEU	ALA	ALA	ASP	THR	THR	ASP	THR	VAL	VAL	K479	L423	A358	A292	L228	L168
GLY	TRP	THR	ALA	THR	PRO	THR	THR	ASP	ASP	THR	L480	L424	L359	G283	E229	W169
TRP	TYR	GLY	TYR	GLY	PRO	GLY	GLY	PRO	ASN	THR	E481	Q425	L360	F294	V230	D170
GLY	VAL	GLY	TYR	THR	LEU	THR	THR	ASP	ASN	THR	G482	D426	E361	R295	V231	V171
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	I427	I427	S362	D296	G232	A172
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	A428	A428	L365	L299	I233	L173
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	P429	P429	T366	R300	G234	E174
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	E430	E430	T367	V235	V234	T175
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	A431	A431	V371	Q236	Q237	A176
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	Q432	Q432	G377	E238	G238	Q177
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	Q433	Q433	H373	G239	G239	Q178
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	PRO	PRO	G374	M239	M239	Q179
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	ASP	ASP	G375	L243	L243	A180
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	H376	T244	T244	P181
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	G377	G245	G245	A182
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	H378	T246	T246	V183
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	A377	R247	R247	V184
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	G379	T248	T248	L185
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	L380	G249	G249	W186
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	E381	T250	T250	Q187
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	E382	Q251	Q251	G188
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	V382	G252	G252	A189
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	D383	Q253	Q253	Q190
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	E384	D254	D254	L191
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	E385	G255	G255	W192
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	E386	A256	A256	A193
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	L443	P256	P256	Q194
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	Q387	A257	A257	G195
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	V388	L258	L258	L196
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	S389	Q259	Q259	V197
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	L391	V260	V260	V198
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	G392	E261	E261	Q199
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	G393	D262	D262	V200
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	A394	A263	A263	N201
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	R395	G264	G264	G202
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	L396	T265	T265	A203
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	G455	H266	H266	G204
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	Q400	V267	V267	V205
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	ALA	S268	S268	S206
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	P401	M269	M269	A207
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	T402	N270	N270	I208
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	A403	G271	G271	H209
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	I404	G272	G272	A210
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	R405	A273	A273	Q211
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	L406	L274	L274	Q212
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	I407	G277	G277	A213
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	D408	S278	S278	G214
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	P409	A279	A279	S215
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	R410	N280	N280	F216
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	S411	G281	G281	T217
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	V412	S281	S281	L218
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	L413	P282	P282	S219
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	N414	A283	A283	G220
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	L415	L286	L286	D222
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	D416			
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	I417			
ALA	VAL	VAL	VAL	VAL	THR	THR	THR	ASP	THR	THR	GLY	GLY	S472			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	687883	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0122	Depositor
Map size (Å)	271.584, 271.584, 271.584	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/3043	0.33	0/4127
2	G	0.19	0/3008	0.46	1/4091 (0.0%)
All	All	0.18	0/6051	0.40	1/8218 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	163	PRO	N-CA-CB	7.44	111.06	103.25

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	A	2979	0	3025	396	0
2	G	2977	245	2914	518	0
All	All	5956	245	5939	910	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 76.

All (910) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:131:HIS:HB2	2:G:161:SER:HB2	1.26	1.12
2:G:417:ILE:HG23	2:G:421:ALA:HB3	1.25	1.10
1:A:402:LYS:HG2	1:A:448:GLU:HG3	1.35	1.07
2:G:132:GLU:HG2	2:G:133:PRO:HD2	1.33	1.07
2:G:210:ALA:HB1	2:G:239:MET:HE2	1.28	1.06
2:G:252:GLY:HA3	2:G:278:GLY:HA3	1.35	1.04
2:G:348:LEU:HD21	2:G:350:GLU:HG3	1.04	1.03
1:A:430:LEU:HG	1:A:431:THR:HG23	1.38	1.03
2:G:168:LEU:HD13	2:G:171:VAL:HG21	1.38	1.01
2:G:158:LEU:HB2	2:G:183:VAL:HG12	1.43	1.01
2:G:78:ARG:HD3	2:G:112:PHE:HB2	1.40	1.00
2:G:171:VAL:HG11	2:G:173:LEU:HD23	1.43	0.99
1:A:301:THR:HG23	1:A:457:ALA:HB3	1.44	0.98
2:G:193:ALA:HB1	2:G:196:LEU:HD11	1.46	0.97
2:G:129:SER:HB2	2:G:159:GLN:HG3	1.44	0.95
2:G:179:GLN:HA	2:G:204:GLY:HA2	1.47	0.95
2:G:403:ALA:HB2	2:G:425:GLY:HA3	1.49	0.94
1:A:346:GLN:HB2	1:A:386:LEU:HD21	1.47	0.94
1:A:359:VAL:HG21	1:A:473:VAL:HG12	1.48	0.93
2:G:160:LEU:HD22	2:G:164:ALA:HB1	1.51	0.93
2:G:262:ASP:HB2	2:G:265:THR:HG23	1.50	0.92
1:A:221:VAL:HG21	1:A:270:THR:HG22	1.51	0.91
1:A:160:MET:HE3	1:A:415:LYS:HG2	1.51	0.91
2:G:348:LEU:CD2	2:G:350:GLU:HG3	1.99	0.91
2:G:61:THR:HB	2:G:86:THR:HG22	1.51	0.91
1:A:310:MET:HE1	1:A:323:PRO:HG3	1.49	0.90
1:A:395:LEU:HB3	1:A:470:VAL:HG23	1.53	0.89
1:A:483:ASP:O	1:A:484:GLN:HG2	1.74	0.88
2:G:467:TRP:HH2	2:G:475:VAL:HG21	1.39	0.88
2:G:235:VAL:HG23	2:G:260:VAL:HG13	1.54	0.88
2:G:269:MET:HE1	2:G:274:LEU:HD21	1.57	0.87
2:G:116:LEU:O	2:G:146:THR:HA	1.73	0.87
2:G:210:ALA:CB	2:G:239:MET:HE2	2.05	0.87
2:G:400:GLN:HG2	2:G:401:PRO:HD2	1.57	0.86
1:A:185:ALA:HA	1:A:427:LEU:HD23	1.58	0.85
1:A:180:GLN:HG2	1:A:244:TYR:CE1	2.12	0.85
2:G:140:ARG:NH1	2:G:165:SER:OG	2.10	0.85
2:G:262:ASP:CB	2:G:265:THR:HG23	2.06	0.85
2:G:452:ARG:HH21	2:G:471:GLY:HA3	1.42	0.84
2:G:319:LEU:HD11	2:G:324:VAL:HG21	1.59	0.84
2:G:210:ALA:HB1	2:G:239:MET:CE	2.08	0.83
1:A:324:MET:HE3	1:A:399:PRO:HD3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:207:ALA:HB3	2:G:232:GLY:O	1.80	0.81
1:A:123:CYS:SG	1:A:233:ARG:NH1	2.53	0.81
2:G:193:ALA:HB1	2:G:196:LEU:CD1	2.09	0.81
2:G:208:ILE:HB	2:G:233:ILE:HD13	1.61	0.81
2:G:237:GLU:HA	2:G:262:ASP:OD1	1.80	0.81
1:A:162:LYS:HB2	1:A:165:THR:HG21	1.63	0.81
2:G:143:MET:HB2	2:G:168:LEU:HD22	1.62	0.81
2:G:360:LEU:HD23	2:G:380:LEU:HD11	1.63	0.81
1:A:409:MET:CB	1:A:441:MET:HE2	2.11	0.80
1:A:259:LEU:HD12	1:A:281:LEU:HB2	1.62	0.80
2:G:183:VAL:HG22	2:G:208:ILE:HG12	1.62	0.80
2:G:360:LEU:HD21	2:G:365:LEU:HD22	1.64	0.80
1:A:367:LEU:HD23	1:A:496:TYR:HE1	1.45	0.80
1:A:235:THR:HA	1:A:238:ASN:HD21	1.45	0.80
1:A:144:ASP:OD1	1:A:145:ALA:N	2.15	0.80
1:A:353:LEU:HD22	1:A:481:LEU:HD21	1.63	0.80
2:G:173:LEU:HG	2:G:198:VAL:HG12	1.64	0.79
1:A:134:GLU:OE1	1:A:137:SER:OG	2.01	0.79
2:G:160:LEU:HB2	2:G:185:LEU:HD23	1.64	0.79
2:G:300:ARG:NH1	2:G:327:ASP:OD2	2.15	0.79
2:G:383:ASP:OD1	2:G:407:ILE:N	2.15	0.79
2:G:243:LEU:HD23	2:G:246:THR:HG21	1.64	0.79
2:G:449:TRP:HH2	2:G:453:THR:HB	1.47	0.78
2:G:274:LEU:HD12	2:G:299:LEU:CD2	2.13	0.78
2:G:438:ARG:CZ	2:G:438:ARG:HA	2.12	0.78
2:G:261:GLU:O	2:G:261:GLU:HG2	1.82	0.78
2:G:413:LEU:CD2	2:G:415:LEU:HB2	2.13	0.78
1:A:324:MET:HE2	1:A:397:THR:HG22	1.66	0.77
2:G:183:VAL:HG23	2:G:208:ILE:HG23	1.64	0.77
2:G:351:SER:OG	2:G:355:GLY:O	2.03	0.77
2:G:417:ILE:CG2	2:G:421:ALA:HB3	2.12	0.77
1:A:310:MET:HE1	1:A:323:PRO:CG	2.15	0.77
2:G:477:GLU:OE1	2:G:479:LYS:HE2	1.85	0.77
1:A:317:ASN:OD1	1:A:318:SER:N	2.18	0.77
2:G:269:MET:HE1	2:G:274:LEU:HD11	1.67	0.76
2:G:348:LEU:HD21	2:G:350:GLU:CG	2.00	0.76
2:G:407:ILE:HA	2:G:430:GLU:HG2	1.66	0.76
2:G:168:LEU:HB3	2:G:171:VAL:HG23	1.68	0.76
2:G:313:ALA:HA	2:G:338:ARG:HG3	1.67	0.76
1:A:156:ALA:HB2	1:A:416:LEU:HD21	1.68	0.76
1:A:304:ASP:OD2	1:A:307:LYS:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD13	1:A:203:PHE:HE1	1.50	0.76
1:A:142:LEU:HD21	1:A:210:LEU:HD22	1.68	0.76
1:A:160:MET:CE	1:A:415:LYS:HG2	2.16	0.76
1:A:327:SER:HB3	1:A:330:TYR:HB2	1.68	0.76
2:G:405:ARG:NH1	2:G:429:PRO:O	2.19	0.76
2:G:348:LEU:HD23	2:G:349:VAL:N	2.01	0.75
1:A:124:PRO:HD2	1:A:428:CYS:SG	2.26	0.75
2:G:337:THR:OG1	2:G:361:GLU:OE2	2.04	0.75
2:G:332:HIS:ND1	2:G:356:ALA:O	2.18	0.75
1:A:157:PHE:HZ	1:A:409:MET:HE1	1.51	0.75
2:G:296:ASP:OD1	2:G:321:HIS:ND1	2.19	0.75
2:G:168:LEU:HB3	2:G:171:VAL:CG2	2.16	0.75
2:G:402:THR:HG21	2:G:405:ARG:HH21	1.52	0.74
1:A:181:VAL:CG2	1:A:289:LEU:HD21	2.17	0.74
1:A:329:LYS:HD3	1:A:465:ALA:HB3	1.69	0.74
1:A:259:LEU:HD12	1:A:281:LEU:CB	2.17	0.74
1:A:378:VAL:O	1:A:382:ILE:HG13	1.86	0.74
2:G:65:GLU:HA	2:G:91:ALA:CB	2.17	0.74
2:G:249:THR:HG22	2:G:250:THR:H	1.52	0.74
1:A:346:GLN:HE21	1:A:354:SER:HB2	1.52	0.74
2:G:168:LEU:CD1	2:G:171:VAL:HG21	2.15	0.74
2:G:342:MET:SD	2:G:344:ARG:HB2	2.28	0.74
2:G:342:MET:HE1	2:G:344:ARG:HE	1.51	0.74
2:G:184:VAL:HG23	2:G:209:HIS:HD2	1.53	0.74
2:G:199:GLN:OE1	2:G:226:ARG:NH1	2.21	0.73
1:A:299:TRP:O	1:A:454:VAL:N	2.17	0.73
2:G:360:LEU:HD11	2:G:365:LEU:HB2	1.71	0.73
1:A:368:GLU:O	1:A:372:GLN:HG3	1.90	0.72
1:A:173:SER:HB3	1:A:291:ASN:HD21	1.53	0.72
1:A:175:ALA:O	1:A:179:THR:HG23	1.88	0.72
1:A:409:MET:HE3	1:A:443:HIS:HB3	1.72	0.72
2:G:190:GLN:HG2	2:G:215:SER:HB3	1.71	0.72
2:G:442:ALA:C	2:G:443:LEU:HD12	2.14	0.72
2:G:274:LEU:HD12	2:G:299:LEU:HD21	1.72	0.72
1:A:254:ASN:O	1:A:258:ASN:ND2	2.22	0.71
2:G:417:ILE:HG23	2:G:421:ALA:CB	2.13	0.71
2:G:402:THR:HA	2:G:426:ASP:HB2	1.72	0.71
1:A:447:LEU:HD11	1:A:491:PHE:CD2	2.25	0.71
2:G:380:LEU:HG	2:G:382:VAL:HG23	1.73	0.71
2:G:208:ILE:HB	2:G:233:ILE:CD1	2.20	0.71
2:G:446:GLY:O	2:G:448:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:HG22	1:A:210:LEU:HD23	1.73	0.71
1:A:443:HIS:NE2	1:A:445:THR:OG1	2.22	0.71
2:G:110:SER:HA	2:G:140:ARG:O	1.90	0.71
2:G:197:VAL:HA	2:G:222:ASP:OD1	1.90	0.71
2:G:79:VAL:HB	2:G:113:LEU:HD13	1.72	0.70
2:G:404:ILE:CD1	2:G:423:LEU:HD11	2.21	0.70
2:G:116:LEU:HD23	2:G:117:ILE:N	2.07	0.70
2:G:94:LEU:HD23	2:G:128:VAL:HB	1.72	0.70
2:G:221:SER:O	2:G:246:THR:HA	1.90	0.70
2:G:234:TYR:CZ	2:G:236:GLN:HG2	2.26	0.70
2:G:171:VAL:CG1	2:G:173:LEU:HD23	2.18	0.70
2:G:449:TRP:CH2	2:G:453:THR:HB	2.27	0.70
1:A:226:HIS:HB2	1:A:230:LEU:HD23	1.74	0.70
2:G:412:VAL:HA	2:G:438:ARG:O	1.92	0.70
1:A:149:PHE:CD1	1:A:197:LEU:HA	2.26	0.70
1:A:206:VAL:HA	1:A:209:ALA:HB3	1.74	0.70
2:G:236:GLN:HA	2:G:265:THR:HG21	1.74	0.70
2:G:71:THR:HA	2:G:97:GLY:O	1.92	0.69
2:G:299:LEU:HD12	2:G:324:VAL:HG22	1.74	0.69
2:G:382:VAL:HG11	2:G:386:SER:HB3	1.73	0.69
2:G:173:LEU:O	2:G:198:VAL:HA	1.92	0.69
2:G:287:LEU:HD23	2:G:312:ALA:CB	2.21	0.69
2:G:442:ALA:O	2:G:443:LEU:HD12	1.92	0.69
1:A:203:PHE:CD1	1:A:206:VAL:HB	2.28	0.69
1:A:368:GLU:HA	1:A:371:GLU:OE1	1.93	0.69
2:G:184:VAL:HG23	2:G:209:HIS:CD2	2.27	0.69
2:G:260:VAL:HB	2:G:286:LEU:HD13	1.75	0.69
1:A:481:LEU:HD22	1:A:490:VAL:CG1	2.22	0.69
2:G:160:LEU:HD22	2:G:164:ALA:CB	2.22	0.69
1:A:352:ASN:ND2	1:A:485:GLN:OE1	2.25	0.69
1:A:367:LEU:HD23	1:A:496:TYR:CE1	2.26	0.69
2:G:382:VAL:HB	2:G:413:LEU:HD12	1.73	0.69
1:A:200:PRO:O	1:A:203:PHE:HB2	1.93	0.69
2:G:155:SER:O	2:G:180:ALA:HB1	1.92	0.69
2:G:453:THR:OG1	2:G:456:VAL:HG23	1.93	0.69
1:A:304:ASP:OD2	1:A:307:LYS:HG2	1.93	0.69
2:G:390:LEU:HB2	2:G:417:ILE:HD13	1.73	0.69
1:A:157:PHE:CZ	1:A:409:MET:HE1	2.28	0.68
1:A:174:ILE:O	1:A:178:LEU:HD23	1.94	0.68
1:A:185:ALA:HA	1:A:427:LEU:CD2	2.22	0.68
1:A:346:GLN:HB3	1:A:386:LEU:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HD22	1:A:490:VAL:HG11	1.76	0.68
2:G:168:LEU:HD13	2:G:171:VAL:CG2	2.21	0.68
2:G:400:GLN:CG	2:G:401:PRO:HD2	2.22	0.68
2:G:404:ILE:HB	2:G:427:ILE:CD1	2.24	0.68
1:A:409:MET:HB3	1:A:441:MET:HE2	1.76	0.68
2:G:312:ALA:O	2:G:315:SER:OG	2.08	0.68
2:G:235:VAL:CG2	2:G:260:VAL:HG13	2.22	0.68
2:G:269:MET:CE	2:G:274:LEU:HD21	2.24	0.68
2:G:390:LEU:HD21	2:G:396:LEU:HB2	1.74	0.68
2:G:125:ALA:O	2:G:155:SER:HA	1.94	0.68
1:A:253:ASN:OD1	1:A:254:ASN:N	2.27	0.68
1:A:327:SER:CB	1:A:330:TYR:HB2	2.24	0.68
1:A:194:GLU:OE1	1:A:199:TYR:HB2	1.93	0.68
2:G:140:ARG:HH11	2:G:165:SER:HG	1.40	0.68
2:G:382:VAL:CG1	2:G:386:SER:HB3	2.24	0.68
2:G:96:VAL:HB	2:G:130:VAL:HG23	1.75	0.67
2:G:152:GLY:O	2:G:177:GLY:HA3	1.94	0.67
1:A:383:MET:HE2	1:A:482:TRP:CG	2.29	0.67
1:A:192:ASN:O	1:A:196:ILE:HG12	1.94	0.67
1:A:251:LEU:HB3	1:A:258:ASN:ND2	2.08	0.67
2:G:287:LEU:HD23	2:G:312:ALA:HB3	1.76	0.67
2:G:342:MET:HE1	2:G:344:ARG:NE	2.10	0.67
1:A:329:LYS:HD3	1:A:465:ALA:CB	2.26	0.66
2:G:61:THR:CB	2:G:86:THR:HG22	2.24	0.66
2:G:393:GLY:N	2:G:420:ARG:HB3	2.08	0.66
1:A:466:ARG:HG3	2:G:234:TYR:CD1	2.29	0.66
1:A:482:TRP:NE1	1:A:487:LYS:HA	2.11	0.66
2:G:62:LYS:HE3	2:G:64:SER:OG	1.93	0.66
2:G:262:ASP:HB2	2:G:265:THR:CG2	2.26	0.66
1:A:341:LYS:C	1:A:361:GLN:HG3	2.21	0.66
1:A:353:LEU:HD22	1:A:481:LEU:CD2	2.26	0.66
2:G:371:VAL:HG21	2:G:395:ARG:NH2	2.10	0.66
1:A:187:GLU:O	1:A:191:THR:HG23	1.95	0.66
1:A:277:LEU:HD23	1:A:290:LEU:HD11	1.78	0.66
2:G:437:ALA:O	2:G:438:ARG:NH1	2.28	0.66
1:A:384:GLU:O	1:A:387:GLU:HG3	1.96	0.66
1:A:420:ASP:O	1:A:425:LEU:HB2	1.96	0.66
1:A:206:VAL:HG22	1:A:210:LEU:CD2	2.27	0.65
1:A:233:ARG:NE	1:A:432:GLU:OE2	2.23	0.65
2:G:456:VAL:HG11	2:G:459:VAL:HG22	1.78	0.65
2:G:415:LEU:HD23	2:G:416:ASP:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:129:SER:HB2	2:G:159:GLN:CG	2.23	0.65
2:G:416:ASP:OD2	2:G:418:LYS:HG3	1.97	0.65
1:A:148:ASP:O	1:A:152:LYS:HG3	1.96	0.64
2:G:56:VAL:HG12	2:G:80:THR:CG2	2.27	0.64
2:G:319:LEU:HD11	2:G:324:VAL:CG2	2.27	0.64
1:A:299:TRP:HH2	1:A:355:LEU:HD23	1.63	0.64
2:G:56:VAL:HG12	2:G:80:THR:HG21	1.78	0.64
2:G:402:THR:HG21	2:G:405:ARG:NH2	2.11	0.64
1:A:238:ASN:O	1:A:242:THR:HG23	1.98	0.64
2:G:84:ILE:HD12	2:G:116:LEU:CD2	2.27	0.64
2:G:131:HIS:CB	2:G:161:SER:HB2	2.15	0.64
2:G:360:LEU:HD21	2:G:365:LEU:CD2	2.28	0.64
1:A:301:THR:HB	1:A:330:TYR:CZ	2.33	0.64
1:A:300:LYS:HA	1:A:454:VAL:HG12	1.78	0.64
1:A:324:MET:HG2	1:A:399:PRO:CA	2.27	0.64
2:G:263:ALA:HA	2:G:289:GLY:HA3	1.80	0.64
2:G:333:GLY:H	2:G:357:ALA:HA	1.62	0.64
1:A:469:LEU:HD12	1:A:469:LEU:O	1.98	0.64
2:G:216:PHE:HD2	2:G:218:LEU:HD13	1.63	0.63
1:A:411:SER:O	1:A:415:LYS:HD3	1.98	0.63
1:A:314:HIS:ND1	1:A:319:VAL:HG22	2.13	0.63
1:A:332:VAL:CG2	1:A:396:LEU:HD22	2.28	0.63
2:G:225:ALA:O	2:G:226:ARG:HD2	1.99	0.63
1:A:180:GLN:HG2	1:A:244:TYR:CD1	2.33	0.63
2:G:315:SER:O	2:G:339:SER:HB2	1.99	0.63
1:A:201:LYS:HD2	1:A:201:LYS:N	2.14	0.63
2:G:96:VAL:HB	2:G:130:VAL:CG2	2.28	0.63
2:G:388:VAL:HG12	2:G:415:LEU:HA	1.81	0.63
1:A:177:LEU:HD22	1:A:291:ASN:HB2	1.79	0.63
1:A:300:LYS:HA	1:A:454:VAL:CG1	2.29	0.63
2:G:246:THR:O	2:G:272:GLY:HA2	1.98	0.63
1:A:454:VAL:HG13	1:A:455:GLU:HG3	1.81	0.62
2:G:262:ASP:HB3	2:G:264:GLY:H	1.64	0.62
1:A:157:PHE:CE1	1:A:412:ILE:HG13	2.34	0.62
2:G:390:LEU:HD23	2:G:394:ALA:HB3	1.81	0.62
2:G:92:GLN:HB3	2:G:126:LEU:HD23	1.81	0.62
2:G:452:ARG:NH2	2:G:471:GLY:HA3	2.13	0.62
2:G:118:ILE:HB	2:G:148:VAL:HG22	1.81	0.62
1:A:218:VAL:HG23	1:A:295:LEU:HA	1.79	0.62
1:A:324:MET:HG2	1:A:399:PRO:HA	1.81	0.62
2:G:94:LEU:CD2	2:G:113:LEU:HG	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD11	1:A:374:LEU:HD13	1.81	0.62
1:A:478:LEU:HD12	1:A:493:GLY:O	2.01	0.61
2:G:69:ASN:HA	2:G:95:ARG:O	2.00	0.61
2:G:443:LEU:HD23	2:G:447:GLY:O	2.00	0.61
2:G:236:GLN:OE1	2:G:237:GLU:HG2	2.00	0.61
2:G:404:ILE:HD11	2:G:423:LEU:HD11	1.80	0.61
1:A:298:LYS:HE3	1:A:452:THR:O	2.00	0.61
1:A:447:LEU:HD11	1:A:491:PHE:HD2	1.64	0.61
2:G:173:LEU:HD11	2:G:182:ALA:HB1	1.83	0.61
2:G:311:VAL:HG21	2:G:317:VAL:CG1	2.30	0.61
2:G:419:ASP:O	2:G:420:ARG:NE	2.33	0.61
1:A:234:ASP:O	1:A:238:ASN:ND2	2.34	0.61
1:A:475:GLN:HB2	1:A:476:PRO:HD2	1.82	0.61
2:G:409:PRO:O	2:G:437:ALA:HB1	2.00	0.61
2:G:443:LEU:HD21	2:G:449:TRP:H	1.65	0.61
2:G:173:LEU:CG	2:G:198:VAL:HG12	2.30	0.61
2:G:183:VAL:CG2	2:G:208:ILE:HG12	2.29	0.61
1:A:219:THR:O	1:A:293:ILE:HG13	2.01	0.61
2:G:263:ALA:HA	2:G:289:GLY:C	2.25	0.61
2:G:362:SER:HA	2:G:385:GLU:O	2.01	0.61
2:G:457:HIS:O	2:G:476:ALA:HB3	2.00	0.61
2:G:82:GLY:C	2:G:116:LEU:HG	2.25	0.61
1:A:304:ASP:HB3	1:A:307:LYS:HG2	1.83	0.61
2:G:337:THR:HG22	2:G:338:ARG:HG2	1.83	0.61
1:A:335:PHE:O	1:A:336:ILE:HD13	2.00	0.60
2:G:84:ILE:HD12	2:G:116:LEU:HD21	1.83	0.60
1:A:398:LEU:HD23	1:A:399:PRO:O	2.02	0.60
2:G:65:GLU:HA	2:G:91:ALA:HB1	1.83	0.60
2:G:92:GLN:HB3	2:G:126:LEU:CD2	2.32	0.60
1:A:220:SER:HB2	1:A:293:ILE:HD12	1.82	0.60
2:G:332:HIS:HB2	2:G:335:VAL:CG2	2.32	0.60
2:G:271:GLY:HA2	2:G:296:ASP:O	2.01	0.60
1:A:196:ILE:HG13	1:A:418:PHE:HD1	1.67	0.60
1:A:420:ASP:HA	1:A:423:TYR:O	2.01	0.60
1:A:305:PRO:O	1:A:308:THR:HG22	2.02	0.60
2:G:80:THR:O	2:G:114:GLN:HB3	2.02	0.60
2:G:132:GLU:HG2	2:G:133:PRO:CD	2.21	0.60
2:G:422:GLN:N	2:G:422:GLN:OE1	2.34	0.60
1:A:183:LEU:HB2	1:A:207:HIS:NE2	2.16	0.60
1:A:241:ARG:CD	1:A:247:SER:HB3	2.32	0.60
1:A:324:MET:HE3	1:A:399:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:296:ASP:HA	2:G:321:HIS:O	2.01	0.60
1:A:225:PHE:CD2	1:A:249:ARG:HB3	2.37	0.59
2:G:294:PHE:CE2	2:G:299:LEU:HD11	2.36	0.59
1:A:169:PHE:CE1	1:A:171:PRO:HG3	2.37	0.59
1:A:169:PHE:HE1	1:A:171:PRO:HG3	1.67	0.59
2:G:309:VAL:HB	2:G:334:LEU:HD12	1.84	0.59
2:G:108:VAL:N	2:G:139:THR:HA	2.17	0.59
2:G:338:ARG:HA	2:G:362:SER:O	2.01	0.59
1:A:163:VAL:HG13	1:A:164:GLU:H	1.67	0.59
1:A:204:THR:HG23	1:A:205:CYS:N	2.17	0.59
2:G:452:ARG:HH21	2:G:471:GLY:CA	2.12	0.59
2:G:144:SER:O	2:G:146:THR:HG23	2.02	0.59
2:G:161:SER:HA	2:G:186:TRP:HB2	1.84	0.59
2:G:463:ASP:HB3	2:G:464:ARG:NH1	2.17	0.59
1:A:476:PRO:HB3	1:A:496:TYR:HA	1.83	0.59
2:G:360:LEU:HD23	2:G:380:LEU:CD1	2.32	0.59
1:A:360:PRO:HD2	1:A:475:GLN:NE2	2.18	0.59
2:G:208:ILE:CD1	2:G:218:LEU:HD21	2.32	0.59
2:G:320:ALA:HA	2:G:344:ARG:O	2.03	0.59
2:G:162:GLY:HA2	2:G:187:GLN:O	2.03	0.59
2:G:263:ALA:HA	2:G:289:GLY:O	2.03	0.59
1:A:285:THR:HG23	1:A:439:SER:HB2	1.84	0.59
2:G:94:LEU:HD22	2:G:113:LEU:HG	1.85	0.59
2:G:112:PHE:CD1	2:G:142:SER:HB3	2.38	0.58
2:G:226:ARG:HG3	2:G:251:GLN:CG	2.33	0.58
2:G:301:THR:HG22	2:G:306:SER:OG	2.03	0.58
1:A:163:VAL:HG13	1:A:164:GLU:N	2.17	0.58
1:A:228:PRO:HD3	1:A:251:LEU:O	2.03	0.58
1:A:362:ASN:HD21	1:A:364:LYS:HB3	1.67	0.58
2:G:191:LEU:HD21	2:G:193:ALA:HB2	1.83	0.58
2:G:402:THR:H	2:G:426:ASP:HB2	1.69	0.58
1:A:325:MET:HE1	1:A:400:ARG:HA	1.84	0.58
2:G:440:ARG:O	2:G:441:VAL:HG23	2.03	0.58
1:A:466:ARG:HG3	2:G:234:TYR:CE1	2.37	0.58
2:G:55:ASP:HB2	2:G:79:VAL:HG22	1.85	0.58
2:G:404:ILE:HD11	2:G:423:LEU:CD1	2.33	0.58
1:A:394:THR:HG23	1:A:469:LEU:O	2.04	0.58
1:A:217:GLY:O	1:A:296:SER:OG	2.18	0.58
1:A:301:THR:HG23	1:A:457:ALA:CB	2.28	0.58
1:A:413:MET:HE2	1:A:421:PHE:HB2	1.85	0.58
2:G:71:THR:HG23	2:G:72:GLY:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:198:VAL:CG2	2:G:223:ILE:HD12	2.33	0.58
2:G:269:MET:CE	2:G:274:LEU:HD11	2.34	0.58
2:G:404:ILE:HB	2:G:427:ILE:HD12	1.85	0.58
1:A:149:PHE:CD1	1:A:197:LEU:HD13	2.39	0.58
1:A:409:MET:HB2	1:A:441:MET:HG2	1.86	0.58
2:G:54:GLY:HA2	2:G:77:VAL:O	2.03	0.58
2:G:228:LEU:HB2	2:G:253:ASP:HB3	1.86	0.58
2:G:453:THR:HG23	2:G:454:ASP:N	2.19	0.58
1:A:427:LEU:HD13	1:A:430:LEU:HD23	1.85	0.58
1:A:497:ASP:OD2	1:A:499:ARG:HG2	2.03	0.58
1:A:482:TRP:HE1	1:A:487:LYS:HA	1.68	0.58
1:A:305:PRO:HA	1:A:451:GLU:HG2	1.86	0.57
1:A:360:PRO:HB3	1:A:365:HIS:HB3	1.87	0.57
2:G:249:THR:O	2:G:250:THR:OG1	2.14	0.57
1:A:164:GLU:HA	1:A:496:TYR:CD2	2.39	0.57
1:A:233:ARG:HE	1:A:432:GLU:CD	2.12	0.57
1:A:315:PHE:HE1	1:A:320:ILE:HG23	1.67	0.57
1:A:343:LYS:HE2	1:A:471:PHE:CE1	2.39	0.57
1:A:466:ARG:O	1:A:468:LEU:HD12	2.04	0.57
2:G:130:VAL:O	2:G:160:LEU:HD23	2.04	0.57
1:A:466:ARG:HD2	2:G:231:VAL:CB	2.34	0.57
2:G:259:GLN:HE21	2:G:287:LEU:HD12	1.68	0.57
2:G:302:VAL:HG13	2:G:302:VAL:O	2.03	0.57
2:G:407:ILE:HG12	2:G:430:GLU:CG	2.35	0.57
2:G:460:ARG:HG3	2:G:460:ARG:O	2.05	0.57
1:A:182:LEU:HA	1:A:185:ALA:HB2	1.86	0.57
1:A:225:PHE:HE2	1:A:249:ARG:HD2	1.70	0.57
2:G:336:VAL:HG13	2:G:339:SER:OG	2.05	0.57
2:G:410:ARG:HG2	2:G:438:ARG:HG2	1.86	0.57
2:G:452:ARG:HD3	2:G:472:ASP:O	2.05	0.57
2:G:459:VAL:HG12	2:G:459:VAL:O	2.04	0.57
2:G:413:LEU:HD23	2:G:415:LEU:HB2	1.87	0.57
2:G:226:ARG:HG3	2:G:251:GLN:HG3	1.85	0.57
1:A:341:LYS:HE2	1:A:365:HIS:CE1	2.40	0.57
2:G:262:ASP:O	2:G:263:ALA:HB3	2.05	0.57
1:A:342:ALA:HB2	1:A:370:MET:SD	2.45	0.56
2:G:438:ARG:HH12	2:G:457:HIS:CG	2.23	0.56
1:A:162:LYS:HB2	1:A:165:THR:CG2	2.35	0.56
1:A:182:LEU:CD1	1:A:190:LYS:HG3	2.35	0.56
1:A:221:VAL:CG2	1:A:270:THR:HG22	2.30	0.56
1:A:477:PHE:CE2	1:A:495:VAL:HB	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:65:GLU:CB	2:G:91:ALA:HA	2.35	0.56
2:G:336:VAL:HB	2:G:360:LEU:HD13	1.87	0.56
1:A:218:VAL:HG22	1:A:293:ILE:HG12	1.87	0.56
1:A:415:LYS:HD2	1:A:415:LYS:N	2.20	0.56
2:G:157:ALA:HB3	2:G:182:ALA:O	2.06	0.56
2:G:188:GLY:O	2:G:214:GLY:HA2	2.05	0.56
2:G:200:VAL:O	2:G:201:ASN:ND2	2.37	0.56
1:A:266:VAL:O	1:A:270:THR:HG23	2.05	0.56
2:G:269:MET:HE1	2:G:274:LEU:CD2	2.33	0.56
1:A:304:ASP:HB3	1:A:307:LYS:CG	2.36	0.56
1:A:329:LYS:HZ3	1:A:465:ALA:HB3	1.70	0.56
2:G:402:THR:CA	2:G:426:ASP:HB2	2.35	0.56
1:A:132:ASP:OD1	1:A:135:SER:HB2	2.04	0.56
1:A:357:ILE:HD11	1:A:471:PHE:HE2	1.71	0.56
1:A:174:ILE:HD11	1:A:443:HIS:ND1	2.21	0.56
2:G:237:GLU:HA	2:G:237:GLU:OE1	2.06	0.56
2:G:116:LEU:HD22	2:G:118:ILE:CD1	2.35	0.55
2:G:356:ALA:HB2	2:G:378:ALA:HB3	1.87	0.55
2:G:373:HIS:HD2	2:G:395:ARG:HH22	1.53	0.55
2:G:438:ARG:HA	2:G:438:ARG:NE	2.20	0.55
1:A:150:SER:HB2	1:A:492:MET:CE	2.36	0.55
1:A:285:THR:HG23	1:A:439:SER:CB	2.35	0.55
2:G:147:THR:O	2:G:149:ARG:HG3	2.07	0.55
1:A:285:THR:CG2	1:A:288:VAL:HG23	2.36	0.55
2:G:358:ALA:HB3	2:G:380:LEU:HA	1.88	0.55
1:A:305:PRO:CA	1:A:451:GLU:HG2	2.37	0.55
2:G:92:GLN:OE1	2:G:126:LEU:HD21	2.07	0.55
2:G:141:LEU:HD12	2:G:142:SER:H	1.72	0.55
2:G:443:LEU:O	2:G:462:LEU:HB2	2.05	0.55
1:A:302:THR:HB	1:A:456:ALA:HA	1.87	0.55
2:G:96:VAL:HB	2:G:130:VAL:CB	2.37	0.55
2:G:118:ILE:CG1	2:G:148:VAL:HG22	2.37	0.55
2:G:216:PHE:CD2	2:G:218:LEU:HD13	2.41	0.55
2:G:388:VAL:CG1	2:G:415:LEU:HA	2.36	0.55
2:G:406:LEU:HD12	2:G:411:SER:OG	2.07	0.55
1:A:419:PHE:O	1:A:422:SER:N	2.36	0.55
2:G:78:ARG:HD3	2:G:112:PHE:CB	2.26	0.55
2:G:108:VAL:N	2:G:138:GLY:O	2.40	0.55
2:G:143:MET:O	2:G:144:SER:OG	2.21	0.55
2:G:260:VAL:HG12	2:G:265:THR:OG1	2.06	0.55
1:A:147:VAL:HG22	1:A:489:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLY:O	1:A:190:LYS:HB2	2.07	0.55
1:A:277:LEU:CD2	1:A:290:LEU:HD21	2.37	0.55
2:G:179:GLN:HA	2:G:204:GLY:CA	2.31	0.55
1:A:206:VAL:O	1:A:210:LEU:N	2.28	0.55
1:A:186:GLY:O	1:A:190:LYS:HD2	2.07	0.54
1:A:383:MET:HE2	1:A:482:TRP:CD1	2.42	0.54
2:G:117:ILE:C	2:G:118:ILE:HD13	2.31	0.54
2:G:435:GLU:OE2	2:G:435:GLU:N	2.35	0.54
2:G:467:TRP:HD1	2:G:467:TRP:O	1.89	0.54
1:A:287:LEU:HD12	1:A:288:VAL:H	1.72	0.54
1:A:304:ASP:CG	1:A:307:LYS:HG2	2.31	0.54
2:G:250:THR:HG21	2:G:255:ALA:O	2.07	0.54
2:G:347:SER:O	2:G:348:LEU:HB2	2.08	0.54
1:A:235:THR:HA	1:A:238:ASN:ND2	2.19	0.54
2:G:212:ASP:HA	2:G:237:GLU:O	2.07	0.54
1:A:194:GLU:CD	1:A:199:TYR:HB2	2.33	0.54
2:G:283:ALA:HB3	2:G:308:GLY:O	2.08	0.54
1:A:153:LEU:HD22	1:A:169:PHE:CD1	2.43	0.54
1:A:312:PRO:HB3	1:A:319:VAL:CG1	2.36	0.54
1:A:316:LYS:HG3	1:A:317:ASN:H	1.72	0.54
1:A:320:ILE:HG21	1:A:499:ARG:HH12	1.72	0.54
2:G:158:LEU:HD12	2:G:183:VAL:CG1	2.38	0.54
2:G:72:GLY:O	2:G:73:ARG:HG2	2.07	0.54
2:G:384:GLY:O	2:G:411:SER:HB2	2.08	0.54
1:A:337:ASP:OD2	1:A:339:THR:OG1	2.25	0.54
1:A:460:SER:OG	1:A:462:ILE:HG12	2.08	0.54
2:G:478:VAL:O	2:G:479:LYS:HD3	2.08	0.54
2:G:94:LEU:O	2:G:128:VAL:HG23	2.08	0.54
2:G:194:GLN:HG3	2:G:219:SER:HB2	1.89	0.54
1:A:154:TYR:CE1	1:A:478:LEU:HD11	2.43	0.53
1:A:277:LEU:CD2	1:A:290:LEU:HD11	2.38	0.53
1:A:403:VAL:CG1	1:A:447:LEU:HB2	2.38	0.53
1:A:403:VAL:HG12	1:A:447:LEU:HB2	1.90	0.53
1:A:181:VAL:HG21	1:A:289:LEU:HD21	1.90	0.53
1:A:416:LEU:O	1:A:417:GLU:HB2	2.07	0.53
1:A:173:SER:HB3	1:A:291:ASN:ND2	2.23	0.53
2:G:178:GLN:O	2:G:204:GLY:N	2.41	0.53
2:G:262:ASP:HB3	2:G:265:THR:HG23	1.87	0.53
2:G:96:VAL:HB	2:G:130:VAL:HB	1.90	0.53
2:G:200:VAL:HG12	2:G:201:ASN:N	2.24	0.53
2:G:254:THR:HA	2:G:280:ASN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:THR:O	2:G:61:THR:OG1	2.22	0.53
2:G:94:LEU:O	2:G:94:LEU:HG	2.07	0.53
2:G:147:THR:O	2:G:147:THR:HG23	2.08	0.53
2:G:175:THR:HG23	2:G:200:VAL:HG13	1.89	0.53
2:G:373:HIS:CD2	2:G:395:ARG:HH22	2.27	0.53
1:A:197:LEU:O	1:A:198:SER:OG	2.26	0.53
1:A:255:SER:HA	1:A:258:ASN:HB2	1.90	0.53
1:A:367:LEU:HD22	1:A:476:PRO:C	2.33	0.53
1:A:384:GLU:HG3	1:A:385:LYS:N	2.23	0.53
2:G:94:LEU:HB3	2:G:128:VAL:HB	1.91	0.53
1:A:255:SER:O	1:A:258:ASN:HB2	2.09	0.53
1:A:315:PHE:CE1	1:A:320:ILE:HG23	2.43	0.53
2:G:119:GLU:HG3	2:G:119:GLU:O	2.09	0.53
1:A:395:LEU:HD23	1:A:470:VAL:CG2	2.39	0.53
2:G:263:ALA:HA	2:G:289:GLY:CA	2.39	0.53
1:A:335:PHE:C	1:A:336:ILE:HD13	2.34	0.52
1:A:398:LEU:HG	1:A:399:PRO:HD2	1.90	0.52
2:G:81:GLY:C	2:G:116:LEU:HD12	2.34	0.52
1:A:164:GLU:HA	1:A:496:TYR:CE2	2.44	0.52
1:A:359:VAL:CG1	1:A:475:GLN:HE21	2.21	0.52
1:A:407:GLN:OE1	1:A:409:MET:HE2	2.09	0.52
2:G:295:ARG:HH12	2:G:296:ASP:CG	2.17	0.52
1:A:150:SER:HB2	1:A:492:MET:HE2	1.90	0.52
1:A:302:THR:HA	1:A:453:GLY:HA3	1.92	0.52
1:A:332:VAL:O	1:A:391:PHE:HA	2.10	0.52
1:A:446:VAL:O	1:A:447:LEU:HD22	2.09	0.52
2:G:318:GLU:HG3	2:G:318:GLU:O	2.08	0.52
1:A:381:ALA:HA	1:A:384:GLU:HG2	1.90	0.52
1:A:428:CYS:SG	1:A:429:GLY:N	2.81	0.52
2:G:351:SER:O	2:G:352:THR:OG1	2.23	0.52
2:G:459:VAL:O	2:G:461:LEU:HG	2.10	0.52
1:A:312:PRO:HB3	1:A:319:VAL:HG11	1.91	0.52
1:A:332:VAL:HG21	1:A:396:LEU:HD22	1.90	0.52
1:A:497:ASP:OD1	1:A:499:ARG:NE	2.43	0.52
2:G:90:GLN:O	2:G:90:GLN:HG2	2.10	0.52
1:A:225:PHE:O	1:A:287:LEU:HD12	2.10	0.52
1:A:304:ASP:CB	1:A:307:LYS:HG2	2.40	0.52
1:A:308:THR:HA	1:A:324:MET:O	2.10	0.52
2:G:229:GLU:HG3	2:G:254:THR:OG1	2.08	0.52
2:G:263:ALA:N	2:G:288:ALA:O	2.42	0.52
2:G:410:ARG:CG	2:G:438:ARG:HG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:426:ASP:O	2:G:427:ILE:HD13	2.10	0.52
1:A:153:LEU:HD22	1:A:169:PHE:CE1	2.44	0.52
2:G:247:ARG:HB3	2:G:247:ARG:NH1	2.25	0.52
2:G:367:VAL:O	2:G:391:LEU:HD23	2.10	0.52
1:A:205:CYS:O	1:A:209:ALA:N	2.24	0.52
1:A:340:LEU:HD11	1:A:374:LEU:CD1	2.39	0.52
2:G:250:THR:HG22	2:G:251:GLN:N	2.23	0.52
2:G:319:LEU:HD23	2:G:320:ALA:N	2.25	0.52
1:A:314:HIS:CD2	1:A:363:LEU:HD21	2.45	0.52
2:G:117:ILE:HG13	2:G:147:THR:HG22	1.92	0.52
1:A:164:GLU:HG2	1:A:496:TYR:CD2	2.45	0.51
1:A:299:TRP:HB2	1:A:453:GLY:HA2	1.92	0.51
1:A:329:LYS:NZ	1:A:465:ALA:HB3	2.25	0.51
1:A:359:VAL:HG12	1:A:475:GLN:HE21	1.75	0.51
1:A:413:MET:CE	1:A:421:PHE:HB2	2.39	0.51
2:G:83:THR:HA	2:G:116:LEU:CD2	2.40	0.51
2:G:311:VAL:HG21	2:G:317:VAL:HG11	1.91	0.51
1:A:181:VAL:HG22	1:A:289:LEU:HD21	1.93	0.51
1:A:300:LYS:HB2	1:A:349:LEU:O	2.10	0.51
1:A:324:MET:CE	1:A:397:THR:HG22	2.40	0.51
1:A:455:GLU:OE2	1:A:457:ALA:HB2	2.11	0.51
2:G:132:GLU:OE1	2:G:138:GLY:HA2	2.10	0.51
2:G:207:ALA:O	2:G:208:ILE:C	2.53	0.51
1:A:225:PHE:CE2	1:A:249:ARG:HD2	2.45	0.51
1:A:241:ARG:CG	1:A:247:SER:HB3	2.41	0.51
1:A:276:ARG:NH1	1:A:279:ASP:OD1	2.38	0.51
1:A:310:MET:HE1	1:A:323:PRO:CB	2.40	0.51
1:A:418:PHE:CE2	1:A:420:ASP:HB2	2.45	0.51
2:G:249:THR:HG22	2:G:250:THR:N	2.23	0.51
2:G:434:PRO:HD2	2:G:435:GLU:OE1	2.09	0.51
1:A:204:THR:HG23	1:A:205:CYS:H	1.76	0.51
1:A:446:VAL:C	1:A:447:LEU:HD22	2.35	0.51
2:G:70:VAL:HG21	2:G:77:VAL:HG11	1.93	0.51
2:G:83:THR:CA	2:G:116:LEU:HD21	2.41	0.51
2:G:198:VAL:HG22	2:G:223:ILE:CD1	2.40	0.51
2:G:306:SER:O	2:G:307:HIS:ND1	2.42	0.51
2:G:358:ALA:O	2:G:380:LEU:HD12	2.10	0.51
2:G:380:LEU:HD22	2:G:388:VAL:HG21	1.93	0.51
1:A:189:THR:HG21	1:A:426:ASN:O	2.11	0.51
1:A:260:GLU:OE2	1:A:264:THR:HG21	2.10	0.51
2:G:118:ILE:O	2:G:120:THR:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:371:VAL:HG13	2:G:371:VAL:O	2.11	0.51
2:G:386:SER:OG	2:G:413:LEU:HG	2.11	0.51
1:A:360:PRO:HA	1:A:370:MET:SD	2.51	0.51
2:G:167:THR:O	2:G:168:LEU:HD23	2.11	0.51
2:G:412:VAL:HG22	2:G:438:ARG:CB	2.41	0.51
1:A:241:ARG:O	1:A:245:SER:HA	2.11	0.51
1:A:335:PHE:CZ	1:A:344:VAL:HG11	2.46	0.51
1:A:384:GLU:HG3	1:A:385:LYS:H	1.76	0.51
1:A:166:ASN:HB3	1:A:496:TYR:H	1.76	0.51
1:A:329:LYS:CD	1:A:465:ALA:HB3	2.38	0.51
2:G:65:GLU:H	2:G:65:GLU:CD	2.18	0.51
2:G:348:LEU:HD23	2:G:349:VAL:CA	2.41	0.51
1:A:341:LYS:O	1:A:361:GLN:HG3	2.11	0.51
2:G:83:THR:HG22	2:G:85:ARG:HG3	1.93	0.51
2:G:76:GLU:HA	2:G:110:SER:O	2.10	0.50
2:G:191:LEU:C	2:G:191:LEU:HD23	2.37	0.50
2:G:329:GLN:HG3	2:G:330:GLY:H	1.75	0.50
1:A:359:VAL:HG13	1:A:360:PRO:HD2	1.93	0.50
2:G:94:LEU:HD23	2:G:128:VAL:CB	2.40	0.50
2:G:367:VAL:HG21	2:G:372:VAL:HG21	1.92	0.50
1:A:234:ASP:OD1	1:A:235:THR:N	2.45	0.50
1:A:252:SER:N	1:A:258:ASN:OD1	2.29	0.50
2:G:187:GLN:CD	2:G:187:GLN:H	2.19	0.50
2:G:70:VAL:HG12	2:G:70:VAL:O	2.11	0.50
2:G:238:GLY:H	2:G:265:THR:HG22	1.76	0.50
2:G:301:THR:HG22	2:G:301:THR:O	2.11	0.50
2:G:419:ASP:HA	2:G:445:ASP:O	2.10	0.50
2:G:183:VAL:CG2	2:G:208:ILE:HG23	2.37	0.50
2:G:382:VAL:HG11	2:G:386:SER:CB	2.40	0.50
2:G:419:ASP:O	2:G:419:ASP:OD2	2.29	0.50
1:A:413:MET:HG2	1:A:418:PHE:HB3	1.92	0.50
2:G:84:ILE:HD13	2:G:118:ILE:HD12	1.92	0.50
2:G:219:SER:HA	2:G:244:THR:O	2.12	0.50
1:A:156:ALA:HB2	1:A:416:LEU:CD2	2.40	0.50
1:A:343:LYS:HE2	1:A:471:PHE:HE1	1.76	0.50
1:A:431:THR:OG1	1:A:436:LEU:HD21	2.12	0.50
2:G:257:ALA:HB3	2:G:283:ALA:O	2.12	0.50
1:A:123:CYS:SG	1:A:124:PRO:HD2	2.52	0.50
2:G:238:GLY:N	2:G:265:THR:HG22	2.27	0.50
1:A:332:VAL:HG12	1:A:333:ALA:N	2.26	0.49
1:A:399:PRO:HD3	1:A:473:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:228:LEU:HD23	2:G:228:LEU:H	1.76	0.49
2:G:402:THR:N	2:G:426:ASP:HB2	2.26	0.49
1:A:286:ARG:HB2	1:A:437:GLN:HE21	1.76	0.49
2:G:181:PRO:HA	2:G:206:SER:O	2.12	0.49
2:G:208:ILE:HD12	2:G:233:ILE:HD11	1.94	0.49
2:G:269:MET:HE1	2:G:274:LEU:CD1	2.40	0.49
1:A:290:LEU:HD23	1:A:291:ASN:N	2.27	0.49
1:A:447:LEU:HD11	1:A:491:PHE:CE2	2.47	0.49
2:G:84:ILE:HD12	2:G:116:LEU:HD22	1.95	0.49
2:G:469:VAL:HG22	2:G:470:THR:N	2.27	0.49
2:G:305:ALA:HA	2:G:330:GLY:O	2.12	0.49
2:G:467:TRP:CH2	2:G:475:VAL:HG21	2.32	0.49
2:G:453:THR:HG23	2:G:454:ASP:H	1.78	0.49
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.94	0.49
1:A:398:LEU:HG	1:A:473:VAL:HG21	1.95	0.49
2:G:65:GLU:HB3	2:G:91:ALA:HA	1.95	0.49
2:G:198:VAL:HG22	2:G:223:ILE:HD12	1.94	0.49
2:G:256:PRO:HA	2:G:282:PRO:O	2.13	0.49
2:G:342:MET:HE1	2:G:344:ARG:CD	2.43	0.49
1:A:281:LEU:HD23	1:A:282:PRO:O	2.12	0.49
1:A:303:PHE:CE2	1:A:327:SER:HB2	2.48	0.49
2:G:237:GLU:CA	2:G:262:ASP:OD1	2.54	0.49
2:G:294:PHE:O	2:G:295:ARG:HG2	2.12	0.49
2:G:406:LEU:O	2:G:429:PRO:HA	2.13	0.49
2:G:196:LEU:N	2:G:196:LEU:HD12	2.27	0.49
1:A:189:THR:HA	1:A:420:ASP:OD2	2.13	0.49
2:G:235:VAL:HG22	2:G:260:VAL:HG22	1.94	0.49
2:G:311:VAL:HG12	2:G:315:SER:OG	2.13	0.49
1:A:396:LEU:HD13	1:A:471:PHE:HB3	1.95	0.49
2:G:419:ASP:OD2	2:G:420:ARG:NH2	2.46	0.49
1:A:144:ASP:OD1	1:A:144:ASP:C	2.56	0.48
2:G:407:ILE:HG12	2:G:430:GLU:HG3	1.95	0.48
2:G:260:VAL:HB	2:G:286:LEU:CD1	2.40	0.48
2:G:292:ALA:HB1	2:G:294:PHE:CE1	2.48	0.48
1:A:181:VAL:O	1:A:185:ALA:N	2.46	0.48
1:A:340:LEU:HD12	1:A:382:ILE:HD11	1.94	0.48
2:G:72:GLY:C	2:G:73:ARG:HG2	2.38	0.48
2:G:210:ALA:HB3	2:G:235:VAL:HG12	1.95	0.48
1:A:259:LEU:HD12	1:A:281:LEU:HB3	1.94	0.48
1:A:305:PRO:N	1:A:451:GLU:HG2	2.28	0.48
1:A:433:ASP:OD1	1:A:435:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:HD1	1:A:197:LEU:HA	1.77	0.48
2:G:226:ARG:O	2:G:230:VAL:HG11	2.13	0.48
2:G:380:LEU:HG	2:G:382:VAL:CG2	2.42	0.48
1:A:183:LEU:O	1:A:183:LEU:HD12	2.13	0.48
1:A:256:ASP:OD1	1:A:257:ALA:N	2.42	0.48
1:A:273:LYS:HG3	1:A:294:TYR:CZ	2.49	0.48
1:A:346:GLN:CB	1:A:386:LEU:HD11	2.42	0.48
1:A:352:ASN:ND2	1:A:485:GLN:HB2	2.29	0.48
2:G:94:LEU:HG	2:G:128:VAL:HG23	1.96	0.48
2:G:128:VAL:HG13	2:G:158:LEU:CD2	2.44	0.48
2:G:396:LEU:O	2:G:396:LEU:HD23	2.13	0.48
1:A:281:LEU:HD23	1:A:282:PRO:N	2.29	0.48
2:G:118:ILE:CB	2:G:148:VAL:HG22	2.44	0.48
2:G:212:ASP:OD2	2:G:237:GLU:HB3	2.14	0.48
2:G:459:VAL:HG11	2:G:467:TRP:CE3	2.49	0.48
1:A:385:LYS:O	1:A:388:MET:HG3	2.13	0.48
2:G:94:LEU:HD21	2:G:113:LEU:CD2	2.44	0.48
2:G:141:LEU:HD12	2:G:142:SER:N	2.29	0.48
2:G:173:LEU:O	2:G:173:LEU:HD12	2.13	0.48
2:G:467:TRP:C	2:G:467:TRP:CD1	2.92	0.48
2:G:250:THR:CG2	2:G:251:GLN:N	2.77	0.47
2:G:431:ALA:HB3	2:G:433:GLN:OE1	2.14	0.47
2:G:434:PRO:HD2	2:G:435:GLU:CD	2.39	0.47
2:G:456:VAL:CG1	2:G:457:HIS:N	2.76	0.47
2:G:77:VAL:HG23	2:G:78:ARG:N	2.28	0.47
2:G:85:ARG:HG2	2:G:119:GLU:CG	2.44	0.47
1:A:304:ASP:C	1:A:451:GLU:HG2	2.39	0.47
2:G:190:GLN:CG	2:G:215:SER:HB3	2.42	0.47
2:G:460:ARG:NE	2:G:462:LEU:HD11	2.29	0.47
1:A:123:CYS:CB	1:A:233:ARG:HH12	2.27	0.47
1:A:164:GLU:HG2	1:A:496:TYR:CE2	2.49	0.47
2:G:194:GLN:O	2:G:196:LEU:HD12	2.14	0.47
2:G:332:HIS:HB2	2:G:335:VAL:HG22	1.96	0.47
2:G:403:ALA:CB	2:G:425:GLY:HA3	2.32	0.47
1:A:300:LYS:CA	1:A:454:VAL:HG12	2.44	0.47
1:A:383:MET:HE2	1:A:482:TRP:CD2	2.49	0.47
2:G:156:PHE:CE1	2:G:181:PRO:HD2	2.50	0.47
2:G:393:GLY:H	2:G:420:ARG:HB3	1.78	0.47
1:A:259:LEU:C	1:A:259:LEU:HD23	2.39	0.47
1:A:325:MET:SD	1:A:398:LEU:O	2.73	0.47
1:A:376:PRO:O	1:A:380:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:56:VAL:HA	2:G:80:THR:OG1	2.14	0.47
2:G:58:ILE:HD12	2:G:58:ILE:H	1.79	0.47
2:G:173:LEU:CD1	2:G:198:VAL:HG12	2.45	0.47
2:G:200:VAL:HG12	2:G:201:ASN:H	1.80	0.47
1:A:176:SER:O	1:A:179:THR:OG1	2.27	0.47
2:G:145:GLY:H	2:G:170:ASP:HB3	1.80	0.47
1:A:362:ASN:CG	1:A:364:LYS:H	2.23	0.47
1:A:490:VAL:HG13	1:A:491:PHE:N	2.29	0.47
1:A:320:ILE:CG2	1:A:499:ARG:HH12	2.28	0.47
2:G:130:VAL:HG13	2:G:160:LEU:CD2	2.45	0.47
2:G:466:VAL:HG12	2:G:468:THR:OG1	2.15	0.47
1:A:346:GLN:OE1	1:A:386:LEU:HG	2.16	0.46
2:G:438:ARG:HA	2:G:438:ARG:NH1	2.30	0.46
1:A:386:LEU:O	1:A:389:SER:HB2	2.15	0.46
2:G:274:LEU:HB2	2:G:299:LEU:HD23	1.98	0.46
2:G:319:LEU:CD1	2:G:324:VAL:HG21	2.39	0.46
2:G:382:VAL:HB	2:G:413:LEU:CD1	2.41	0.46
2:G:83:THR:HA	2:G:116:LEU:HD21	1.97	0.46
1:A:340:LEU:CD1	1:A:374:LEU:HD13	2.45	0.46
1:A:400:ARG:NH2	1:A:451:GLU:OE1	2.47	0.46
1:A:497:ASP:CG	1:A:499:ARG:HG2	2.40	0.46
1:A:151:LEU:HD21	1:A:379:PHE:CD2	2.50	0.46
1:A:409:MET:CG	1:A:441:MET:HE2	2.45	0.46
2:G:201:ASN:HD21	2:G:226:ARG:HH11	1.62	0.46
1:A:150:SER:CB	1:A:492:MET:HE1	2.46	0.46
1:A:384:GLU:HA	1:A:387:GLU:HG3	1.97	0.46
2:G:159:GLN:HA	2:G:184:VAL:O	2.15	0.46
2:G:289:GLY:HA2	2:G:314:HIS:O	2.15	0.46
1:A:218:VAL:HG22	1:A:293:ILE:CG1	2.46	0.46
1:A:218:VAL:HG21	1:A:491:PHE:CZ	2.51	0.46
1:A:299:TRP:CE3	1:A:349:LEU:HD23	2.51	0.46
1:A:413:MET:HE3	1:A:413:MET:HB3	1.78	0.46
1:A:413:MET:SD	1:A:421:PHE:HB2	2.56	0.46
2:G:433:GLN:HB3	2:G:435:GLU:OE2	2.16	0.46
1:A:367:LEU:HD22	1:A:476:PRO:O	2.16	0.46
1:A:335:PHE:CE1	1:A:344:VAL:HG11	2.51	0.46
2:G:416:ASP:O	2:G:417:ILE:HG12	2.16	0.46
1:A:178:LEU:HD12	1:A:193:LEU:HD21	1.98	0.45
1:A:154:TYR:OH	1:A:478:LEU:HD13	2.16	0.45
2:G:130:VAL:CG1	2:G:160:LEU:HD21	2.46	0.45
2:G:196:LEU:HB2	2:G:221:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:222:ASP:CB	2:G:247:ARG:HG2	2.46	0.45
2:G:301:THR:HG22	2:G:306:SER:CB	2.46	0.45
1:A:310:MET:HE2	1:A:323:PRO:HA	1.99	0.45
2:G:460:ARG:CZ	2:G:462:LEU:HD11	2.47	0.45
1:A:241:ARG:HG2	1:A:247:SER:HB3	1.99	0.45
2:G:114:GLN:O	2:G:115:ASN:C	2.58	0.45
2:G:234:TYR:CE2	2:G:236:GLN:HG2	2.51	0.45
2:G:405:ARG:HG2	2:G:430:GLU:OE2	2.17	0.45
1:A:226:HIS:CB	1:A:230:LEU:HD23	2.42	0.45
1:A:447:LEU:HD21	1:A:491:PHE:CE2	2.52	0.45
2:G:321:HIS:H	2:G:346:GLY:HA2	1.80	0.45
2:G:407:ILE:HG12	2:G:430:GLU:CD	2.41	0.45
2:G:452:ARG:HE	2:G:471:GLY:CA	2.29	0.45
2:G:477:GLU:HG2	2:G:478:VAL:N	2.30	0.45
1:A:203:PHE:O	1:A:206:VAL:HG12	2.16	0.45
1:A:362:ASN:ND2	1:A:364:LYS:HB3	2.29	0.45
2:G:193:ALA:HB1	2:G:196:LEU:HD21	1.97	0.45
2:G:380:LEU:HB3	2:G:404:ILE:HG13	1.99	0.45
2:G:390:LEU:HD23	2:G:394:ALA:CB	2.46	0.45
2:G:402:THR:CG2	2:G:405:ARG:HH21	2.25	0.45
1:A:347:LEU:HD12	1:A:347:LEU:N	2.32	0.45
2:G:158:LEU:CB	2:G:183:VAL:HG12	2.30	0.45
1:A:479:PHE:CE1	1:A:495:VAL:HG23	2.52	0.45
2:G:158:LEU:HD12	2:G:183:VAL:HG11	1.99	0.45
2:G:453:THR:O	2:G:454:ASP:HB2	2.17	0.45
1:A:337:ASP:OD1	1:A:382:ILE:HG12	2.17	0.45
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.81	0.45
1:A:304:ASP:OD1	1:A:306:LYS:HE2	2.17	0.45
2:G:410:ARG:HG2	2:G:410:ARG:O	2.17	0.45
1:A:162:LYS:HE2	1:A:165:THR:HG21	1.98	0.44
1:A:409:MET:HG3	1:A:441:MET:HE2	1.99	0.44
2:G:71:THR:O	2:G:98:THR:HB	2.17	0.44
2:G:74:THR:O	2:G:74:THR:HG22	2.17	0.44
2:G:85:ARG:HG2	2:G:119:GLU:HG2	1.98	0.44
2:G:90:GLN:N	2:G:123:THR:O	2.49	0.44
2:G:238:GLY:CA	2:G:265:THR:HG22	2.48	0.44
2:G:262:ASP:O	2:G:263:ALA:CB	2.64	0.44
2:G:329:GLN:O	2:G:330:GLY:C	2.59	0.44
2:G:443:LEU:HD23	2:G:447:GLY:C	2.42	0.44
1:A:182:LEU:HD12	1:A:190:LYS:HG3	1.98	0.44
1:A:254:ASN:OD1	1:A:254:ASN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HB2	1:A:437:GLN:NE2	2.32	0.44
1:A:420:ASP:HB3	1:A:425:LEU:HD12	1.99	0.44
2:G:127:GLY:O	2:G:128:VAL:C	2.59	0.44
2:G:380:LEU:H	2:G:396:LEU:HD21	1.81	0.44
1:A:166:ASN:HB2	1:A:495:VAL:HA	1.99	0.44
2:G:77:VAL:HG22	2:G:111:VAL:HB	1.99	0.44
2:G:201:ASN:ND2	2:G:226:ARG:HH11	2.16	0.44
2:G:82:GLY:N	2:G:116:LEU:HG	2.33	0.44
2:G:365:LEU:HD12	2:G:366:THR:N	2.33	0.44
1:A:159:ALA:CB	1:A:160:MET:HE2	2.48	0.44
1:A:206:VAL:O	1:A:210:LEU:HD23	2.17	0.44
2:G:65:GLU:CG	2:G:91:ALA:HA	2.47	0.44
2:G:261:GLU:HB3	2:G:287:LEU:HB2	2.00	0.44
2:G:318:GLU:OE2	2:G:342:MET:HE3	2.18	0.44
2:G:309:VAL:HB	2:G:334:LEU:CD1	2.48	0.44
1:A:225:PHE:HA	1:A:249:ARG:O	2.18	0.44
2:G:112:PHE:HA	2:G:142:SER:O	2.17	0.44
2:G:197:VAL:HG12	2:G:197:VAL:O	2.18	0.44
2:G:216:PHE:HD2	2:G:218:LEU:CD1	2.28	0.44
1:A:266:VAL:HG11	1:A:277:LEU:HD23	2.00	0.43
1:A:291:ASN:OD1	1:A:292:ALA:N	2.51	0.43
2:G:158:LEU:HB2	2:G:183:VAL:CG1	2.31	0.43
2:G:209:HIS:NE2	2:G:211:GLN:OE1	2.49	0.43
2:G:260:VAL:HG21	2:G:267:VAL:HG21	2.00	0.43
2:G:456:VAL:HG12	2:G:457:HIS:N	2.33	0.43
1:A:447:LEU:HD21	1:A:491:PHE:CD2	2.54	0.43
2:G:263:ALA:CA	2:G:289:GLY:HA3	2.46	0.43
1:A:138:THR:O	1:A:141:VAL:N	2.50	0.43
1:A:316:LYS:HD2	1:A:316:LYS:HA	1.86	0.43
1:A:344:VAL:HG23	1:A:358:LEU:CD2	2.48	0.43
1:A:427:LEU:HD13	1:A:430:LEU:CD2	2.48	0.43
2:G:115:ASN:HA	2:G:144:SER:O	2.17	0.43
1:A:148:ASP:CG	1:A:152:LYS:HE3	2.43	0.43
1:A:298:LYS:NZ	1:A:452:THR:HB	2.34	0.43
1:A:338:GLN:O	1:A:341:LYS:N	2.51	0.43
1:A:383:MET:HG2	1:A:482:TRP:CH2	2.54	0.43
2:G:58:ILE:HG23	2:G:83:THR:O	2.18	0.43
2:G:419:ASP:OD2	2:G:419:ASP:C	2.62	0.43
1:A:142:LEU:HD13	1:A:203:PHE:CE1	2.39	0.43
1:A:178:LEU:HD12	1:A:193:LEU:HD11	2.01	0.43
1:A:241:ARG:HD2	1:A:247:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG21	1:A:277:LEU:HB3	2.00	0.43
2:G:238:GLY:O	2:G:239:MET:HG2	2.18	0.43
1:A:142:LEU:O	1:A:146:LEU:HG	2.18	0.43
1:A:153:LEU:HD21	1:A:157:PHE:CE1	2.54	0.43
1:A:206:VAL:HG13	1:A:207:HIS:N	2.33	0.43
1:A:259:LEU:HD11	1:A:279:ASP:O	2.17	0.43
2:G:89:ASN:O	2:G:90:GLN:HB3	2.19	0.43
2:G:94:LEU:HD23	2:G:128:VAL:CG2	2.48	0.43
2:G:193:ALA:HB1	2:G:196:LEU:CD2	2.49	0.43
2:G:225:ALA:C	2:G:226:ARG:HD2	2.44	0.43
2:G:463:ASP:O	2:G:464:ARG:HB2	2.19	0.43
1:A:299:TRP:CE3	1:A:299:TRP:HA	2.53	0.43
1:A:300:LYS:C	1:A:454:VAL:HG12	2.44	0.43
2:G:395:ARG:HG3	2:G:424:LEU:HD12	2.01	0.43
2:G:463:ASP:HB3	2:G:464:ARG:CZ	2.49	0.43
1:A:206:VAL:CA	1:A:209:ALA:HB3	2.45	0.43
2:G:97:GLY:HA3	2:G:131:HIS:O	2.18	0.43
2:G:183:VAL:HG23	2:G:183:VAL:O	2.19	0.43
2:G:243:LEU:HD12	2:G:243:LEU:N	2.34	0.43
2:G:412:VAL:HG22	2:G:438:ARG:HB3	2.01	0.43
1:A:403:VAL:HG13	1:A:403:VAL:O	2.18	0.43
1:A:483:ASP:C	1:A:485:GLN:H	2.26	0.43
2:G:348:LEU:HD23	2:G:349:VAL:C	2.44	0.42
1:A:149:PHE:CE1	1:A:197:LEU:HD13	2.54	0.42
1:A:226:HIS:O	1:A:251:LEU:HB2	2.18	0.42
1:A:263:ASN:ND2	1:A:278:LEU:O	2.46	0.42
1:A:466:ARG:HA	2:G:234:TYR:CZ	2.53	0.42
1:A:182:LEU:HD11	1:A:190:LYS:HG3	2.00	0.42
2:G:68:ILE:O	2:G:94:LEU:HA	2.20	0.42
2:G:230:VAL:O	2:G:255:ALA:HB1	2.19	0.42
2:G:457:HIS:ND1	2:G:458:THR:HG23	2.34	0.42
1:A:427:LEU:HB3	1:A:430:LEU:HB3	2.00	0.42
2:G:238:GLY:H	2:G:265:THR:CG2	2.32	0.42
2:G:381:GLU:HG2	2:G:405:ARG:HB3	2.02	0.42
2:G:469:VAL:HG22	2:G:470:THR:H	1.84	0.42
2:G:252:GLY:HA2	2:G:277:SER:O	2.20	0.42
2:G:478:VAL:C	2:G:479:LYS:HG2	2.43	0.42
1:A:134:GLU:HA	1:A:137:SER:OG	2.19	0.42
1:A:154:TYR:CD2	1:A:154:TYR:C	2.98	0.42
1:A:327:SER:OG	1:A:330:TYR:HB2	2.20	0.42
1:A:400:ARG:HH21	1:A:450:THR:HB	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:C	1:A:481:LEU:HD23	2.45	0.42
2:G:352:THR:HA	2:G:376:GLY:HA3	2.02	0.42
2:G:464:ARG:O	2:G:466:VAL:HG23	2.20	0.42
1:A:483:ASP:O	1:A:484:GLN:CG	2.57	0.42
1:A:219:THR:OG1	1:A:294:TYR:CE1	2.72	0.42
1:A:276:ARG:NH1	1:A:276:ARG:HG3	2.34	0.42
1:A:298:LYS:HB3	1:A:452:THR:O	2.20	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.89	0.42
1:A:480:VAL:HG22	1:A:492:MET:HG3	2.00	0.42
1:A:261:LEU:C	1:A:261:LEU:HD23	2.45	0.42
1:A:277:LEU:HD21	1:A:290:LEU:HD21	2.02	0.42
2:G:56:VAL:HG12	2:G:80:THR:HG23	2.00	0.42
2:G:342:MET:HE1	2:G:344:ARG:HD3	2.01	0.42
2:G:478:VAL:HG12	2:G:479:LYS:N	2.34	0.42
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.82	0.41
1:A:345:GLY:O	1:A:357:ILE:HG12	2.20	0.41
1:A:462:ILE:N	1:A:462:ILE:HD13	2.36	0.41
1:A:467:THR:O	1:A:467:THR:HG23	2.19	0.41
2:G:228:LEU:CG	2:G:229:GLU:OE2	2.69	0.41
2:G:243:LEU:HD22	2:G:269:MET:HE2	2.03	0.41
2:G:266:HIS:NE2	2:G:268:SER:OG	2.53	0.41
1:A:204:THR:CG2	1:A:205:CYS:N	2.83	0.41
2:G:114:GLN:OE1	2:G:115:ASN:N	2.53	0.41
2:G:226:ARG:HG3	2:G:251:GLN:HG2	2.01	0.41
2:G:260:VAL:CG2	2:G:267:VAL:HG21	2.50	0.41
2:G:400:GLN:HG2	2:G:401:PRO:CD	2.40	0.41
2:G:404:ILE:HD13	2:G:423:LEU:HD21	2.02	0.41
1:A:133:LEU:HG	1:A:134:GLU:OE2	2.20	0.41
1:A:307:LYS:O	1:A:326:ASN:ND2	2.54	0.41
2:G:65:GLU:HG3	2:G:91:ALA:HA	2.01	0.41
2:G:349:VAL:HG12	2:G:357:ALA:HB1	2.02	0.41
2:G:395:ARG:O	2:G:395:ARG:HG2	2.19	0.41
1:A:288:VAL:HG13	1:A:440:ALA:O	2.21	0.41
1:A:496:TYR:O	1:A:498:PRO:HD3	2.20	0.41
2:G:158:LEU:HD12	2:G:183:VAL:HG12	2.02	0.41
2:G:236:GLN:CD	2:G:237:GLU:HG2	2.44	0.41
2:G:259:GLN:HG2	2:G:261:GLU:OE1	2.20	0.41
2:G:404:ILE:HB	2:G:427:ILE:HD13	2.01	0.41
2:G:452:ARG:HE	2:G:471:GLY:C	2.28	0.41
1:A:346:GLN:C	1:A:347:LEU:HD12	2.45	0.41
2:G:295:ARG:HB3	2:G:295:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:459:VAL:O	2:G:460:ARG:C	2.62	0.41
1:A:233:ARG:O	1:A:237:VAL:HG23	2.21	0.41
1:A:356:VAL:HG22	1:A:386:LEU:CD2	2.51	0.41
2:G:228:LEU:HG	2:G:229:GLU:OE2	2.21	0.41
2:G:468:THR:HG22	2:G:468:THR:O	2.19	0.41
2:G:475:VAL:HG12	2:G:477:GLU:H	1.86	0.41
1:A:143:GLY:O	1:A:147:VAL:HG23	2.20	0.41
1:A:218:VAL:O	1:A:218:VAL:HG13	2.19	0.41
1:A:346:GLN:HE21	1:A:354:SER:CB	2.25	0.41
1:A:228:PRO:HD3	1:A:251:LEU:C	2.45	0.41
1:A:295:LEU:HB3	1:A:447:LEU:HD13	2.03	0.41
1:A:334:HIS:CE1	1:A:336:ILE:HD11	2.55	0.41
1:A:398:LEU:HD23	1:A:399:PRO:N	2.35	0.41
2:G:87:SER:HA	2:G:121:SER:O	2.21	0.41
2:G:266:HIS:HA	2:G:291:SER:O	2.21	0.41
2:G:269:MET:HG2	2:G:270:ASN:N	2.35	0.41
2:G:311:VAL:HG21	2:G:317:VAL:HG12	2.02	0.41
2:G:311:VAL:CG1	2:G:315:SER:OG	2.69	0.41
2:G:390:LEU:HD23	2:G:394:ALA:O	2.21	0.41
2:G:416:ASP:C	2:G:417:ILE:HG12	2.45	0.41
1:A:307:LYS:HB3	1:A:326:ASN:HB2	2.03	0.41
1:A:481:LEU:HD23	1:A:482:TRP:N	2.36	0.41
2:G:202:GLY:O	2:G:227:GLY:HA3	2.20	0.41
2:G:319:LEU:HD22	2:G:343:VAL:HG13	2.03	0.41
2:G:406:LEU:O	2:G:406:LEU:HG	2.20	0.41
1:A:189:THR:HA	1:A:192:ASN:OD1	2.21	0.41
2:G:324:VAL:O	2:G:349:VAL:HA	2.21	0.41
1:A:157:PHE:HA	1:A:412:ILE:HD11	2.03	0.40
1:A:332:VAL:CG1	1:A:333:ALA:N	2.83	0.40
2:G:70:VAL:O	2:G:71:THR:C	2.64	0.40
2:G:114:GLN:CD	2:G:115:ASN:H	2.29	0.40
2:G:178:GLN:O	2:G:204:GLY:CA	2.68	0.40
2:G:186:TRP:O	2:G:187:GLN:C	2.64	0.40
2:G:243:LEU:HB3	2:G:246:THR:CG2	2.51	0.40
2:G:460:ARG:NH2	2:G:462:LEU:HD11	2.36	0.40
1:A:168:ALA:HB2	1:A:403:VAL:HG11	2.04	0.40
2:G:365:LEU:HD12	2:G:366:THR:H	1.86	0.40
1:A:480:VAL:HG22	1:A:492:MET:CG	2.51	0.40
2:G:77:VAL:CG2	2:G:111:VAL:HB	2.51	0.40
2:G:225:ALA:HB1	2:G:230:VAL:CG2	2.51	0.40
2:G:235:VAL:CG2	2:G:260:VAL:HG22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:382:VAL:O	2:G:406:LEU:HA	2.21	0.40
2:G:474:ARG:NE	2:G:474:ARG:HA	2.35	0.40
2:G:65:GLU:HG3	2:G:91:ALA:CA	2.51	0.40
2:G:117:ILE:O	2:G:118:ILE:HD13	2.21	0.40
2:G:373:HIS:ND1	2:G:375:HIS:HB2	2.36	0.40
2:G:413:LEU:HD21	2:G:415:LEU:HB2	2.01	0.40
2:G:417:ILE:HG22	2:G:447:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/403 (93%)	339 (90%)	37 (10%)	0	100	100
2	G	417/877 (48%)	313 (75%)	103 (25%)	1 (0%)	43	72
All	All	793/1280 (62%)	652 (82%)	140 (18%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	163	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/366 (94%)	342 (100%)	1 (0%)	86	83
2	G	302/637 (47%)	302 (100%)	0	100	100
All	All	645/1003 (64%)	644 (100%)	1 (0%)	85	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	238	ASN
1	A	271	ASN
1	A	272	ASN
1	A	334	HIS
1	A	346	GLN
1	A	365	HIS
1	A	475	GLN
2	G	66	HIS
2	G	92	GLN
2	G	314	HIS
2	G	364	HIS
2	G	375	HIS
2	G	387	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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-11814. These allow visual inspection of the internal detail of the map and identification of artifacts.

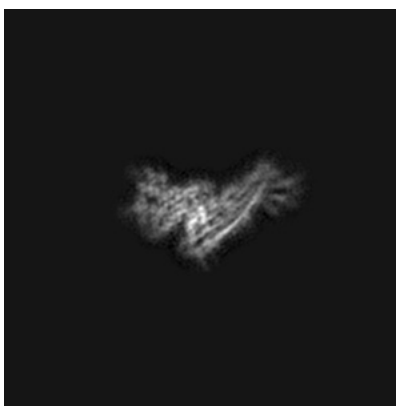
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

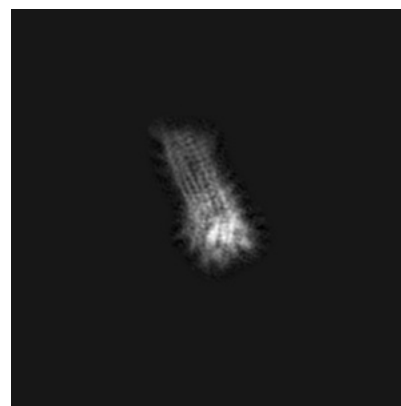
6.1.1 Primary map



X

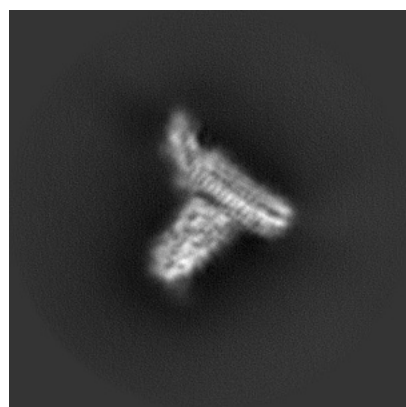


Y

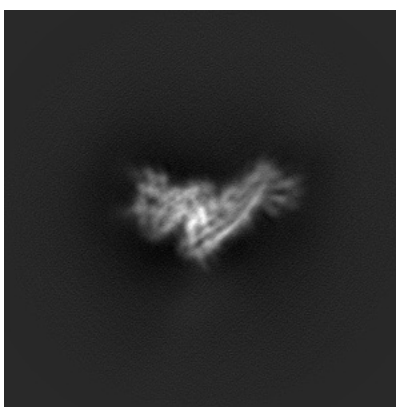


Z

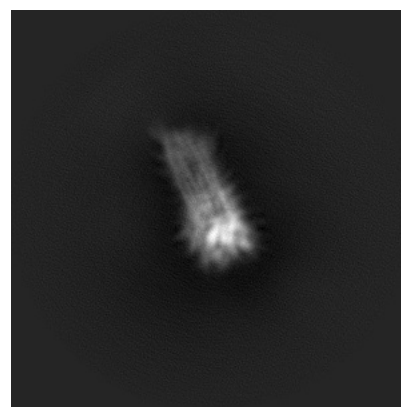
6.1.2 Raw map



X



Y

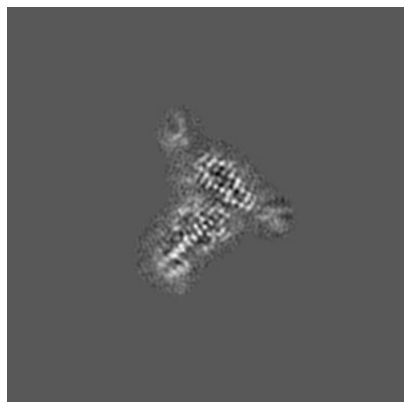


Z

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

6.2 Central slices [i](#)

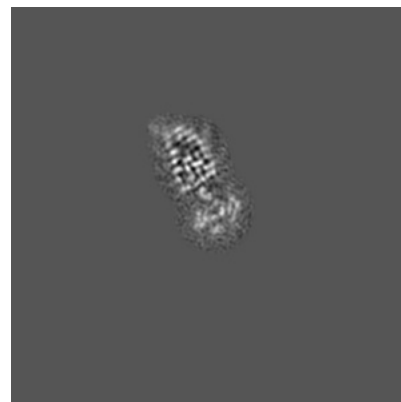
6.2.1 Primary map



X Index: 164

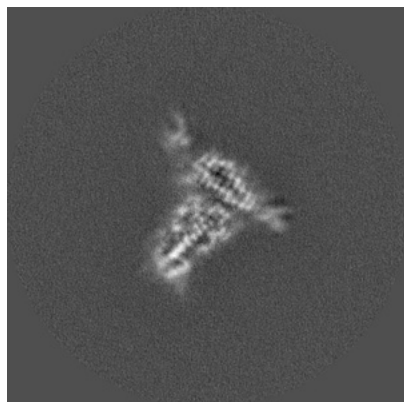


Y Index: 164

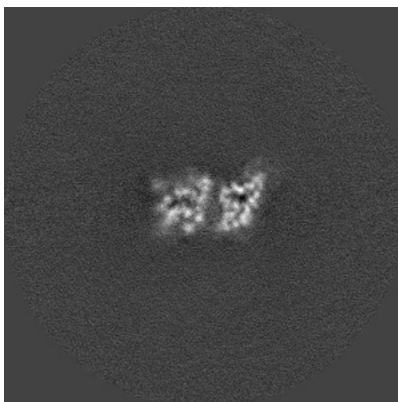


Z Index: 164

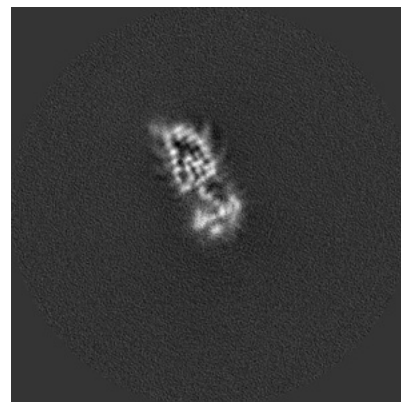
6.2.2 Raw map



X Index: 164



Y Index: 164

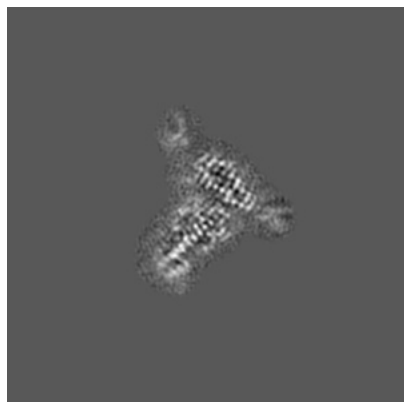


Z Index: 164

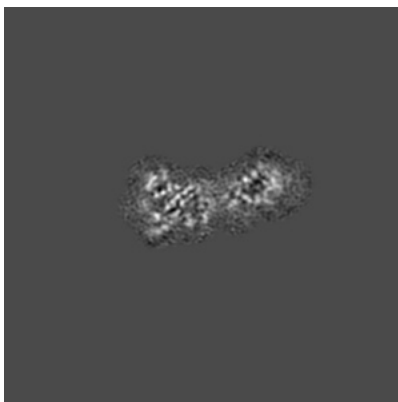
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

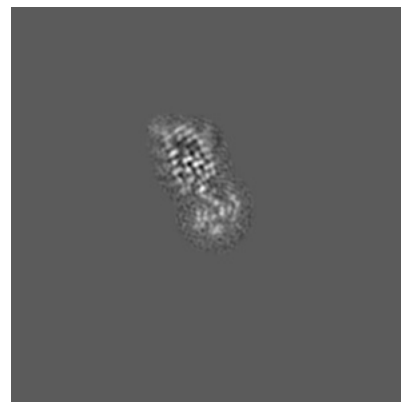
6.3.1 Primary map



X Index: 164

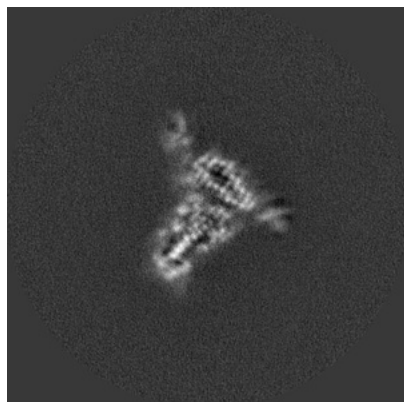


Y Index: 149

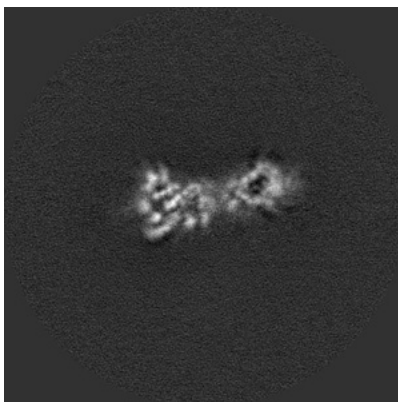


Z Index: 163

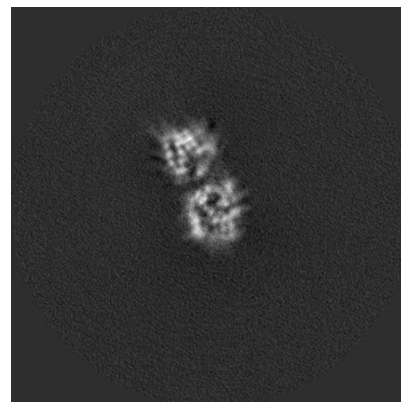
6.3.2 Raw map



X Index: 165



Y Index: 148

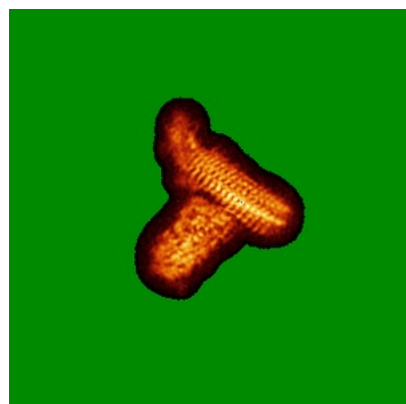


Z Index: 154

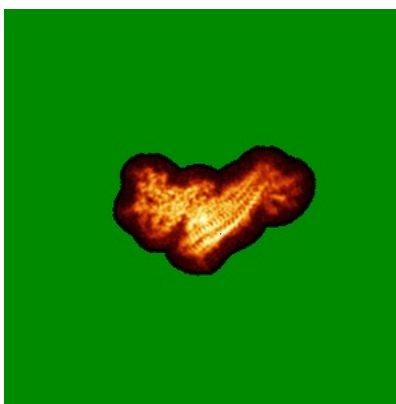
The images above show the largest variance slices of the map in three orthogonal directions.

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

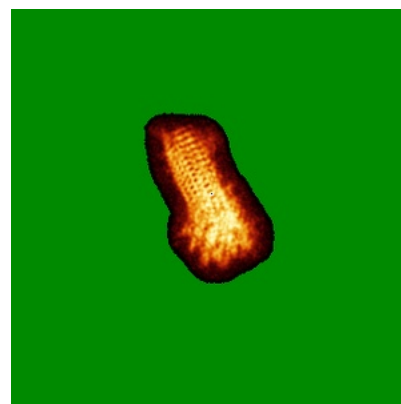
6.4.1 Primary map



X



Y

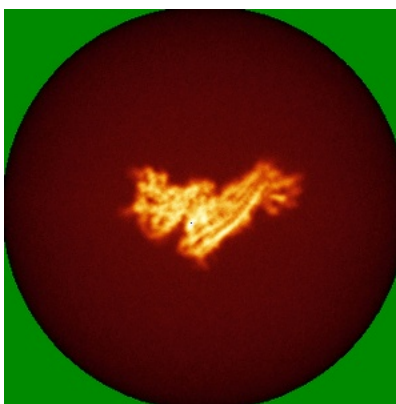


Z

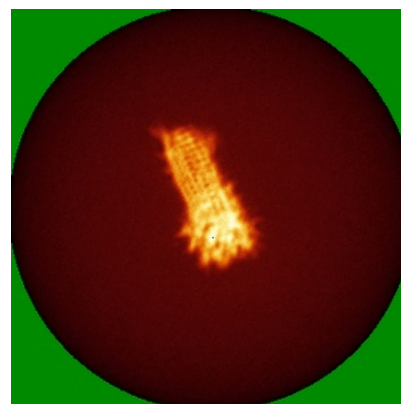
6.4.2 Raw map



X



Y

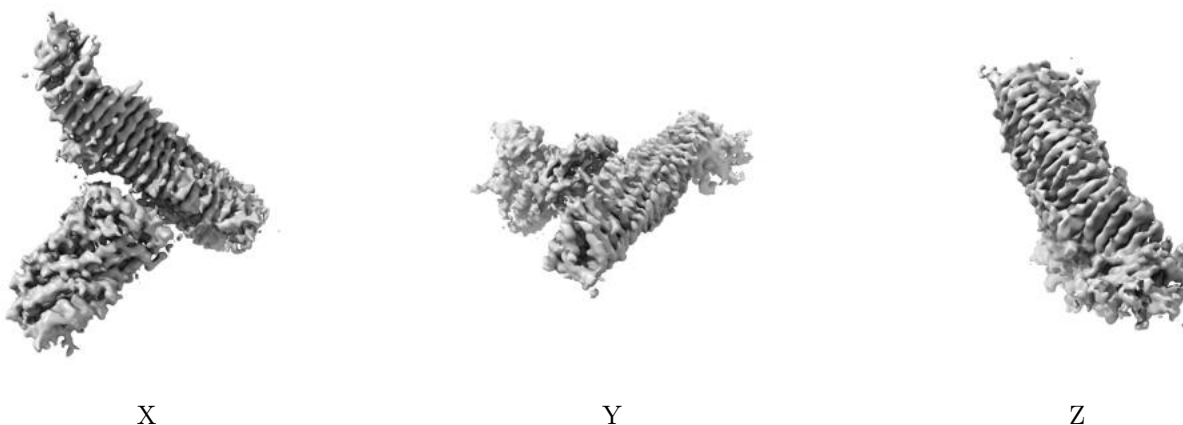


Z

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.

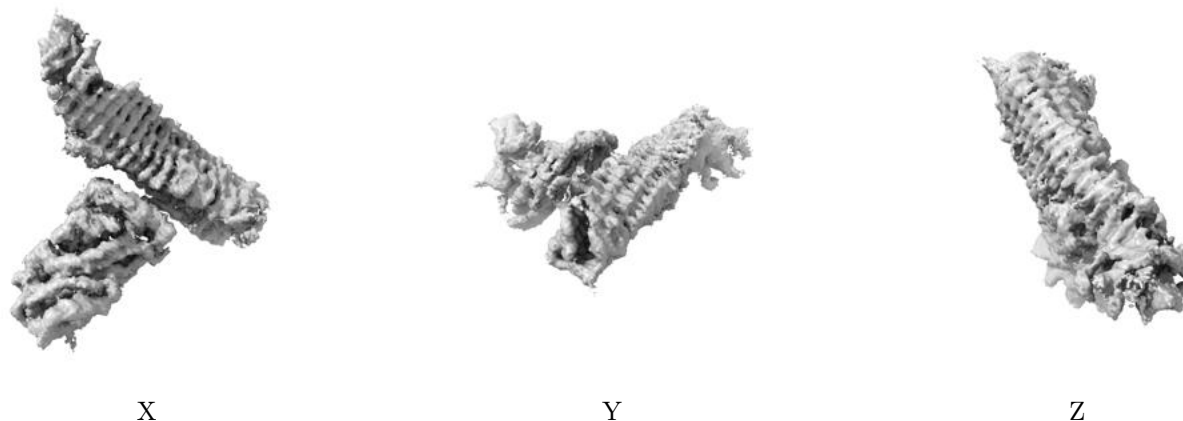
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0122. 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.

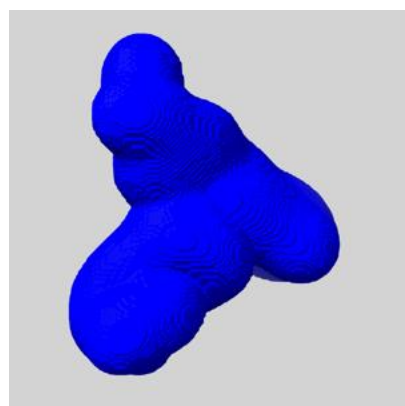
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

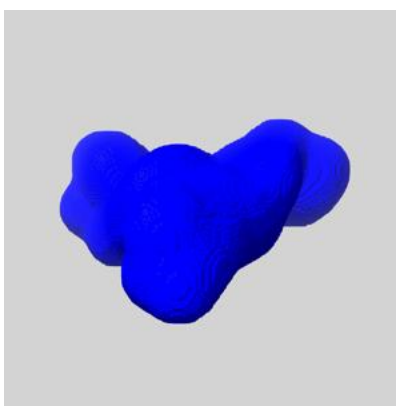
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

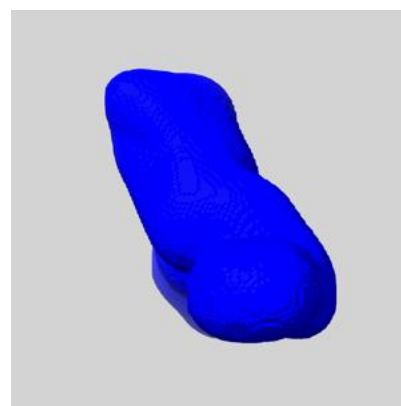
6.6.1 emd_11814_msk_1.map [i](#)



X



Y

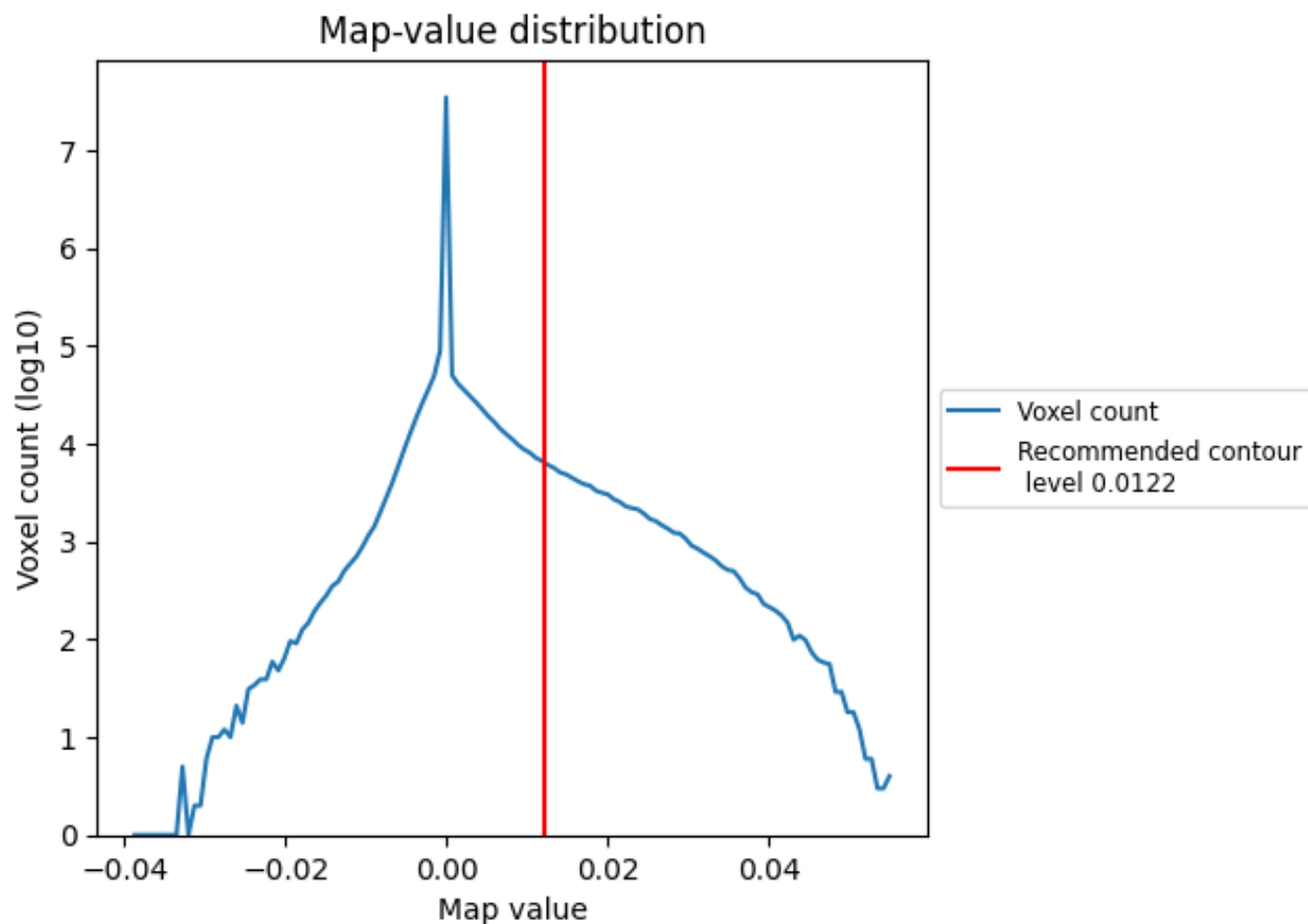


Z

7 Map analysis [i](#)

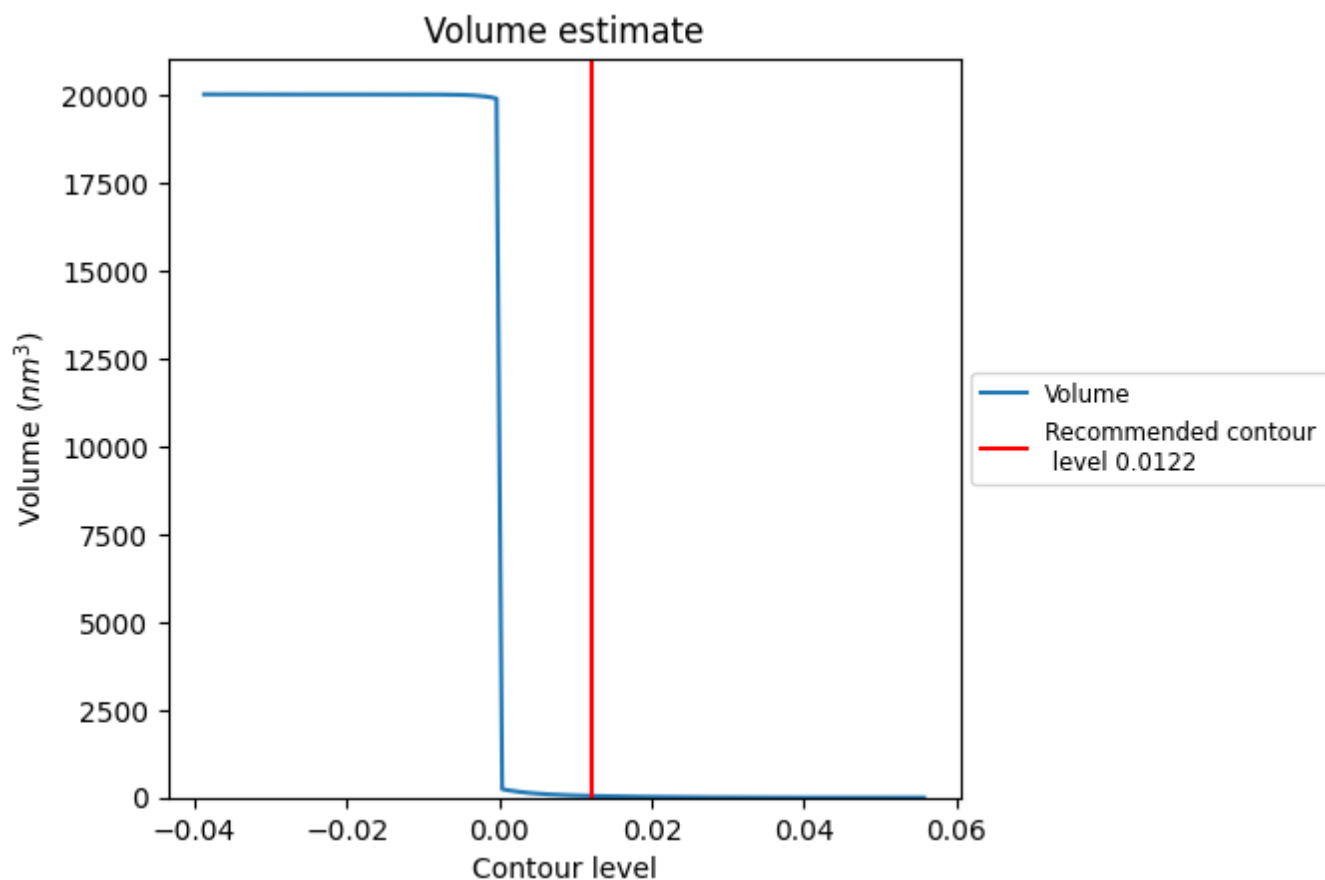
This section contains the results of statistical analysis of the map.

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.

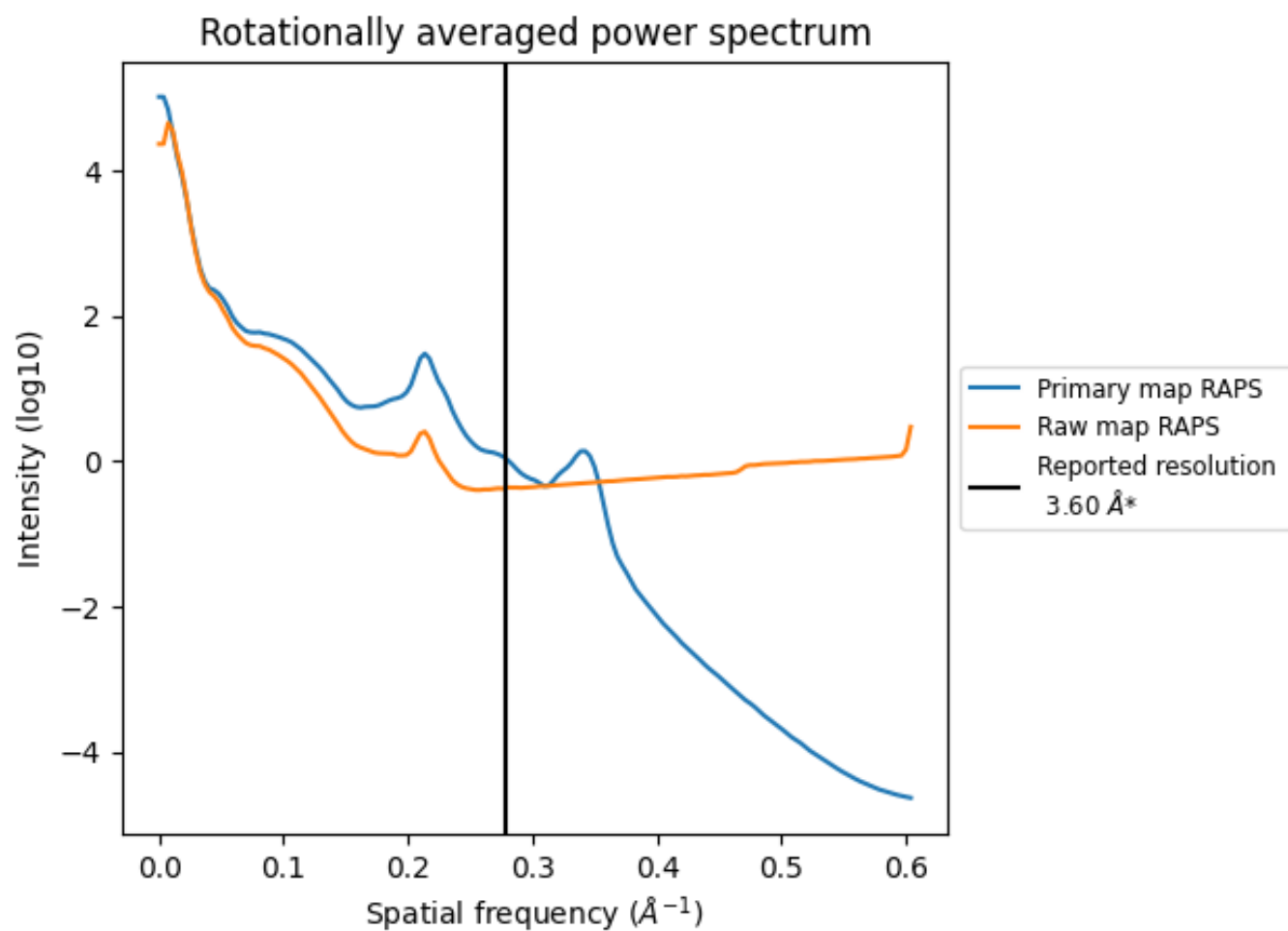
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm³; this corresponds to an approximate mass of 42 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 ⓘ

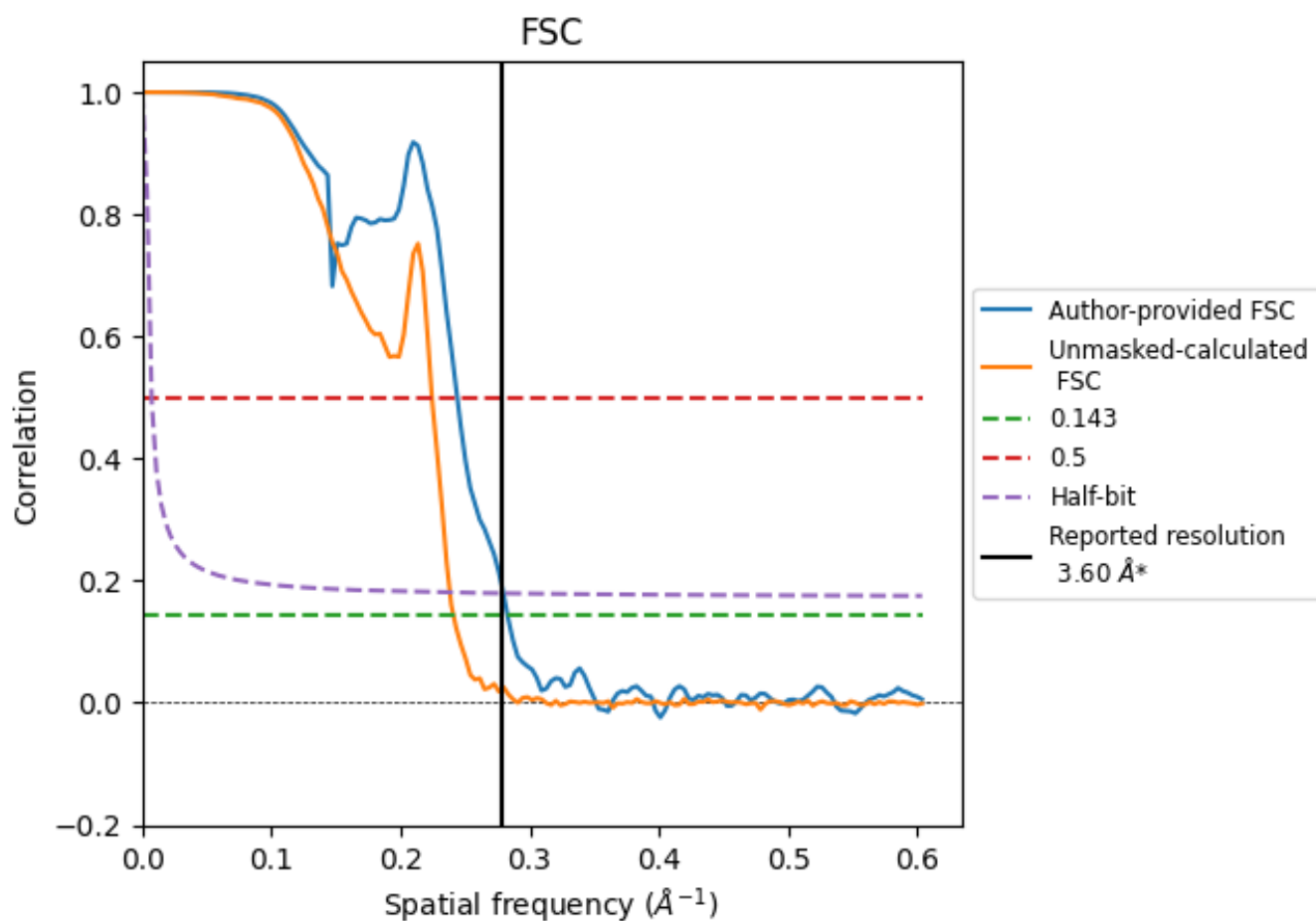


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

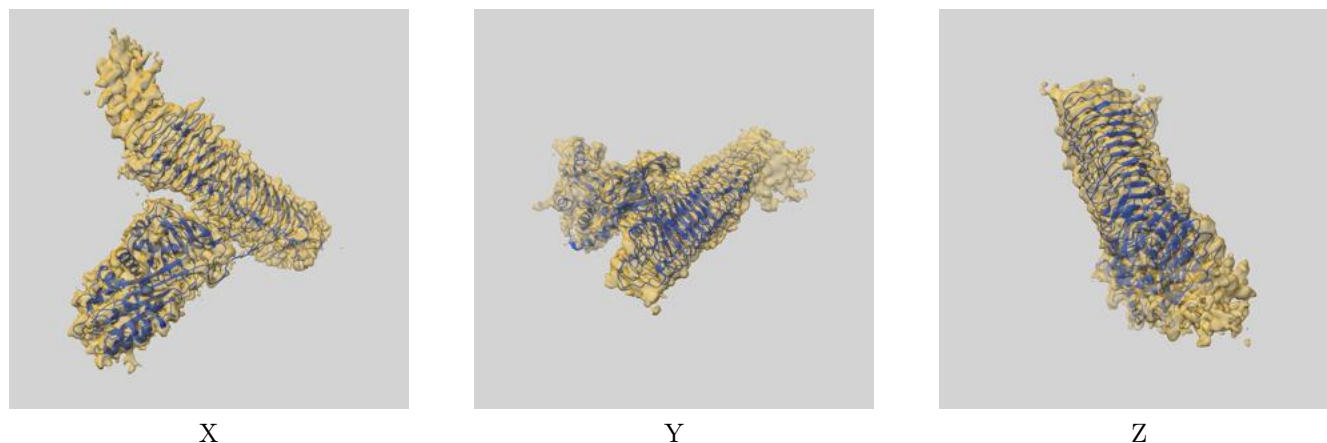
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	4.10	3.58
Unmasked-calculated*	4.15	4.46	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

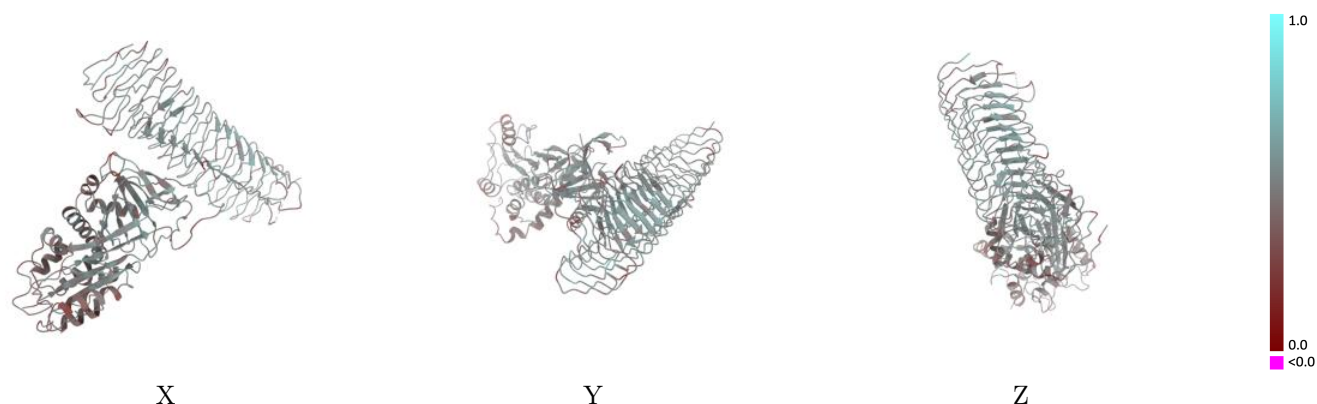
This section contains information regarding the fit between EMDB map EMD-11814 and PDB model 7AKV. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



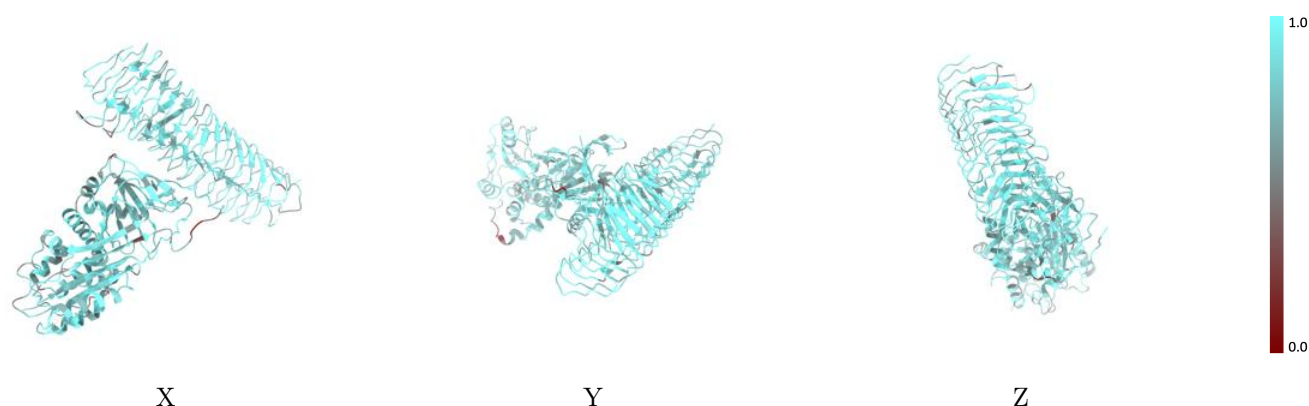
The images above show the 3D surface view of the map at the recommended contour level 0.0122 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



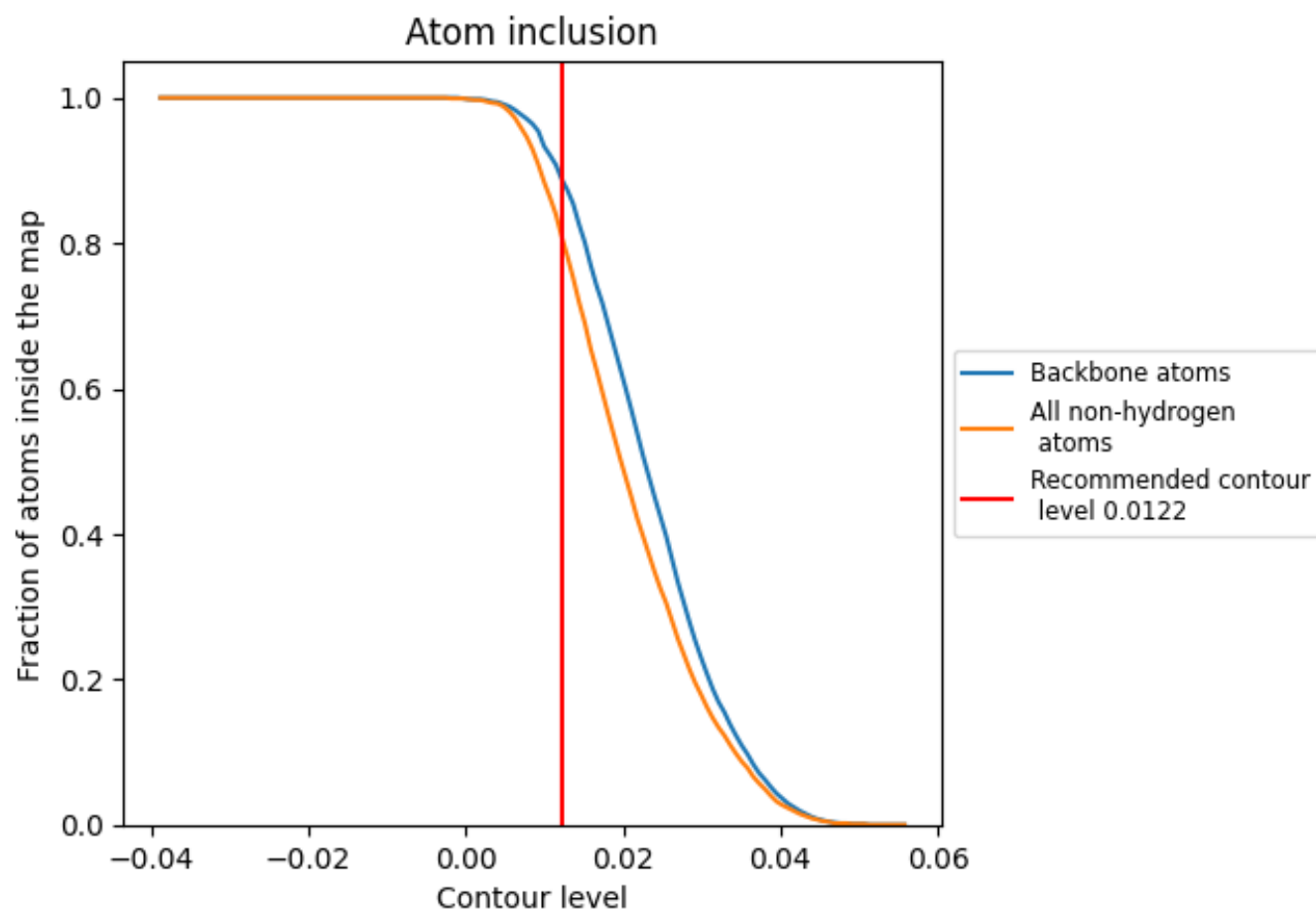
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0122).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.0122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.4770
A	0.7960	0.4570
G	0.8320	0.4970

