W O R L D W I D E
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P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

May 15, 2025 – 10:39 AM EDT

PDB ID	:	9E2I / pdb_00009e2i
EMDB ID	:	EMD-47453
Title	:	Variediene synthase with six cyclases
Authors	:	Wenger, E.S.; Christianson, D.W.
Deposited on	:	2024-10-22
Resolution	:	3.18 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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 3.18 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	Percentile Ranks	Value
Clashscore		19
Ramachandran outliers		0.9%
Sidechain outliers		8.0%

Worse *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
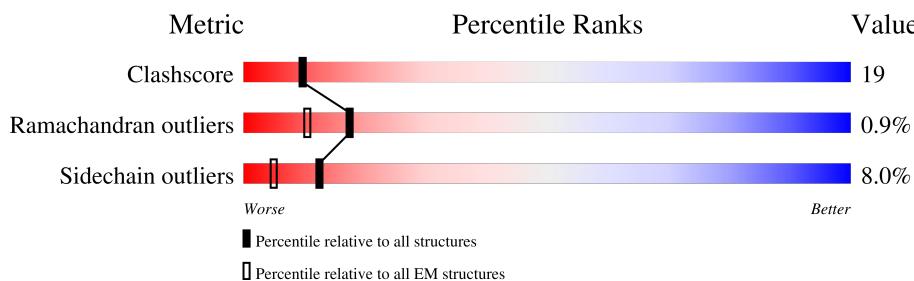
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	725	17% — 50% / 25% / • / 21%
1	B	725	15% — 47% / 32% / • / 18%
1	C	725	22% — 50% / 26% / • / 21%
1	D	725	12% — 50% / 29% / • / 19%
1	E	725	22% — 50% / 28% / • / 19%
1	F	725	18% — 52% / 27% / • / 17%
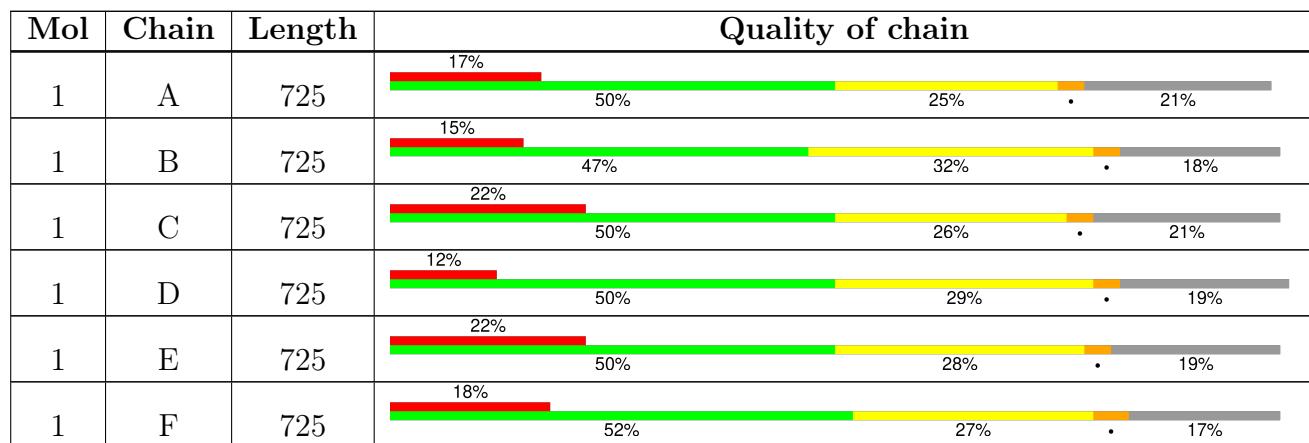
2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 28392 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 Variediene synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	572	Total	C	N	O	S	0	0
			4611	2931	789	862	29		
1	B	595	Total	C	N	O	S	0	0
			4800	3045	825	900	30		
1	C	573	Total	C	N	O	S	0	0
			4622	2935	794	864	29		
1	D	589	Total	C	N	O	S	0	0
			4745	3010	816	890	29		
1	E	589	Total	C	N	O	S	0	0
			4753	3018	818	887	30		
1	F	604	Total	C	N	O	S	0	0
			4861	3079	836	916	30		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0P0ZD79
A	2	GLY	-	expression tag	UNP A0A0P0ZD79
A	3	SER	-	expression tag	UNP A0A0P0ZD79
A	4	SER	-	expression tag	UNP A0A0P0ZD79
A	5	HIS	-	expression tag	UNP A0A0P0ZD79
A	6	HIS	-	expression tag	UNP A0A0P0ZD79
A	7	HIS	-	expression tag	UNP A0A0P0ZD79
A	8	HIS	-	expression tag	UNP A0A0P0ZD79
A	9	HIS	-	expression tag	UNP A0A0P0ZD79
A	10	HIS	-	expression tag	UNP A0A0P0ZD79
A	11	SER	-	expression tag	UNP A0A0P0ZD79
A	12	SER	-	expression tag	UNP A0A0P0ZD79
A	13	GLY	-	expression tag	UNP A0A0P0ZD79
A	14	LEU	-	expression tag	UNP A0A0P0ZD79
A	15	VAL	-	expression tag	UNP A0A0P0ZD79
A	16	PRO	-	expression tag	UNP A0A0P0ZD79
A	17	ARG	-	expression tag	UNP A0A0P0ZD79
A	18	GLY	-	expression tag	UNP A0A0P0ZD79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	expression tag	UNP A0A0P0ZD79
A	20	HIS	-	expression tag	UNP A0A0P0ZD79
B	1	MET	-	initiating methionine	UNP A0A0P0ZD79
B	2	GLY	-	expression tag	UNP A0A0P0ZD79
B	3	SER	-	expression tag	UNP A0A0P0ZD79
B	4	SER	-	expression tag	UNP A0A0P0ZD79
B	5	HIS	-	expression tag	UNP A0A0P0ZD79
B	6	HIS	-	expression tag	UNP A0A0P0ZD79
B	7	HIS	-	expression tag	UNP A0A0P0ZD79
B	8	HIS	-	expression tag	UNP A0A0P0ZD79
B	9	HIS	-	expression tag	UNP A0A0P0ZD79
B	10	HIS	-	expression tag	UNP A0A0P0ZD79
B	11	SER	-	expression tag	UNP A0A0P0ZD79
B	12	SER	-	expression tag	UNP A0A0P0ZD79
B	13	GLY	-	expression tag	UNP A0A0P0ZD79
B	14	LEU	-	expression tag	UNP A0A0P0ZD79
B	15	VAL	-	expression tag	UNP A0A0P0ZD79
B	16	PRO	-	expression tag	UNP A0A0P0ZD79
B	17	ARG	-	expression tag	UNP A0A0P0ZD79
B	18	GLY	-	expression tag	UNP A0A0P0ZD79
B	19	SER	-	expression tag	UNP A0A0P0ZD79
B	20	HIS	-	expression tag	UNP A0A0P0ZD79
C	1	MET	-	initiating methionine	UNP A0A0P0ZD79
C	2	GLY	-	expression tag	UNP A0A0P0ZD79
C	3	SER	-	expression tag	UNP A0A0P0ZD79
C	4	SER	-	expression tag	UNP A0A0P0ZD79
C	5	HIS	-	expression tag	UNP A0A0P0ZD79
C	6	HIS	-	expression tag	UNP A0A0P0ZD79
C	7	HIS	-	expression tag	UNP A0A0P0ZD79
C	8	HIS	-	expression tag	UNP A0A0P0ZD79
C	9	HIS	-	expression tag	UNP A0A0P0ZD79
C	10	HIS	-	expression tag	UNP A0A0P0ZD79
C	11	SER	-	expression tag	UNP A0A0P0ZD79
C	12	SER	-	expression tag	UNP A0A0P0ZD79
C	13	GLY	-	expression tag	UNP A0A0P0ZD79
C	14	LEU	-	expression tag	UNP A0A0P0ZD79
C	15	VAL	-	expression tag	UNP A0A0P0ZD79
C	16	PRO	-	expression tag	UNP A0A0P0ZD79
C	17	ARG	-	expression tag	UNP A0A0P0ZD79
C	18	GLY	-	expression tag	UNP A0A0P0ZD79
C	19	SER	-	expression tag	UNP A0A0P0ZD79
C	20	HIS	-	expression tag	UNP A0A0P0ZD79

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A0A0P0ZD79
D	2	GLY	-	expression tag	UNP A0A0P0ZD79
D	3	SER	-	expression tag	UNP A0A0P0ZD79
D	4	SER	-	expression tag	UNP A0A0P0ZD79
D	5	HIS	-	expression tag	UNP A0A0P0ZD79
D	6	HIS	-	expression tag	UNP A0A0P0ZD79
D	7	HIS	-	expression tag	UNP A0A0P0ZD79
D	8	HIS	-	expression tag	UNP A0A0P0ZD79
D	9	HIS	-	expression tag	UNP A0A0P0ZD79
D	10	HIS	-	expression tag	UNP A0A0P0ZD79
D	11	SER	-	expression tag	UNP A0A0P0ZD79
D	12	SER	-	expression tag	UNP A0A0P0ZD79
D	13	GLY	-	expression tag	UNP A0A0P0ZD79
D	14	LEU	-	expression tag	UNP A0A0P0ZD79
D	15	VAL	-	expression tag	UNP A0A0P0ZD79
D	16	PRO	-	expression tag	UNP A0A0P0ZD79
D	17	ARG	-	expression tag	UNP A0A0P0ZD79
D	18	GLY	-	expression tag	UNP A0A0P0ZD79
D	19	SER	-	expression tag	UNP A0A0P0ZD79
D	20	HIS	-	expression tag	UNP A0A0P0ZD79
E	1	MET	-	initiating methionine	UNP A0A0P0ZD79
E	2	GLY	-	expression tag	UNP A0A0P0ZD79
E	3	SER	-	expression tag	UNP A0A0P0ZD79
E	4	SER	-	expression tag	UNP A0A0P0ZD79
E	5	HIS	-	expression tag	UNP A0A0P0ZD79
E	6	HIS	-	expression tag	UNP A0A0P0ZD79
E	7	HIS	-	expression tag	UNP A0A0P0ZD79
E	8	HIS	-	expression tag	UNP A0A0P0ZD79
E	9	HIS	-	expression tag	UNP A0A0P0ZD79
E	10	HIS	-	expression tag	UNP A0A0P0ZD79
E	11	SER	-	expression tag	UNP A0A0P0ZD79
E	12	SER	-	expression tag	UNP A0A0P0ZD79
E	13	GLY	-	expression tag	UNP A0A0P0ZD79
E	14	LEU	-	expression tag	UNP A0A0P0ZD79
E	15	VAL	-	expression tag	UNP A0A0P0ZD79
E	16	PRO	-	expression tag	UNP A0A0P0ZD79
E	17	ARG	-	expression tag	UNP A0A0P0ZD79
E	18	GLY	-	expression tag	UNP A0A0P0ZD79
E	19	SER	-	expression tag	UNP A0A0P0ZD79
E	20	HIS	-	expression tag	UNP A0A0P0ZD79
F	1	MET	-	initiating methionine	UNP A0A0P0ZD79
F	2	GLY	-	expression tag	UNP A0A0P0ZD79

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| Chain	Residue	Modelled	Actual	Comment	Reference
F	3	SER	-	expression tag	UNP A0A0P0ZD79
F	4	SER	-	expression tag	UNP A0A0P0ZD79
F	5	HIS	-	expression tag	UNP A0A0P0ZD79
F	6	HIS	-	expression tag	UNP A0A0P0ZD79
F	7	HIS	-	expression tag	UNP A0A0P0ZD79
F	8	HIS	-	expression tag	UNP A0A0P0ZD79
F	9	HIS	-	expression tag	UNP A0A0P0ZD79
F	10	HIS	-	expression tag	UNP A0A0P0ZD79
F	11	SER	-	expression tag	UNP A0A0P0ZD79
F	12	SER	-	expression tag	UNP A0A0P0ZD79
F	13	GLY	-	expression tag	UNP A0A0P0ZD79
F	14	LEU	-	expression tag	UNP A0A0P0ZD79
F	15	VAL	-	expression tag	UNP A0A0P0ZD79
F	16	PRO	-	expression tag	UNP A0A0P0ZD79
F	17	ARG	-	expression tag	UNP A0A0P0ZD79
F	18	GLY	-	expression tag	UNP A0A0P0ZD79
F	19	SER	-	expression tag	UNP A0A0P0ZD79
F	20	HIS	-	expression tag	UNP A0A0P0ZD79

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: Variediene synthase


• Molecule 1: Variediene synthase

Chain B:

• Molecule 1: Variediene synthase

Chain C:

• Molecule 1: Variediene synthase

Chain D:

12%

50% 29% 19%

V522 D526 M531 D532 I533 Y534 M538 K570 T571 L574 F575 R576 M582 Q589 Q590 K591 Q596 L597 L600 S601 D602 E606 V610 Y614 T618 E619 GLU TYR THR GLY GLN LYS GLY PHE CYS GLU ASP L631 D632 E633 C634 K649 N650 V651

S660 R661 L666 E672 I684 T687 M695 I698 L705 E706 G707 E708 T709 G710 S711 P712 R717 L718 L719 I720 L723 K724 VAL

• Molecule 1: Variediene synthase

Chain E:

22%

50% 28% • 19%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER GLN SER SER ASP F27 I28 L29 N30 S31 T32 L33 S34 S35 VAL GLU VAL GLU ARG SER T41 P42 D43 I44 F47 C48 S49 G50 TYR GLU L53 R54 R55 H56 H57 H58 E59 H60 L61

A62 N63 E64 L67 R68 C69 R70 T71 D72 W73 E74 Q75 G78 P79 I80 E81 R82 W83 G84 S85 C86 N87 P88 W89 E90 G91 H92 F93 G94 A95 V96 V97 L98 P99 F100 C101 K102 P103 E104 R105 L106 A107 V108 I109 C110 Y111 I112 F113 F117 L118 Y119 D120 N121 VAL VAL GLU SER

ALA ALA LYS SER THR LEU ASN LEU ASN THR ASP ASN ILE ALA LEU ASP GLU THR GLU Y145 R146 T147 V148 R149 L152 Q156 I157 Q158 S159 K160 M161 L166 D169 R172 A173 E174 V175 V176 I177 N178 S179 W180 K181 E182 M183 I184 S185 T186 T187 A188 LYS LYS ASP LYS THR

ARG ALA PHE ASN LEU GLU GLU Y202 V203 D204 Y205 R206 I207 I208 D209 T210 G211 A212 P213 F214 V215 D216 M217 L218 M219 R220 F221 G222 M223 G224 I225 T228 M226 L227 T228 Q229 E230 R234 I235 E236 P237 I238 V239 K240 P241 C242 Y243 A244 A245 L246 G247 L248 A249 N250 D261 Y252 F263 S254 F255

D256 I257 E258 W259 E260 E261 F262 Q263 A264 D267 K268 T269 T270 M271 T272 N273 A274 V275 W276 L277 F278 M279 Q280 W281 E282 N283 L284 N285 A286 E287 Q288 A289 K290 R291 R292 V293 Q294 E295 V296 T297 K298 Q299 Y300 E301 Q302 Q303 Y304 L305 R306 N307 I308 A309 D310 F311 A312 A313 G314 E315 G316

K317 E318 N319 I320 K321 L322 Q323 T324 Y325 L326 K327 A328 Q329 G330 Y331 Q332 V333 N336 V337 A338 W339 S340 L341 R342 C343 P344 R345 Y346 H347 P348 W349 L350 C351 K352 E353 A354 A355 S356 L357 L358 H359 Q360 ASP THR ILE GLN GLU LEU GLU ALA GLY LYS ARG LYS PRO GLN ALA LEU GLU GLU

TYR ARG SER SER HIS SER GLU SER ASP LEU SER ASP ALA SER PRO THR PHE TRP SER GLY SER CYS ARG SER ALA ARG SER VAL SER SER ALA PHE GLY PRO PRO ASP LYS ASP SER ILE SER ILE THR PRO ALA ILE LEU G427 I438 R447 D452 G453 L454 V459

L460 P461 D462 H463 R464 L468 L475 S479 L482 E486 P490 L491 R492 R493 L515 V518 M519 V522 M531 Y534 L535 E536 R539 C557 P558 L564 I567 R568 Q569 K570 T571 R576 R580 M581 M582 P587 V588 Q589 Q590 K591 G592 L593

D602 E606 Q609 Y614 K615 N616 L617 T618 E619 E620 Y621 T622 G623 Q624 K625 G626 F627 C628 E629 D630 L631 D632 E633 C634 P639 V651 K671 V674 L675 T687 E706 N713 I720 K724 VAL

• Molecule 1: Variediene synthase

Chain F:

18%

52% 27% • 17%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER GLN S24 S25 D26 F27 I28 L29 N30 S31 T32 L33 S34 S35 V36 VAL GLU ARG S40 T41 P42 D43 I44 A45 G46 F47 C48 S49 G50 TYR GLU L53 R54 R55 H56 H57 H58 E59 H60

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	60587	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	43	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.642	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.31	0/4706	0.63	2/6361 (0.0%)
1	B	0.33	0/4903	0.62	2/6627 (0.0%)
1	C	0.31	0/4719	0.57	1/6378 (0.0%)
1	D	0.30	0/4844	0.61	1/6549 (0.0%)
1	E	0.23	0/4855	0.54	0/6563
1	F	0.30	0/4962	0.57	4/6707 (0.1%)
All	All	0.30	0/28989	0.59	10/39185 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	308	ILE	N-CA-C	-7.05	104.11	111.58
1	F	297	THR	N-CA-C	-6.42	104.28	111.28
1	F	311	PHE	N-CA-C	-6.38	104.33	111.28
1	F	296	VAL	N-CA-C	-6.01	104.45	111.00
1	D	32	THR	CB-CA-C	-5.85	109.82	116.54
1	A	297	THR	N-CA-C	-5.79	105.47	112.54
1	A	48	CYS	N-CA-C	5.69	118.96	111.28
1	C	331	TYR	N-CA-C	-5.58	105.82	113.30
1	B	331	TYR	N-CA-C	-5.48	106.96	113.97
1	F	305	LEU	N-CA-C	-5.10	105.63	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4611	0	4538	182	0
1	B	4800	0	4716	205	0
1	C	4622	0	4546	176	0
1	D	4745	0	4663	189	0
1	E	4753	0	4673	191	0
1	F	4861	0	4773	176	0
All	All	28392	0	27909	1094	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 19.

All (1094) 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:D:312:ALA:HA	1:D:316:GLY:HA3	1.34	1.06
1:D:197:ASN:N	1:D:197:ASN:HD22	1.48	1.06
1:D:234:ARG:HH22	1:D:315:GLU:HG2	1.20	1.06
1:C:89:TRP:CB	1:C:342:ARG:HD3	1.87	1.05
1:B:284:LEU:HD11	1:B:292:ARG:NH1	1.73	1.03
1:A:302:GLN:HA	1:A:305:LEU:HB2	1.42	1.01
1:A:245:ALA:HB2	1:A:304:TYR:CE2	1.97	0.99
1:C:241:PRO:HB2	1:C:304:TYR:HB2	1.46	0.95
1:A:262:PHE:CE1	1:A:271:MET:HA	2.07	0.89
1:F:251:ASP:HB3	1:F:273:ASN:HA	1.52	0.89
1:C:177:ILE:HA	1:C:180:TRP:HB3	1.53	0.89
1:C:89:TRP:HB2	1:C:342:ARG:HD3	1.54	0.88
1:E:27:PHE:HB3	1:E:323:GLN:H	1.38	0.87
1:E:251:ASP:HB3	1:E:274:ALA:H	1.36	0.87
1:C:89:TRP:HB3	1:C:342:ARG:HD3	1.54	0.86
1:C:298:LYS:HD2	1:C:302:GLN:HG3	1.57	0.86
1:E:169:ASP:HB3	1:E:172:ARG:HE	1.43	0.84
1:D:206:ARG:HH22	1:D:248:LEU:HD23	1.42	0.83
1:B:284:LEU:HD11	1:B:292:ARG:CZ	2.09	0.82
1:E:177:ILE:HA	1:E:180:TRP:HB3	1.61	0.82
1:A:241:PRO:HB2	1:A:304:TYR:CE1	2.14	0.81
1:E:588:VAL:HG12	1:E:589:GLN:H	1.42	0.81
1:C:89:TRP:HB2	1:C:342:ARG:CD	2.10	0.81
1:C:356:SER:HA	1:C:359:HIS:CE1	2.16	0.81
1:D:251:ASP:HB3	1:D:273:ASN:HA	1.62	0.81
1:F:304:TYR:HA	1:F:307:ASN:HB3	1.63	0.80
1:A:347:HIS:O	1:A:347:HIS:ND1	2.14	0.80
1:D:197:ASN:N	1:D:197:ASN:ND2	2.23	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:HB3	1:A:240:LYS:HE2	1.63	0.79
1:B:304:TYR:HA	1:B:307:ASN:HB2	1.65	0.79
1:A:618:THR:HG22	1:A:619:GLU:HG3	1.63	0.79
1:C:89:TRP:CB	1:C:342:ARG:CD	2.61	0.78
1:F:307:ASN:HA	1:F:310:ASP:HB2	1.66	0.78
1:A:245:ALA:HB2	1:A:304:TYR:HE2	1.46	0.77
1:B:85:SER:HB2	1:B:93:PHE:HB3	1.64	0.77
1:A:48:CYS:HA	1:A:305:LEU:HD11	1.66	0.77
1:C:271:MET:HE2	1:C:273:ASN:HB2	1.66	0.77
1:C:519:MET:HE3	1:D:519:MET:HE3	1.66	0.77
1:D:55:ARG:NH1	1:D:56:HIS:O	2.17	0.76
1:D:284:LEU:HB3	1:D:288:GLN:HB2	1.65	0.76
1:B:251:ASP:HB3	1:B:274:ALA:H	1.48	0.76
1:B:307:ASN:HA	1:B:310:ASP:HB3	1.67	0.76
1:D:337:VAL:HA	1:D:340:SER:HB2	1.65	0.76
1:A:301:GLU:O	1:A:305:LEU:HD23	1.85	0.76
1:C:172:ARG:HH21	1:C:226:MET:HG2	1.51	0.75
1:E:215:VAL:HA	1:E:218:LEU:HD12	1.69	0.75
1:B:183:MET:HE1	1:B:214:PHE:HB2	1.67	0.75
1:B:101:CYS:HB3	1:B:222:GLY:HA2	1.67	0.75
1:B:322:LEU:HA	1:B:325:TYR:HB3	1.69	0.75
1:F:55:ARG:NH1	1:F:56:HIS:O	2.20	0.75
1:E:203:VAL:HG21	1:E:248:LEU:HG	1.67	0.74
1:A:66:SER:O	1:A:70:ARG:N	2.20	0.74
1:E:296:VAL:HG22	1:E:300:TYR:HE1	1.53	0.74
1:A:236:GLU:O	1:A:240:LYS:N	2.21	0.73
1:A:71:THR:O	1:A:75:GLN:N	2.21	0.72
1:E:27:PHE:HB3	1:E:322:LEU:H	1.54	0.72
1:E:254:SER:OG	1:E:273:ASN:ND2	2.21	0.72
1:F:113:PHE:HE1	1:F:218:LEU:HD13	1.52	0.72
1:F:444:LYS:HD3	1:F:493:ARG:HH22	1.54	0.72
1:F:634:CYS:SG	1:F:661:ARG:NH2	2.63	0.72
1:F:242:CYS:HA	1:F:304:TYR:CE2	2.25	0.71
1:A:232:GLN:O	1:A:236:GLU:N	2.24	0.71
1:F:56:HIS:CE1	1:F:99:PRO:HA	2.25	0.71
1:A:291:ARG:O	1:A:295:GLU:HG3	1.90	0.71
1:C:340:SER:HA	1:C:343:CYS:HB2	1.71	0.71
1:E:218:LEU:O	1:E:222:GLY:N	2.20	0.71
1:B:88:PRO:HB2	1:B:357:LEU:HD13	1.72	0.70
1:A:262:PHE:CE2	1:A:268:LYS:HB2	2.26	0.70
1:A:292:ARG:O	1:A:296:VAL:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASP:HA	1:C:219:MET:HG3	1.73	0.70
1:D:32:THR:O	1:D:54:ARG:NH2	2.25	0.70
1:F:279:MET:HE2	1:F:285:ASN:HA	1.74	0.70
1:F:29:LEU:HD23	1:F:324:THR:HG22	1.74	0.70
1:F:292:ARG:O	1:F:296:VAL:N	2.25	0.70
1:D:312:ALA:HA	1:D:316:GLY:CA	2.19	0.69
1:B:448:GLU:N	1:B:448:GLU:OE1	2.23	0.69
1:D:273:ASN:OD1	1:D:276:TRP:N	2.20	0.69
1:B:204:ASP:OD1	1:B:205:TYR:N	2.24	0.69
1:B:460:LEU:HD23	1:B:461:PRO:HD2	1.74	0.69
1:D:519:MET:HA	1:D:522:VAL:HG22	1.75	0.69
1:E:291:ARG:O	1:E:295:GLU:N	2.25	0.69
1:A:87:ASN:HD21	1:A:90:GLU:HB3	1.58	0.69
1:E:292:ARG:O	1:E:296:VAL:HG12	1.93	0.69
1:A:712:PRO:O	1:B:156:GLN:NE2	2.25	0.68
1:B:324:THR:HA	1:B:327:LYS:HB3	1.76	0.68
1:B:176:VAL:HG22	1:B:217:MET:HB3	1.76	0.68
1:D:248:LEU:O	1:D:252:TYR:N	2.24	0.68
1:E:287:GLU:HG3	1:E:291:ARG:HE	1.59	0.68
1:A:44:ILE:N	1:A:47:PHE:O	2.25	0.68
1:E:216:ASP:HA	1:E:219:MET:HG3	1.74	0.68
1:F:268:LYS:HD3	1:F:271:MET:HE1	1.75	0.68
1:E:43:ASP:HB3	1:E:50:GLY:H	1.59	0.68
1:F:235:ILE:HA	1:F:238:ILE:HB	1.77	0.67
1:D:31:SER:OG	1:D:54:ARG:NE	2.26	0.67
1:E:251:ASP:O	1:E:273:ASN:ND2	2.28	0.67
1:D:234:ARG:NH2	1:D:315:GLU:HG2	2.03	0.67
1:E:27:PHE:HB3	1:E:323:GLN:N	2.11	0.66
1:C:245:ALA:HA	1:C:248:LEU:HD12	1.77	0.66
1:D:206:ARG:NH2	1:D:248:LEU:HD23	2.09	0.66
1:E:258:GLU:HA	1:E:261:GLU:HB2	1.78	0.66
1:F:588:VAL:O	1:F:590:GLN:N	2.28	0.66
1:A:49:SER:N	1:A:305:LEU:HD12	2.10	0.66
1:A:293:VAL:O	1:A:297:THR:HB	1.95	0.66
1:E:303:GLN:O	1:E:307:ASN:N	2.26	0.66
1:B:284:LEU:HD11	1:B:292:ARG:HH11	1.58	0.66
1:C:218:LEU:O	1:C:222:GLY:N	2.28	0.66
1:B:35:SER:O	1:B:55:ARG:N	2.28	0.66
1:A:269:THR:HG22	1:A:270:THR:HG23	1.77	0.65
1:A:65:GLY:HA2	1:A:68:ARG:HH11	1.60	0.65
1:B:706:GLU:HG2	1:B:712:PRO:HA	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:LEU:HB3	1:D:326:LEU:HD23	1.79	0.65
1:B:61:LEU:HD11	1:B:106:LEU:HB3	1.77	0.65
1:D:25:SER:OG	1:D:30:ASN:N	2.29	0.65
1:E:28:ILE:O	1:E:324:THR:N	2.29	0.65
1:B:245:ALA:HB2	1:B:300:TYR:HB2	1.79	0.65
1:E:176:VAL:O	1:E:180:TRP:N	2.28	0.65
1:E:291:ARG:O	1:E:295:GLU:HG3	1.95	0.65
1:F:475:LEU:HD11	1:F:534:TYR:HE1	1.61	0.65
1:A:285:ASN:O	1:A:289:ALA:N	2.27	0.65
1:E:218:LEU:HA	1:E:221:PHE:HB3	1.79	0.65
1:D:216:ASP:O	1:D:220:ARG:NH1	2.30	0.64
1:B:100:PHE:HB3	1:B:223:MET:HE1	1.79	0.64
1:C:444:LYS:HG3	1:C:446:VAL:HG23	1.79	0.64
1:F:216:ASP:O	1:F:220:ARG:HG3	1.96	0.64
1:B:284:LEU:CD1	1:B:292:ARG:HD2	2.26	0.64
1:A:206:ARG:HH22	1:A:244:ALA:HA	1.62	0.64
1:D:238:ILE:O	1:D:329:GLN:NE2	2.31	0.64
1:A:176:VAL:O	1:A:180:TRP:N	2.21	0.64
1:B:258:GLU:HG3	1:B:271:MET:HE2	1.78	0.64
1:C:109:ILE:HG23	1:C:218:LEU:HD13	1.78	0.64
1:C:253:PHE:HB3	1:C:346:TYR:CZ	2.33	0.64
1:A:50:GLY:HA3	1:A:305:LEU:O	1.95	0.64
1:D:206:ARG:HA	1:D:209:ASP:HB3	1.79	0.64
1:F:326:LEU:HA	1:F:329:GLN:HB3	1.80	0.64
1:F:282:GLU:N	1:F:282:GLU:OE2	2.31	0.64
1:B:628:CYS:O	1:B:671:LYS:NZ	2.30	0.63
1:F:48:CYS:HB2	1:F:337:VAL:HG21	1.79	0.63
1:F:481:MET:HE2	1:F:507:THR:HG23	1.80	0.63
1:B:271:MET:SD	1:B:276:TRP:HB3	2.39	0.63
1:F:519:MET:HA	1:F:522:VAL:HG12	1.79	0.63
1:B:239:VAL:HG13	1:B:329:GLN:HE21	1.62	0.63
1:F:32:THR:O	1:F:54:ARG:NH2	2.31	0.63
1:C:301:GLU:HA	1:C:304:TYR:HB3	1.81	0.63
1:E:288:GLN:O	1:E:292:ARG:N	2.29	0.63
1:F:76:PHE:HD2	1:F:157:ILE:HB	1.63	0.63
1:F:297:THR:O	1:F:301:GLU:N	2.30	0.63
1:F:34:SER:O	1:F:54:ARG:NH2	2.32	0.63
1:D:277:LEU:O	1:D:281:TRP:N	2.29	0.63
1:B:215:VAL:HA	1:B:218:LEU:HD12	1.79	0.63
1:A:301:GLU:HA	1:A:304:TYR:CD2	2.35	0.62
1:F:519:MET:HE2	1:F:534:TYR:HE2	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:O	1:B:252:TYR:N	2.32	0.62
1:F:31:SER:OG	1:F:54:ARG:NH1	2.33	0.62
1:F:329:GLN:HA	1:F:332:GLN:HB2	1.79	0.62
1:B:87:ASN:O	1:B:91:GLY:N	2.32	0.62
1:E:27:PHE:HA	1:E:321:LYS:H	1.64	0.62
1:F:289:ALA:O	1:F:293:VAL:N	2.21	0.62
1:D:457:TRP:CD1	1:D:709:THR:HG21	2.35	0.62
1:B:173:ALA:O	1:B:177:ILE:HG13	2.00	0.62
1:B:352:LYS:HA	1:B:355:ALA:HB3	1.80	0.62
1:B:693:GLU:OE2	1:B:697:LYS:HE2	1.99	0.62
1:C:350:LEU:O	1:C:354:ALA:N	2.26	0.62
1:B:206:ARG:NH2	1:B:250:ASN:OD1	2.32	0.61
1:B:290:LYS:NZ	1:B:291:ARG:HG3	2.14	0.61
1:C:220:ARG:HA	1:C:225:ILE:HB	1.81	0.61
1:C:468:LEU:HD13	1:C:582:MET:HG2	1.81	0.61
1:D:61:LEU:HD22	1:D:107:ALA:HB2	1.83	0.61
1:F:260:GLU:O	1:F:264:ALA:N	2.32	0.61
1:A:324:THR:HA	1:A:327:LYS:HD3	1.80	0.61
1:B:107:ALA:O	1:B:111:TYR:N	2.32	0.61
1:B:290:LYS:HZ3	1:B:291:ARG:HG3	1.65	0.61
1:E:475:LEU:HD13	1:E:518:VAL:HG21	1.81	0.61
1:B:64:GLU:OE2	1:B:68:ARG:NH1	2.34	0.61
1:B:231:GLU:HA	1:B:234:ARG:HB2	1.83	0.61
1:B:284:LEU:HB3	1:B:288:GLN:HB3	1.81	0.61
1:B:322:LEU:O	1:B:326:LEU:N	2.22	0.61
1:F:277:LEU:HA	1:F:280:GLN:HG2	1.82	0.61
1:C:356:SER:HA	1:C:359:HIS:HE1	1.63	0.61
1:D:48:CYS:HB2	1:D:337:VAL:HG21	1.82	0.61
1:A:294:GLN:O	1:A:298:LYS:HB2	2.01	0.61
1:C:303:GLN:O	1:C:307:ASN:N	2.31	0.61
1:D:87:ASN:ND2	1:D:343:CYS:SG	2.66	0.61
1:D:197:ASN:N	1:D:280:GLN:HE22	1.99	0.61
1:D:231:GLU:O	1:D:235:ILE:N	2.24	0.61
1:F:660:SER:HB3	1:F:666:LEU:HG	1.83	0.61
1:D:231:GLU:HA	1:D:234:ARG:HB2	1.81	0.60
1:A:215:VAL:HA	1:A:218:LEU:HB2	1.83	0.60
1:C:319:ASN:O	1:C:323:GLN:NE2	2.34	0.60
1:B:258:GLU:HB3	1:B:273:ASN:ND2	2.16	0.60
1:B:287:GLU:O	1:B:291:ARG:HG3	2.02	0.60
1:C:89:TRP:HB3	1:C:342:ARG:HH11	1.65	0.60
1:D:322:LEU:O	1:D:326:LEU:N	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:LEU:O	1:E:325:TYR:N	2.23	0.60
1:F:47:PHE:HD2	1:F:294:GLN:HG2	1.66	0.60
1:F:322:LEU:HB3	1:F:326:LEU:HG	1.82	0.60
1:C:278:PHE:HB3	1:C:289:ALA:HB1	1.83	0.60
1:A:515:LEU:O	1:A:519:MET:HG3	2.01	0.60
1:B:29:LEU:H	1:B:324:THR:HG21	1.66	0.60
1:E:296:VAL:HG22	1:E:300:TYR:CE1	2.34	0.60
1:A:301:GLU:HG2	1:A:305:LEU:HD23	1.82	0.60
1:C:89:TRP:HB3	1:C:342:ARG:CD	2.26	0.60
1:E:568:ARG:NH2	1:E:606:GLU:OE2	2.32	0.60
1:A:568:ARG:NE	1:A:606:GLU:OE1	2.30	0.60
1:E:27:PHE:CB	1:E:322:LEU:H	2.14	0.60
1:E:49:SER:HB3	1:E:302:GLN:HG2	1.84	0.60
1:B:356:SER:O	1:B:359:HIS:ND1	2.34	0.60
1:E:589:GLN:O	1:E:591:LYS:NZ	2.33	0.59
1:F:56:HIS:HE1	1:F:99:PRO:HA	1.65	0.59
1:F:327:LYS:O	1:F:331:TYR:N	2.34	0.59
1:C:70:ARG:HH22	1:C:84:GLY:H	1.50	0.59
1:D:35:SER:O	1:D:55:ARG:N	2.35	0.59
1:E:152:LEU:HB3	1:F:456:VAL:HG12	1.84	0.59
1:F:83:TRP:HB3	1:F:345:ARG:HG2	1.84	0.59
1:B:206:ARG:HA	1:B:209:ASP:HB2	1.84	0.59
1:E:111:TYR:CE2	1:E:161:MET:HE1	2.38	0.59
1:D:217:MET:O	1:D:221:PHE:N	2.28	0.59
1:E:29:LEU:HD11	1:E:327:LYS:HD3	1.84	0.59
1:A:475:LEU:HD13	1:A:518:VAL:HG21	1.85	0.59
1:D:206:ARG:NH1	1:D:244:ALA:O	2.36	0.59
1:D:254:SER:O	1:D:258:GLU:HG2	2.02	0.59
1:E:74:GLU:HG2	1:E:79:PRO:HA	1.83	0.59
1:F:82:ARG:HB2	1:F:121:ASN:HD21	1.68	0.59
1:C:65:GLY:HA2	1:C:68:ARG:HD3	1.84	0.59
1:C:220:ARG:O	1:C:225:ILE:N	2.33	0.59
1:E:111:TYR:HE2	1:E:161:MET:HE1	1.66	0.59
1:A:301:GLU:HG2	1:A:305:LEU:CD2	2.32	0.59
1:F:265:GLU:O	1:F:267:ASP:N	2.35	0.59
1:C:173:ALA:O	1:C:177:ILE:N	2.27	0.59
1:F:220:ARG:NH2	1:F:225:ILE:HG22	2.18	0.59
1:F:565:ASP:HA	1:F:568:ARG:HE	1.68	0.58
1:A:85:SER:OG	1:A:114:GLU:OE2	2.20	0.58
1:A:197:ASN:N	1:A:201:GLU:OE1	2.35	0.58
1:A:288:GLN:O	1:A:292:ARG:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ASP:OD2	1:D:256:ASP:N	2.36	0.58
1:C:256:ASP:HB2	1:C:346:TYR:HB2	1.85	0.58
1:E:27:PHE:O	1:E:323:GLN:HB2	2.03	0.58
1:F:457:TRP:CD1	1:F:709:THR:HG21	2.38	0.58
1:B:85:SER:O	1:B:92:HIS:ND1	2.37	0.58
1:D:278:PHE:HB3	1:D:284:LEU:HD12	1.86	0.58
1:F:258:GLU:OE1	1:F:273:ASN:HB2	2.04	0.58
1:A:459:VAL:HG21	1:B:145:TYR:CE1	2.38	0.58
1:B:115:TYR:O	1:B:119:TYR:N	2.33	0.58
1:B:699:THR:HG22	1:B:720:ILE:HD13	1.86	0.58
1:C:284:LEU:HD22	1:C:292:ARG:HB2	1.85	0.58
1:C:588:VAL:O	1:C:591:LYS:NZ	2.36	0.58
1:C:215:VAL:HA	1:C:218:LEU:HB2	1.84	0.58
1:A:298:LYS:HE2	1:A:302:GLN:HG2	1.84	0.58
1:E:102:LYS:HZ3	1:E:105:ARG:HD3	1.69	0.58
1:C:319:ASN:OD1	1:C:321:LYS:HE2	2.04	0.57
1:C:456:VAL:HA	1:D:152:LEU:HD11	1.87	0.57
1:D:213:PRO:O	1:D:217:MET:HE2	2.05	0.57
1:E:285:ASN:O	1:E:289:ALA:N	2.32	0.57
1:E:328:ALA:O	1:E:332:GLN:N	2.37	0.57
1:B:284:LEU:HD11	1:B:292:ARG:HD2	1.86	0.57
1:C:294:GLN:O	1:C:298:LYS:N	2.33	0.57
1:C:515:LEU:O	1:C:519:MET:HG3	2.04	0.57
1:C:564:LEU:HD23	1:C:567:ILE:HD11	1.86	0.57
1:D:35:SER:N	1:D:55:ARG:O	2.33	0.57
1:A:220:ARG:HA	1:A:225:ILE:HG13	1.87	0.57
1:A:235:ILE:O	1:A:239:VAL:HG23	2.05	0.57
1:B:308:ILE:HG12	1:B:326:LEU:HD11	1.86	0.57
1:B:112:ILE:O	1:B:116:ALA:N	2.37	0.57
1:E:43:ASP:HB2	1:E:47:PHE:O	2.03	0.57
1:A:298:LYS:O	1:A:302:GLN:N	2.33	0.57
1:B:607:PHE:HA	1:B:694:LEU:HD13	1.86	0.57
1:F:282:GLU:HG2	1:F:284:LEU:HG	1.87	0.57
1:A:297:THR:O	1:A:301:GLU:N	2.38	0.57
1:E:294:GLN:O	1:E:298:LYS:HB2	2.03	0.57
1:E:622:THR:HG22	1:E:628:CYS:H	1.70	0.57
1:E:304:TYR:O	1:E:308:ILE:N	2.34	0.57
1:A:48:CYS:HA	1:A:305:LEU:CD1	2.33	0.56
1:B:344:PRO:HG3	1:B:350:LEU:HD21	1.87	0.56
1:E:27:PHE:HB3	1:E:322:LEU:N	2.19	0.56
1:D:706:GLU:HG2	1:D:712:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:TYR:HB2	1:D:293:VAL:HG11	1.87	0.56
1:D:351:CYS:HA	1:D:354:ALA:HB3	1.87	0.56
1:B:158:GLN:HE22	1:B:180:TRP:HH2	1.51	0.56
1:B:428:ASP:C	1:B:430:HIS:H	2.13	0.56
1:C:251:ASP:HB3	1:C:273:ASN:HA	1.87	0.56
1:F:242:CYS:HA	1:F:304:TYR:CZ	2.41	0.56
1:B:215:VAL:O	1:B:219:MET:N	2.39	0.56
1:B:468:LEU:HD13	1:B:582:MET:HG2	1.86	0.56
1:C:568:ARG:O	1:C:576:ARG:NH2	2.39	0.56
1:D:113:PHE:HE1	1:D:218:LEU:HD13	1.71	0.56
1:E:219:MET:HE2	1:E:223:MET:HE1	1.88	0.56
1:E:287:GLU:O	1:E:291:ARG:HG3	2.04	0.56
1:E:305:LEU:HD13	1:E:308:ILE:HD12	1.86	0.56
1:D:576:ARG:NH1	1:D:602:ASP:OD1	2.38	0.56
1:A:68:ARG:O	1:A:72:ASP:N	2.30	0.56
1:A:59:GLU:HA	1:A:62:ALA:HB3	1.88	0.56
1:A:706:GLU:OE2	1:A:713:ASN:N	2.38	0.56
1:C:534:TYR:HA	1:C:577:LEU:HD11	1.88	0.56
1:E:83:TRP:CD1	1:E:86:CYS:HG	2.23	0.56
1:D:305:LEU:HA	1:D:308:ILE:HB	1.86	0.56
1:F:301:GLU:O	1:F:302:GLN:C	2.49	0.56
1:A:537:GLU:OE1	1:A:580:ARG:NH1	2.36	0.55
1:B:304:TYR:CE1	1:B:333:VAL:HG21	2.40	0.55
1:F:68:ARG:HB3	1:F:111:TYR:HE1	1.71	0.55
1:B:241:PRO:HB2	1:B:300:TYR:HB3	1.87	0.55
1:C:57:HIS:O	1:C:58:HIS:C	2.48	0.55
1:D:596:GLN:NE2	1:D:708:GLU:OE2	2.34	0.55
1:F:295:GLU:HA	1:F:298:LYS:HB2	1.86	0.55
1:A:62:ALA:HA	1:A:110:CYS:SG	2.46	0.55
1:C:57:HIS:HB2	1:C:98:LEU:O	2.07	0.55
1:F:183:MET:HE1	1:F:214:PHE:HB2	1.87	0.55
1:F:251:ASP:O	1:F:273:ASN:ND2	2.39	0.55
1:F:588:VAL:O	1:F:589:GLN:C	2.49	0.55
1:D:102:LYS:H	1:D:102:LYS:HD2	1.71	0.55
1:D:206:ARG:HH12	1:D:248:LEU:N	2.05	0.55
1:E:342:ARG:HD2	1:E:350:LEU:HD11	1.89	0.55
1:A:475:LEU:HB3	1:A:574:LEU:HD11	1.89	0.55
1:D:278:PHE:HA	1:D:281:TRP:HB2	1.89	0.55
1:D:709:THR:HG23	1:D:711:SER:H	1.72	0.55
1:C:251:ASP:O	1:C:273:ASN:ND2	2.37	0.55
1:D:447:ARG:HD3	1:D:574:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:539:ARG:NH2	1:F:428:ASP:OD2	2.40	0.55
1:F:449:ALA:HB1	1:F:719:LEU:HD21	1.88	0.55
1:D:475:LEU:HD11	1:D:534:TYR:HE1	1.72	0.55
1:B:251:ASP:HB3	1:B:274:ALA:N	2.19	0.55
1:D:301:GLU:HG3	1:D:333:VAL:HG11	1.89	0.55
1:F:206:ARG:NH1	1:F:251:ASP:OD2	2.40	0.55
1:B:254:SER:OG	1:B:273:ASN:OD1	2.24	0.55
1:B:350:LEU:HB2	1:B:353:GLU:HB2	1.89	0.55
1:B:626:GLY:HA3	1:B:629:GLU:HG3	1.88	0.55
1:C:333:VAL:HG23	1:C:334:PRO:HD3	1.89	0.55
1:D:257:ILE:O	1:D:261:GLU:HG2	2.07	0.55
1:E:73:TRP:O	1:E:78:GLY:N	2.32	0.55
1:C:177:ILE:HG23	1:C:180:TRP:HD1	1.72	0.54
1:C:243:TYR:HA	1:C:246:LEU:HD12	1.89	0.54
1:C:310:ASP:OD2	1:C:311:PHE:N	2.41	0.54
1:C:353:GLU:HA	1:C:356:SER:HB2	1.88	0.54
1:D:444:LYS:HD3	1:D:493:ARG:HH22	1.71	0.54
1:E:564:LEU:HD23	1:E:567:ILE:HD11	1.89	0.54
1:F:296:VAL:HA	1:F:299:GLN:HB3	1.88	0.54
1:B:34:SER:O	1:B:54:ARG:NE	2.40	0.54
1:C:519:MET:HG2	1:C:534:TYR:HE2	1.73	0.54
1:D:202:TYR:O	1:D:206:ARG:HG2	2.08	0.54
1:C:354:ALA:O	1:C:358:LEU:HG	2.08	0.54
1:E:249:ALA:HB3	1:E:336:ASN:ND2	2.23	0.54
1:F:199:LEU:HD23	1:F:199:LEU:H	1.73	0.54
1:A:58:HIS:CE1	1:A:61:LEU:HB2	2.42	0.54
1:B:255:PHE:HA	1:B:273:ASN:ND2	2.22	0.54
1:F:322:LEU:O	1:F:326:LEU:N	2.34	0.54
1:E:88:PRO:HG3	1:E:354:ALA:HA	1.89	0.54
1:E:492:ARG:HH11	1:E:493:ARG:NH1	2.05	0.54
1:B:285:ASN:O	1:B:289:ALA:N	2.40	0.54
1:C:458:LEU:O	1:C:459:VAL:C	2.49	0.54
1:E:304:TYR:CZ	1:E:308:ILE:HD11	2.43	0.54
1:F:35:SER:N	1:F:55:ARG:O	2.40	0.54
1:A:505:GLU:HG2	1:B:486:GLU:HB3	1.90	0.54
1:B:73:TRP:HD1	1:B:78:GLY:O	1.91	0.54
1:D:327:LYS:O	1:D:331:TYR:N	2.41	0.54
1:F:608:PHE:CE2	1:F:723:LEU:HD11	2.43	0.54
1:D:325:TYR:HA	1:D:328:ALA:HB3	1.90	0.54
1:E:33:LEU:HD11	1:E:103:PRO:HD3	1.90	0.54
1:A:241:PRO:CB	1:A:304:TYR:CE1	2.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ARG:HH12	1:D:248:LEU:H	1.54	0.54
1:D:257:ILE:O	1:D:260:GLU:HG2	2.07	0.54
1:E:220:ARG:HA	1:E:225:ILE:HB	1.90	0.54
1:F:706:GLU:HG2	1:F:712:PRO:HA	1.90	0.54
1:C:714:TRP:HD1	1:D:156:GLN:HG2	1.72	0.53
1:D:231:GLU:O	1:D:235:ILE:HG12	2.08	0.53
1:E:31:SER:OG	1:E:54:ARG:NH1	2.40	0.53
1:A:243:TYR:HA	1:A:246:LEU:HD12	1.90	0.53
1:B:218:LEU:HA	1:B:221:PHE:HB3	1.90	0.53
1:A:109:ILE:HD12	1:A:109:ILE:H	1.72	0.53
1:E:161:MET:HE2	1:E:161:MET:N	2.22	0.53
1:A:202:TYR:HB3	1:A:281:TRP:CZ2	2.43	0.53
1:A:564:LEU:HD23	1:A:567:ILE:HD11	1.91	0.53
1:B:145:TYR:CZ	1:B:149:ARG:HB2	2.43	0.53
1:B:428:ASP:O	1:B:430:HIS:N	2.41	0.53
1:B:519:MET:HE1	1:B:531:MET:SD	2.49	0.53
1:B:695:MET:HE1	1:B:723:LEU:HD23	1.89	0.53
1:D:183:MET:HE1	1:D:214:PHE:CG	2.43	0.53
1:A:202:TYR:HB3	1:A:281:TRP:HZ2	1.74	0.53
1:B:117:PHE:HA	1:B:120:ASP:HB3	1.89	0.53
1:B:449:ALA:HB1	1:B:719:LEU:HD21	1.91	0.53
1:E:298:LYS:O	1:E:302:GLN:N	2.24	0.53
1:F:454:LEU:HB3	1:F:582:MET:HE1	1.91	0.53
1:D:287:GLU:HA	1:D:290:LYS:HD2	1.90	0.53
1:D:342:ARG:HA	1:D:347:HIS:HD2	1.74	0.53
1:B:320:ILE:HA	1:B:323:GLN:HB2	1.90	0.53
1:F:306:ARG:O	1:F:310:ASP:N	2.41	0.53
1:E:49:SER:OG	1:E:305:LEU:HD23	2.08	0.53
1:B:213:PRO:O	1:B:217:MET:N	2.36	0.53
1:D:177:ILE:O	1:D:181:LYS:N	2.40	0.53
1:F:255:PHE:HA	1:F:258:GLU:HG2	1.90	0.53
1:B:26:ASP:N	1:B:26:ASP:OD1	2.42	0.52
1:C:216:ASP:OD2	1:C:220:ARG:NH2	2.43	0.52
1:E:27:PHE:HA	1:E:321:LYS:N	2.24	0.52
1:E:631:LEU:HD21	1:E:674:VAL:HG11	1.91	0.52
1:F:258:GLU:HA	1:F:261:GLU:HG2	1.91	0.52
1:A:656:ILE:HG23	1:A:670:LEU:HD23	1.90	0.52
1:C:519:MET:HE3	1:D:519:MET:CE	2.39	0.52
1:E:333:VAL:O	1:E:337:VAL:HG23	2.08	0.52
1:A:648:PRO:HG2	1:A:649:LYS:HD3	1.92	0.52
1:E:58:HIS:HB2	1:E:106:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:O	1:A:71:THR:OG1	2.23	0.52
1:C:163:LEU:O	1:C:167:SER:HB3	2.10	0.52
1:C:262:PHE:HB2	1:C:271:MET:HG3	1.92	0.52
1:C:523:ARG:NH2	1:D:532:ASP:OD1	2.42	0.52
1:F:31:SER:O	1:F:33:LEU:N	2.42	0.52
1:B:77:ILE:HG12	1:B:154:THR:HG22	1.92	0.52
1:B:105:ARG:HD3	1:B:221:PHE:CE2	2.45	0.52
1:E:172:ARG:HD2	1:E:221:PHE:HA	1.91	0.52
1:F:82:ARG:HB2	1:F:121:ASN:ND2	2.25	0.52
1:D:223:MET:HB2	1:D:225:ILE:HG13	1.91	0.52
1:E:568:ARG:O	1:E:576:ARG:NH2	2.43	0.52
1:F:257:ILE:O	1:F:260:GLU:HB3	2.09	0.52
1:A:292:ARG:HG3	1:A:296:VAL:CG1	2.40	0.52
1:E:292:ARG:NE	1:E:296:VAL:HG11	2.23	0.52
1:A:88:PRO:HD2	1:A:89:TRP:CZ3	2.44	0.52
1:B:29:LEU:HD22	1:B:223:MET:HE2	1.91	0.52
1:A:278:PHE:HA	1:A:281:TRP:HB2	1.91	0.52
1:C:214:PHE:O	1:C:218:LEU:N	2.41	0.52
1:D:519:MET:HE2	1:D:534:TYR:CE2	2.45	0.52
1:E:252:TYR:HB2	1:E:293:VAL:HG11	1.92	0.52
1:B:77:ILE:HD11	1:B:154:THR:HA	1.91	0.51
1:B:304:TYR:OH	1:B:330:GLY:HA2	2.10	0.51
1:E:217:MET:HA	1:E:220:ARG:HD2	1.92	0.51
1:B:34:SER:HA	1:B:56:HIS:HA	1.90	0.51
1:A:261:GLU:HA	1:A:264:ALA:HB3	1.92	0.51
1:C:90:GLU:HG2	1:C:342:ARG:HD2	1.92	0.51
1:D:112:ILE:O	1:D:116:ALA:N	2.37	0.51
1:D:113:PHE:CE1	1:D:218:LEU:HD13	2.45	0.51
1:B:118:LEU:HA	1:B:121:ASN:HB2	1.92	0.51
1:D:618:THR:OG1	1:D:619:GLU:N	2.44	0.51
1:B:219:MET:HE3	1:B:328:ALA:HB3	1.91	0.51
1:C:83:TRP:O	1:C:345:ARG:NH1	2.44	0.51
1:F:254:SER:O	1:F:258:GLU:N	2.42	0.51
1:F:304:TYR:O	1:F:308:ILE:N	2.43	0.51
1:F:350:LEU:O	1:F:351:CYS:C	2.53	0.51
1:B:172:ARG:NH1	1:B:224:GLY:O	2.43	0.51
1:D:238:ILE:HG22	1:D:329:GLN:HE22	1.76	0.51
1:E:55:ARG:HE	1:E:96:VAL:HG13	1.75	0.51
1:E:101:CYS:SG	1:E:222:GLY:HA3	2.51	0.51
1:A:520:GLU:HG3	1:B:535:LEU:HD13	1.92	0.51
1:B:656:ILE:HG23	1:B:670:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:568:ARG:HD3	1:E:602:ASP:HB3	1.93	0.51
1:F:117:PHE:O	1:F:121:ASN:N	2.43	0.51
1:E:27:PHE:CB	1:E:323:GLN:H	2.19	0.51
1:E:49:SER:OG	1:E:301:GLU:OE2	2.29	0.51
1:F:321:LYS:O	1:F:324:THR:OG1	2.27	0.51
1:A:661:ARG:HG2	1:A:661:ARG:HH11	1.76	0.51
1:D:235:ILE:HD12	1:D:322:LEU:HD21	1.92	0.51
1:D:268:LYS:HZ1	1:D:271:MET:HA	1.76	0.51
1:E:49:SER:HA	1:E:298:LYS:HZ1	1.75	0.51
1:E:275:VAL:HG11	1:E:290:LYS:HZ2	1.76	0.51
1:F:220:ARG:NH2	1:F:227:LEU:HB3	2.26	0.51
1:A:246:LEU:HG	1:A:333:VAL:HG22	1.92	0.51
1:A:83:TRP:CD1	1:A:344:PRO:HB2	2.46	0.50
1:C:90:GLU:HG2	1:C:342:ARG:CD	2.41	0.50
1:C:235:ILE:HG22	1:C:239:VAL:HG13	1.93	0.50
1:F:246:LEU:HG	1:F:336:ASN:ND2	2.26	0.50
1:A:206:ARG:HH12	1:A:244:ALA:HA	1.75	0.50
1:B:105:ARG:O	1:B:105:ARG:HG3	2.12	0.50
1:D:85:SER:HB2	1:D:93:PHE:HB3	1.93	0.50
1:D:101:CYS:SG	1:D:222:GLY:HA3	2.51	0.50
1:D:245:ALA:HB2	1:D:300:TYR:HB3	1.92	0.50
1:E:322:LEU:O	1:E:324:THR:N	2.44	0.50
1:F:275:VAL:HA	1:F:289:ALA:HB1	1.93	0.50
1:A:287:GLU:N	1:A:287:GLU:OE1	2.44	0.50
1:B:342:ARG:HA	1:B:347:HIS:CD2	2.46	0.50
1:D:515:LEU:HD22	1:D:538:MET:HE1	1.92	0.50
1:C:232:GLN:O	1:C:236:GLU:N	2.44	0.50
1:D:276:TRP:O	1:D:279:MET:HB2	2.12	0.50
1:B:35:SER:N	1:B:55:ARG:O	2.41	0.50
1:B:505:GLU:OE2	1:B:505:GLU:N	2.45	0.50
1:D:252:TYR:HE2	1:D:290:LYS:HB2	1.76	0.50
1:E:302:GLN:HB3	1:E:306:ARG:HH21	1.77	0.50
1:F:679:ARG:HH11	1:F:679:ARG:HG2	1.76	0.50
1:A:176:VAL:HG13	1:A:214:PHE:HE1	1.75	0.50
1:B:182:GLU:O	1:B:186:THR:OG1	2.23	0.50
1:D:49:SER:OG	1:D:298:LYS:HD2	2.12	0.50
1:D:301:GLU:O	1:D:305:LEU:N	2.42	0.50
1:A:29:LEU:HG	1:A:324:THR:HB	1.93	0.50
1:A:260:GLU:O	1:A:264:ALA:N	2.35	0.50
1:F:292:ARG:HA	1:F:295:GLU:HG3	1.92	0.50
1:A:49:SER:O	1:A:305:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:O	1:A:116:ALA:N	2.43	0.50
1:C:505:GLU:HG2	1:D:486:GLU:HB3	1.94	0.50
1:C:617:LEU:HD21	1:C:678:LEU:HD13	1.93	0.50
1:D:315:GLU:O	1:D:316:GLY:C	2.55	0.50
1:A:567:ILE:HG21	1:A:609:GLN:HG2	1.93	0.50
1:B:217:MET:O	1:B:221:PHE:N	2.36	0.50
1:C:89:TRP:HB3	1:C:342:ARG:NH1	2.27	0.50
1:E:216:ASP:OD1	1:E:220:ARG:NE	2.43	0.50
1:F:216:ASP:OD1	1:F:332:GLN:NE2	2.45	0.50
1:F:666:LEU:HB2	1:F:671:LYS:NZ	2.27	0.50
1:B:216:ASP:HA	1:B:219:MET:HB3	1.94	0.49
1:B:235:ILE:HA	1:B:238:ILE:HB	1.93	0.49
1:C:27:PHE:HB2	1:C:321:LYS:HB3	1.94	0.49
1:E:56:HIS:CD2	1:E:106:LEU:HD22	2.47	0.49
1:D:115:TYR:OH	1:D:158:GLN:OE1	2.26	0.49
1:D:235:ILE:HG22	1:D:239:VAL:HG23	1.93	0.49
1:F:202:TYR:O	1:F:206:ARG:HD3	2.12	0.49
1:A:206:ARG:NH1	1:A:243:TYR:O	2.44	0.49
1:D:29:LEU:HB2	1:D:324:THR:HA	1.94	0.49
1:E:34:SER:OG	1:E:54:ARG:NH2	2.41	0.49
1:E:54:ARG:HG3	1:E:331:TYR:HE2	1.77	0.49
1:E:112:ILE:HG21	1:E:214:PHE:HZ	1.76	0.49
1:B:276:TRP:HA	1:B:279:MET:HB2	1.93	0.49
1:C:661:ARG:HG2	1:C:661:ARG:O	2.13	0.49
1:D:268:LYS:HZ3	1:D:271:MET:HG2	1.78	0.49
1:A:61:LEU:HA	1:A:64:GLU:HB3	1.94	0.49
1:A:63:ASN:O	1:A:67:LEU:N	2.23	0.49
1:A:475:LEU:HD21	1:A:538:MET:HE1	1.93	0.49
1:B:246:LEU:HD11	1:B:333:VAL:HG22	1.95	0.49
1:B:342:ARG:O	1:B:342:ARG:NE	2.44	0.49
1:E:285:ASN:H	1:E:288:GLN:HB2	1.76	0.49
1:A:81:GLU:O	1:A:82:ARG:HB3	2.13	0.49
1:E:55:ARG:HG3	1:E:95:ALA:HB1	1.95	0.49
1:B:251:ASP:HB3	1:B:273:ASN:HA	1.94	0.49
1:B:431:LEU:O	1:B:510:SER:OG	2.26	0.49
1:D:276:TRP:HA	1:D:279:MET:HG2	1.94	0.49
1:D:454:LEU:HD21	1:D:597:LEU:HD22	1.95	0.49
1:D:519:MET:HE2	1:D:534:TYR:HE2	1.78	0.49
1:E:183:MET:HE3	1:E:214:PHE:HD1	1.78	0.49
1:B:55:ARG:HH21	1:B:59:GLU:HG3	1.77	0.49
1:C:80:ILE:HG21	1:C:118:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:O	1:D:207:ILE:HG12	2.13	0.49
1:E:276:TRP:O	1:E:279:MET:HB2	2.13	0.49
1:F:26:ASP:OD1	1:F:26:ASP:N	2.35	0.49
1:A:246:LEU:O	1:A:336:ASN:ND2	2.45	0.49
1:A:349:TRP:HA	1:A:352:LYS:NZ	2.27	0.49
1:B:691:MET:HA	1:B:694:LEU:HD12	1.94	0.49
1:C:140:LEU:HD22	1:C:141:ASP:H	1.77	0.49
1:E:28:ILE:HG12	1:E:321:LYS:O	2.13	0.49
1:E:275:VAL:HG11	1:E:290:LYS:NZ	2.28	0.49
1:F:577:LEU:HG	1:F:581:MET:HE2	1.95	0.49
1:A:352:LYS:HD3	1:A:352:LYS:N	2.27	0.48
1:D:173:ALA:O	1:D:177:ILE:HG12	2.13	0.48
1:D:312:ALA:CA	1:D:316:GLY:HA3	2.25	0.48
1:F:198:ASN:HA	1:F:281:TRP:HB3	1.95	0.48
1:B:697:LYS:HB2	1:B:697:LYS:HE3	1.51	0.48
1:E:216:ASP:OD2	1:E:243:TYR:OH	2.27	0.48
1:F:320:ILE:HA	1:F:323:GLN:HG3	1.95	0.48
1:B:312:ALA:HA	1:B:316:GLY:CA	2.43	0.48
1:C:89:TRP:C	1:C:342:ARG:HH11	2.20	0.48
1:C:359:HIS:HA	1:C:362:THR:OG1	2.13	0.48
1:C:228:THR:O	1:C:232:GLN:N	2.34	0.48
1:C:352:LYS:O	1:C:356:SER:N	2.45	0.48
1:D:346:TYR:HB2	1:D:347:HIS:CE1	2.48	0.48
1:E:172:ARG:NH2	1:E:173:ALA:HB2	2.28	0.48
1:E:482:LEU:O	1:E:486:GLU:HG3	2.14	0.48
1:F:102:LYS:HB3	1:F:104:GLU:HG2	1.95	0.48
1:A:65:GLY:HA3	1:A:110:CYS:SG	2.54	0.48
1:A:534:TYR:HA	1:A:577:LEU:HD11	1.95	0.48
1:C:176:VAL:O	1:C:180:TRP:N	2.38	0.48
1:C:227:LEU:HD22	1:C:231:GLU:CG	2.43	0.48
1:C:239:VAL:HG12	1:C:326:LEU:HD11	1.95	0.48
1:E:71:THR:O	1:E:75:GLN:N	2.45	0.48
1:E:230:GLU:O	1:E:234:ARG:N	2.47	0.48
1:E:242:CYS:O	1:E:246:LEU:HD12	2.13	0.48
1:F:534:TYR:CD1	1:F:577:LEU:HD21	2.49	0.48
1:B:83:TRP:HH2	1:B:358:LEU:HD11	1.79	0.48
1:B:600:LEU:HD11	1:B:698:ILE:HG23	1.96	0.48
1:C:73:TRP:HD1	1:C:78:GLY:O	1.96	0.48
1:C:706:GLU:CD	1:C:712:PRO:HA	2.39	0.48
1:F:277:LEU:HB3	1:F:281:TRP:CZ2	2.49	0.48
1:F:315:GLU:OE2	1:F:315:GLU:N	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:HB3	1:A:281:TRP:HE1	1.78	0.48
1:A:237:PRO:HA	1:A:240:LYS:HD2	1.96	0.48
1:A:458:LEU:HD21	1:A:583:VAL:HG22	1.95	0.48
1:B:675:LEU:O	1:B:679:ARG:HG3	2.13	0.48
1:C:176:VAL:HG21	1:C:221:PHE:HB2	1.96	0.48
1:F:231:GLU:HA	1:F:234:ARG:HB2	1.96	0.48
1:B:82:ARG:HG3	1:B:83:TRP:H	1.78	0.48
1:B:178:ASN:O	1:B:182:GLU:HG2	2.14	0.48
1:B:298:LYS:O	1:B:299:GLN:C	2.57	0.48
1:C:230:GLU:OE1	1:C:233:LYS:NZ	2.47	0.48
1:D:219:MET:HE3	1:D:219:MET:HB3	1.70	0.48
1:D:706:GLU:OE1	1:D:717:ARG:NH2	2.47	0.48
1:F:82:ARG:HA	1:F:82:ARG:NE	2.28	0.48
1:F:307:ASN:O	1:F:311:PHE:N	2.40	0.48
1:A:279:MET:N	1:A:279:MET:HE2	2.29	0.48
1:B:114:GLU:HA	1:B:117:PHE:CZ	2.49	0.48
1:C:255:PHE:O	1:C:259:TRP:HB3	2.14	0.48
1:D:183:MET:HE1	1:D:214:PHE:CD2	2.49	0.48
1:F:214:PHE:CD2	1:F:218:LEU:HD11	2.48	0.48
1:B:492:ARG:HG2	1:B:493:ARG:HD2	1.95	0.47
1:C:340:SER:O	1:C:346:TYR:OH	2.32	0.47
1:E:460:LEU:HD23	1:E:587:PRO:HD3	1.95	0.47
1:F:276:TRP:O	1:F:279:MET:HB2	2.14	0.47
1:A:253:PHE:CD2	1:A:340:SER:HB2	2.49	0.47
1:B:276:TRP:O	1:B:279:MET:HB2	2.14	0.47
1:C:29:LEU:HB2	1:C:324:THR:HB	1.97	0.47
1:C:212:ALA:O	1:C:216:ASP:N	2.36	0.47
1:C:248:LEU:HD23	1:C:274:ALA:HB1	1.96	0.47
1:D:82:ARG:HB2	1:D:121:ASN:ND2	2.29	0.47
1:E:279:MET:HE1	1:E:286:ALA:N	2.28	0.47
1:F:24:SER:HA	1:F:27:PHE:HB2	1.95	0.47
1:F:237:PRO:HA	1:F:240:LYS:HB2	1.96	0.47
1:F:245:ALA:HB1	1:F:297:THR:HG23	1.96	0.47
1:F:311:PHE:CE2	1:F:316:GLY:HA3	2.49	0.47
1:B:666:LEU:HB2	1:B:671:LYS:HE3	1.96	0.47
1:D:279:MET:CE	1:D:289:ALA:HB2	2.45	0.47
1:F:351:CYS:O	1:F:355:ALA:N	2.33	0.47
1:A:81:GLU:HG2	1:A:82:ARG:N	2.29	0.47
1:B:721:HIS:HA	1:B:724:LYS:NZ	2.30	0.47
1:E:217:MET:N	1:E:217:MET:HE2	2.29	0.47
1:E:323:GLN:HG2	1:E:326:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:THR:HA	1:C:146:ARG:HH21	1.80	0.47
1:C:274:ALA:O	1:C:278:PHE:N	2.45	0.47
1:D:352:LYS:O	1:D:356:SER:OG	2.23	0.47
1:E:62:ALA:HA	1:E:110:CYS:SG	2.54	0.47
1:C:115:TYR:O	1:C:119:TYR:N	2.47	0.47
1:C:217:MET:HA	1:C:220:ARG:HD2	1.96	0.47
1:C:581:MET:O	1:C:585:ILE:HG12	2.15	0.47
1:E:236:GLU:O	1:E:240:LYS:HG2	2.14	0.47
1:B:284:LEU:CD1	1:B:292:ARG:CZ	2.89	0.47
1:C:219:MET:HB3	1:C:223:MET:HE1	1.96	0.47
1:C:258:GLU:HA	1:C:261:GLU:HB2	1.97	0.47
1:C:343:CYS:HB3	1:C:346:TYR:CE1	2.49	0.47
1:D:251:ASP:HB3	1:D:273:ASN:CA	2.40	0.47
1:D:325:TYR:O	1:D:329:GLN:N	2.35	0.47
1:D:342:ARG:HA	1:D:347:HIS:CD2	2.50	0.47
1:D:351:CYS:O	1:D:355:ALA:N	2.31	0.47
1:E:461:PRO:HG2	1:E:464:ARG:HG3	1.97	0.47
1:A:249:ALA:HB3	1:A:336:ASN:ND2	2.30	0.47
1:A:301:GLU:O	1:A:304:TYR:N	2.44	0.47
1:B:83:TRP:CE2	1:B:344:PRO:HG2	2.50	0.47
1:B:115:TYR:HA	1:B:118:LEU:HB2	1.96	0.47
1:B:475:LEU:HD12	1:B:475:LEU:HA	1.80	0.47
1:C:57:HIS:CE1	1:C:101:CYS:HB2	2.49	0.47
1:E:212:ALA:O	1:E:216:ASP:N	2.43	0.47
1:A:180:TRP:HB2	1:A:214:PHE:CE1	2.50	0.47
1:A:233:LYS:HA	1:A:236:GLU:HB2	1.97	0.47
1:B:334:PRO:O	1:B:335:GLY:C	2.57	0.47
1:C:87:ASN:HD22	1:C:344:PRO:HD3	1.80	0.47
1:E:258:GLU:O	1:E:262:PHE:N	2.46	0.47
1:F:213:PRO:O	1:F:217:MET:HE2	2.15	0.47
1:F:475:LEU:HD11	1:F:534:TYR:CE1	2.46	0.47
1:A:468:LEU:HD13	1:A:582:MET:HG3	1.97	0.47
1:B:277:LEU:O	1:B:281:TRP:N	2.44	0.47
1:E:27:PHE:C	1:E:323:GLN:HB2	2.40	0.47
1:F:31:SER:HG	1:F:54:ARG:NH1	2.13	0.47
1:F:40:SER:OG	1:F:41:THR:N	2.44	0.47
1:A:347:HIS:HB2	1:A:349:TRP:CZ2	2.50	0.46
1:C:326:LEU:O	1:C:330:GLY:N	2.45	0.46
1:C:648:PRO:HG2	1:C:649:LYS:HD3	1.97	0.46
1:D:110:CYS:HA	1:D:113:PHE:HB2	1.97	0.46
1:D:220:ARG:CD	1:D:227:LEU:HG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:LEU:HB3	1:D:574:LEU:HD11	1.96	0.46
1:A:230:GLU:HA	1:A:233:LYS:HB3	1.96	0.46
1:F:173:ALA:O	1:F:177:ILE:N	2.33	0.46
1:B:117:PHE:O	1:B:121:ASN:N	2.46	0.46
1:B:150:SER:O	1:B:154:THR:HG23	2.15	0.46
1:B:610:VAL:HG21	1:B:690:LYS:HD3	1.96	0.46
1:B:625:LYS:HD3	1:B:629:GLU:HB2	1.97	0.46
1:C:70:ARG:HH22	1:C:84:GLY:N	2.12	0.46
1:C:535:LEU:HD23	1:D:516:ILE:HG23	1.97	0.46
1:E:70:ARG:HH11	1:E:80:ILE:HD13	1.79	0.46
1:E:323:GLN:O	1:E:327:LYS:N	2.40	0.46
1:A:518:VAL:O	1:A:522:VAL:HG23	2.15	0.46
1:B:285:ASN:ND2	1:B:288:GLN:H	2.14	0.46
1:C:83:TRP:NE1	1:C:86:CYS:SG	2.88	0.46
1:C:563:TYR:O	1:C:567:ILE:HG12	2.15	0.46
1:D:238:ILE:HG23	1:D:311:PHE:CD1	2.50	0.46
1:B:85:SER:HB3	1:B:117:PHE:CE2	2.50	0.46
1:C:215:VAL:O	1:C:219:MET:N	2.43	0.46
1:C:242:CYS:SG	1:C:333:VAL:HG22	2.56	0.46
1:D:660:SER:HB2	1:D:666:LEU:HG	1.98	0.46
1:E:245:ALA:HB1	1:E:333:VAL:HG11	1.97	0.46
1:E:296:VAL:O	1:E:300:TYR:HD1	1.99	0.46
1:F:26:ASP:HB2	1:F:225:ILE:HD11	1.96	0.46
1:E:152:LEU:HD12	1:F:459:VAL:HG13	1.97	0.46
1:D:233:LYS:O	1:D:236:GLU:HB3	2.16	0.46
1:D:297:THR:O	1:D:301:GLU:N	2.49	0.46
1:E:72:ASP:OD2	1:E:111:TYR:OH	2.27	0.46
1:F:597:LEU:HD23	1:F:597:LEU:HA	1.78	0.46
1:A:291:ARG:O	1:A:294:GLN:HB3	2.16	0.46
1:B:83:TRP:CH2	1:B:358:LEU:HD11	2.50	0.46
1:B:695:MET:CE	1:B:723:LEU:HD23	2.45	0.46
1:C:69:CYS:HA	1:C:72:ASP:HB2	1.98	0.46
1:D:90:GLU:HG2	1:D:341:LEU:HD13	1.97	0.46
1:D:614:TYR:HE1	1:D:684:ILE:HG23	1.81	0.46
1:F:182:GLU:O	1:F:186:THR:OG1	2.23	0.46
1:F:468:LEU:HD13	1:F:582:MET:HG2	1.98	0.46
1:E:468:LEU:HD13	1:E:582:MET:HG2	1.98	0.46
1:F:258:GLU:CD	1:F:273:ASN:HD22	2.24	0.46
1:F:269:THR:OG1	1:F:270:THR:N	2.49	0.46
1:F:301:GLU:HA	1:F:304:TYR:CZ	2.50	0.46
1:A:109:ILE:HA	1:A:112:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ILE:HA	1:B:324:THR:HG21	1.98	0.46
1:B:290:LYS:O	1:B:291:ARG:C	2.59	0.46
1:B:608:PHE:CZ	1:B:723:LEU:HD11	2.51	0.46
1:C:89:TRP:HB2	1:C:342:ARG:HD2	1.94	0.46
1:C:160:LYS:O	1:C:164:GLU:HG2	2.16	0.46
1:C:290:LYS:HB3	1:C:290:LYS:HE3	1.52	0.46
1:F:230:GLU:O	1:F:234:ARG:N	2.41	0.46
1:B:315:GLU:O	1:B:315:GLU:HG3	2.16	0.45
1:C:93:PHE:O	1:C:97:VAL:HB	2.16	0.45
1:C:217:MET:HA	1:C:220:ARG:HB2	1.97	0.45
1:C:518:VAL:HA	1:C:521:LYS:HD2	1.98	0.45
1:E:291:ARG:HA	1:E:294:GLN:HB2	1.98	0.45
1:A:163:LEU:O	1:A:167:SER:HB3	2.15	0.45
1:C:253:PHE:HB3	1:C:346:TYR:CE1	2.50	0.45
1:D:614:TYR:O	1:D:614:TYR:CD2	2.69	0.45
1:E:69:CYS:HA	1:E:72:ASP:HB2	1.98	0.45
1:E:223:MET:HB2	1:E:225:ILE:HG13	1.98	0.45
1:F:26:ASP:O	1:F:324:THR:HG21	2.16	0.45
1:A:302:GLN:O	1:A:306:ARG:N	2.49	0.45
1:B:110:CYS:HA	1:B:113:PHE:HB2	1.98	0.45
1:B:180:TRP:HB2	1:B:214:PHE:CE1	2.50	0.45
1:D:83:TRP:CD2	1:D:344:PRO:HB2	2.51	0.45
1:D:695:MET:HE3	1:D:724:LYS:HD2	1.97	0.45
1:E:100:PHE:O	1:E:223:MET:HE3	2.15	0.45
1:E:299:GLN:O	1:E:303:GLN:N	2.42	0.45
1:F:234:ARG:O	1:F:237:PRO:HD2	2.17	0.45
1:A:49:SER:C	1:A:305:LEU:HD12	2.42	0.45
1:A:448:GLU:CD	1:A:448:GLU:H	2.24	0.45
1:B:337:VAL:HA	1:B:340:SER:HB2	1.99	0.45
1:B:339:TRP:C	1:B:341:LEU:HG	2.42	0.45
1:C:304:TYR:O	1:C:308:ILE:HG13	2.17	0.45
1:F:234:ARG:O	1:F:238:ILE:HD12	2.16	0.45
1:B:83:TRP:O	1:B:345:ARG:NH2	2.27	0.45
1:B:89:TRP:CD1	1:B:357:LEU:HD12	2.52	0.45
1:C:101:CYS:SG	1:C:222:GLY:HA3	2.57	0.45
1:D:25:SER:CB	1:D:30:ASN:H	2.29	0.45
1:D:634:CYS:SG	1:D:661:ARG:HG3	2.56	0.45
1:F:160:LYS:HD2	1:F:160:LYS:O	2.16	0.45
1:A:355:ALA:O	1:A:359:HIS:N	2.36	0.45
1:B:284:LEU:HD12	1:B:292:ARG:HD2	1.97	0.45
1:C:69:CYS:HB3	1:C:114:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ARG:O	1:D:71:THR:C	2.59	0.45
1:D:570:LYS:NZ	1:D:571:THR:OG1	2.49	0.45
1:E:536:GLU:OE1	1:E:580:ARG:NH2	2.49	0.45
1:F:203:VAL:HA	1:F:206:ARG:HE	1.81	0.45
1:A:706:GLU:HG2	1:A:712:PRO:HA	1.99	0.45
1:B:278:PHE:HA	1:B:281:TRP:HB2	1.98	0.45
1:C:273:ASN:HB3	1:C:276:TRP:HB3	1.98	0.45
1:E:326:LEU:O	1:E:330:GLY:N	2.31	0.45
1:A:105:ARG:HD2	1:A:221:PHE:CE2	2.52	0.45
1:A:721:HIS:O	1:A:721:HIS:ND1	2.50	0.45
1:C:523:ARG:HD2	1:D:531:MET:HG2	1.98	0.45
1:D:262:PHE:HD1	1:D:268:LYS:HE2	1.81	0.45
1:D:347:HIS:HB3	1:D:349:TRP:CZ2	2.52	0.45
1:D:451:ILE:HG23	1:D:582:MET:SD	2.57	0.45
1:E:300:TYR:O	1:E:303:GLN:HB3	2.16	0.45
1:E:490:PRO:O	1:E:491:LEU:HD23	2.17	0.45
1:A:161:MET:HE3	1:A:161:MET:HB3	1.72	0.45
1:B:33:LEU:HD13	1:B:33:LEU:HA	1.78	0.45
1:B:284:LEU:HD11	1:B:292:ARG:CD	2.46	0.45
1:E:317:LYS:HB3	1:E:317:LYS:HE3	1.58	0.45
1:F:105:ARG:HA	1:F:105:ARG:HD2	1.83	0.45
1:A:220:ARG:HG2	1:A:225:ILE:HB	1.98	0.45
1:A:538:MET:HE2	1:A:538:MET:HB2	1.83	0.45
1:A:608:PHE:CE2	1:A:723:LEU:HD21	2.51	0.45
1:C:49:SER:OG	1:C:302:GLN:HG2	2.17	0.45
1:C:336:ASN:O	1:C:337:VAL:C	2.59	0.45
1:D:698:ILE:HG21	1:D:720:ILE:HD11	1.99	0.45
1:E:246:LEU:HA	1:E:336:ASN:ND2	2.32	0.45
1:E:249:ALA:HB3	1:E:336:ASN:HD21	1.82	0.45
1:E:567:ILE:HG21	1:E:609:GLN:HG2	1.99	0.45
1:F:234:ARG:C	1:F:238:ILE:HD12	2.42	0.45
1:E:217:MET:O	1:E:221:PHE:N	2.49	0.44
1:A:110:CYS:O	1:A:114:GLU:HG2	2.16	0.44
1:A:166:LEU:HD23	1:A:170:ALA:HA	1.99	0.44
1:A:232:GLN:HG3	1:A:236:GLU:HG3	1.99	0.44
1:A:523:ARG:NH1	1:B:531:MET:HG2	2.33	0.44
1:B:563:TYR:O	1:B:567:ILE:HG12	2.16	0.44
1:C:34:SER:HG	1:C:56:HIS:N	2.16	0.44
1:C:81:GLU:HG2	1:C:82:ARG:N	2.32	0.44
1:C:261:GLU:O	1:C:265:GLU:N	2.35	0.44
1:F:667:ASP:OD1	1:F:667:ASP:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:MET:HE1	1:A:285:ASN:C	2.42	0.44
1:A:285:ASN:HB3	1:A:288:GLN:HB2	1.99	0.44
1:A:447:ARG:HD2	1:A:574:LEU:HD23	1.99	0.44
1:B:485:ILE:HD13	1:B:504:THR:HG23	1.98	0.44
1:C:285:ASN:O	1:C:289:ALA:N	2.24	0.44
1:D:219:MET:O	1:D:223:MET:HG3	2.17	0.44
1:E:254:SER:HA	1:E:346:TYR:CD1	2.53	0.44
1:F:27:PHE:C	1:F:324:THR:HG23	2.42	0.44
1:F:333:VAL:HA	1:F:336:ASN:ND2	2.33	0.44
1:A:291:ARG:O	1:A:295:GLU:N	2.49	0.44
1:A:351:CYS:SG	1:A:352:LYS:HD3	2.58	0.44
1:A:355:ALA:C	1:A:359:HIS:HD1	2.25	0.44
1:D:242:CYS:HB2	1:D:304:TYR:CZ	2.52	0.44
1:E:202:TYR:HB3	1:E:281:TRP:HH2	1.81	0.44
1:F:115:TYR:O	1:F:119:TYR:N	2.30	0.44
1:A:251:ASP:O	1:A:273:ASN:ND2	2.38	0.44
1:C:259:TRP:HA	1:C:271:MET:SD	2.57	0.44
1:D:32:THR:OG1	1:D:33:LEU:N	2.50	0.44
1:D:98:LEU:HD21	1:D:113:PHE:HZ	1.83	0.44
1:E:328:ALA:HA	1:E:331:TYR:HB2	1.98	0.44
1:B:312:ALA:HA	1:B:316:GLY:HA3	2.00	0.44
1:C:223:MET:SD	1:C:223:MET:N	2.91	0.44
1:D:308:ILE:HD11	1:D:329:GLN:HG3	1.99	0.44
1:D:438:ILE:HA	1:D:441:LEU:HD12	1.99	0.44
1:E:99:PRO:HD2	1:E:328:ALA:HB1	1.99	0.44
1:B:70:ARG:HH11	1:B:80:ILE:HD13	1.81	0.44
1:B:338:ALA:O	1:B:341:LEU:HD11	2.18	0.44
1:C:253:PHE:CZ	1:C:341:LEU:HG	2.53	0.44
1:D:212:ALA:O	1:D:215:VAL:HG22	2.18	0.44
1:D:285:ASN:HD21	1:D:287:GLU:HB2	1.83	0.44
1:F:85:SER:HB3	1:F:117:PHE:CE2	2.53	0.44
1:F:527:ASP:HB3	1:F:530:CYS:HB2	2.00	0.44
1:A:83:TRP:HD1	1:A:344:PRO:HB2	1.80	0.44
1:B:304:TYR:HE1	1:B:333:VAL:HG21	1.82	0.44
1:C:441:LEU:HD22	1:C:441:LEU:HA	1.85	0.44
1:C:567:ILE:HG21	1:C:609:GLN:HG2	1.99	0.44
1:D:290:LYS:HG2	1:D:291:ARG:N	2.33	0.44
1:D:324:THR:O	1:D:328:ALA:N	2.41	0.44
1:D:723:LEU:HD23	1:D:723:LEU:HA	1.83	0.44
1:E:452:ASP:N	1:E:452:ASP:OD1	2.51	0.44
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:LEU:O	1:B:674:VAL:HG23	2.18	0.44
1:C:342:ARG:O	1:C:343:CYS:C	2.61	0.44
1:D:206:ARG:NH1	1:D:248:LEU:N	2.65	0.44
1:D:273:ASN:OD1	1:D:273:ASN:C	2.61	0.44
1:D:277:LEU:HB3	1:D:281:TRP:CE2	2.53	0.44
1:D:338:ALA:O	1:D:341:LEU:HD11	2.17	0.44
1:F:44:ILE:N	1:F:47:PHE:O	2.42	0.44
1:F:309:ALA:HA	1:F:312:ALA:HB3	2.00	0.44
1:C:519:MET:HG2	1:C:534:TYR:CE2	2.51	0.43
1:E:105:ARG:HG2	1:E:221:PHE:CE1	2.53	0.43
1:E:271:MET:HE3	1:E:276:TRP:HB2	2.00	0.43
1:E:706:GLU:OE2	1:E:713:ASN:N	2.50	0.43
1:A:149:ARG:HA	1:A:149:ARG:HD3	1.87	0.43
1:A:459:VAL:HG21	1:B:145:TYR:HE1	1.83	0.43
1:B:246:LEU:HD22	1:B:336:ASN:HB3	2.00	0.43
1:C:89:TRP:CB	1:C:342:ARG:HH11	2.31	0.43
1:D:98:LEU:HD21	1:D:113:PHE:CZ	2.53	0.43
1:D:220:ARG:HD2	1:D:225:ILE:O	2.18	0.43
1:E:344:PRO:HG3	1:E:350:LEU:HB2	2.01	0.43
1:F:77:ILE:H	1:F:77:ILE:HG13	1.42	0.43
1:B:99:PRO:HD2	1:B:100:PHE:CE2	2.53	0.43
1:B:118:LEU:O	1:B:122:VAL:HG23	2.17	0.43
1:C:705:LEU:O	1:C:709:THR:HG22	2.18	0.43
1:E:47:PHE:O	1:E:48:CYS:HB2	2.17	0.43
1:E:184:ILE:HD13	1:E:184:ILE:HA	1.86	0.43
1:E:236:GLU:N	1:E:237:PRO:HD2	2.33	0.43
1:E:304:TYR:CE2	1:E:330:GLY:HA2	2.53	0.43
1:F:102:LYS:HB2	1:F:102:LYS:HE3	1.51	0.43
1:F:646:SER:O	1:F:648:PRO:HD3	2.18	0.43
1:A:87:ASN:ND2	1:A:90:GLU:HB3	2.30	0.43
1:C:589:GLN:H	1:C:589:GLN:HG3	1.56	0.43
1:E:225:ILE:HD13	1:E:322:LEU:HD22	2.01	0.43
1:E:515:LEU:O	1:E:519:MET:HG2	2.19	0.43
1:F:118:LEU:HA	1:F:121:ASN:HB2	2.00	0.43
1:A:327:LYS:O	1:A:331:TYR:N	2.52	0.43
1:D:117:PHE:O	1:D:121:ASN:N	2.51	0.43
1:D:206:ARG:HH12	1:D:248:LEU:HG	1.83	0.43
1:D:206:ARG:O	1:D:210:THR:HG22	2.18	0.43
1:E:273:ASN:OD1	1:E:275:VAL:HB	2.18	0.43
1:F:104:GLU:HG2	1:F:105:ARG:H	1.83	0.43
1:A:83:TRP:CE2	1:A:351:CYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:SER:O	1:A:154:THR:OG1	2.36	0.43
1:B:83:TRP:CD2	1:B:344:PRO:HG2	2.53	0.43
1:B:112:ILE:HG21	1:B:214:PHE:HZ	1.82	0.43
1:B:293:VAL:HA	1:B:296:VAL:HG22	2.01	0.43
1:B:539:ARG:HG3	1:B:539:ARG:HH11	1.82	0.43
1:C:93:PHE:HB2	1:C:339:TRP:CE2	2.53	0.43
1:D:231:GLU:O	1:D:234:ARG:N	2.52	0.43
1:D:329:GLN:HA	1:D:332:GLN:HG2	2.01	0.43
1:E:213:PRO:HA	1:E:216:ASP:HB3	2.01	0.43
1:F:723:LEU:HD23	1:F:723:LEU:HA	1.89	0.43
1:B:446:VAL:HG11	1:B:608:PHE:CZ	2.54	0.43
1:C:724:LYS:HA	1:C:724:LYS:HD2	1.87	0.43
1:E:159:SER:HB2	1:F:718:LEU:HD23	2.00	0.43
1:E:183:MET:HE3	1:E:214:PHE:CD1	2.54	0.43
1:F:698:ILE:HG21	1:F:720:ILE:HD11	2.00	0.43
1:A:322:LEU:HA	1:A:325:TYR:HB3	2.01	0.43
1:B:285:ASN:OD1	1:B:287:GLU:N	2.48	0.43
1:C:220:ARG:HH22	1:C:232:GLN:CD	2.26	0.43
1:D:213:PRO:O	1:D:216:ASP:HB3	2.18	0.43
1:D:614:TYR:HB2	1:D:687:THR:HG21	2.00	0.43
1:E:619:GLU:O	1:E:621:TYR:N	2.51	0.43
1:F:351:CYS:O	1:F:354:ALA:N	2.52	0.43
1:B:32:THR:C	1:B:34:SER:N	2.77	0.43
1:B:607:PHE:HD1	1:B:694:LEU:HB2	1.82	0.43
1:B:630:ASP:O	1:B:635:LYS:N	2.51	0.43
1:C:90:GLU:OE2	1:C:342:ARG:CZ	2.67	0.43
1:C:151:ILE:HG13	1:C:152:LEU:N	2.33	0.43
1:E:182:GLU:O	1:E:186:THR:N	2.45	0.43
1:F:454:LEU:HD21	1:F:597:LEU:HD21	1.99	0.43
1:A:448:GLU:CD	1:A:448:GLU:N	2.77	0.43
1:A:668:VAL:O	1:A:672:GLU:HG2	2.18	0.43
1:B:706:GLU:OE1	1:B:717:ARG:NH2	2.52	0.43
1:C:462:ASP:OD2	1:C:466:ASN:ND2	2.52	0.43
1:C:652:GLN:O	1:C:656:ILE:HG12	2.19	0.43
1:D:258:GLU:HG3	1:D:259:TRP:N	2.34	0.43
1:D:348:PRO:O	1:D:350:LEU:N	2.52	0.43
1:D:493:ARG:HA	1:D:493:ARG:HD3	1.64	0.43
1:E:27:PHE:HD2	1:E:322:LEU:HB2	1.84	0.43
1:F:249:ALA:O	1:F:253:PHE:HB2	2.19	0.43
1:A:219:MET:HB3	1:A:325:TYR:HE1	1.84	0.42
1:A:426:LEU:HD22	1:A:426:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:GLY:O	1:A:684:ILE:N	2.52	0.42
1:B:85:SER:HA	1:B:339:TRP:CZ2	2.54	0.42
1:C:352:LYS:HA	1:C:352:LYS:HD2	1.83	0.42
1:D:442:PRO:HD3	1:D:495:ARG:NH2	2.33	0.42
1:E:54:ARG:HG3	1:E:331:TYR:CE2	2.54	0.42
1:F:351:CYS:O	1:F:352:LYS:C	2.62	0.42
1:A:90:GLU:HB2	1:A:342:ARG:HB3	2.00	0.42
1:A:196:PHE:HB3	1:A:281:TRP:NE1	2.34	0.42
1:B:312:ALA:O	1:B:317:LYS:HG2	2.19	0.42
1:C:163:LEU:HD21	1:D:718:LEU:HA	2.00	0.42
1:D:253:PHE:CD1	1:D:340:SER:HB3	2.53	0.42
1:F:460:LEU:HD21	1:F:585:ILE:HG13	2.00	0.42
1:A:218:LEU:O	1:A:222:GLY:N	2.53	0.42
1:A:328:ALA:HA	1:A:331:TYR:HB2	2.01	0.42
1:B:169:ASP:HB3	1:B:221:PHE:HE1	1.83	0.42
1:D:235:ILE:HD12	1:D:322:LEU:HD11	2.00	0.42
1:D:95:ALA:O	1:D:99:PRO:HB3	2.20	0.42
1:D:258:GLU:OE1	1:D:273:ASN:ND2	2.44	0.42
1:E:211:GLY:O	1:E:215:VAL:HG23	2.19	0.42
1:F:529:ARG:O	1:F:533:ILE:HG13	2.19	0.42
1:A:257:ILE:HD12	1:A:257:ILE:H	1.85	0.42
1:B:58:HIS:HB3	1:B:60:HIS:CE1	2.55	0.42
1:B:277:LEU:HB3	1:B:281:TRP:CE2	2.55	0.42
1:C:245:ALA:HB3	1:C:333:VAL:HG11	2.01	0.42
1:C:454:LEU:HB2	1:C:582:MET:HE1	2.01	0.42
1:D:241:PRO:O	1:D:300:TYR:HB3	2.20	0.42
1:E:253:PHE:CE2	1:E:341:LEU:HA	2.55	0.42
1:E:323:GLN:HA	1:E:326:LEU:HB2	2.00	0.42
1:F:35:SER:H	1:F:55:ARG:H	1.68	0.42
1:F:56:HIS:HD2	1:F:59:GLU:HB2	1.85	0.42
1:F:537:GLU:HB2	1:F:577:LEU:HD13	2.01	0.42
1:F:615:LYS:HB2	1:F:615:LYS:HE2	1.82	0.42
1:A:212:ALA:HB3	1:A:243:TYR:CD1	2.54	0.42
1:B:257:ILE:O	1:B:261:GLU:N	2.43	0.42
1:C:98:LEU:HD23	1:C:219:MET:HE3	2.02	0.42
1:C:220:ARG:NH2	1:C:232:GLN:OE1	2.51	0.42
1:C:299:GLN:O	1:C:303:GLN:HB3	2.19	0.42
1:C:534:TYR:HD1	1:C:577:LEU:HD11	1.85	0.42
1:E:56:HIS:HD2	1:E:106:LEU:HD13	1.84	0.42
1:E:252:TYR:C	1:E:252:TYR:CD1	2.98	0.42
1:E:619:GLU:O	1:E:620:GLU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:VAL:O	1:F:112:ILE:HG13	2.19	0.42
1:B:234:ARG:O	1:B:237:PRO:HD2	2.20	0.42
1:B:618:THR:O	1:B:619:GLU:HG2	2.19	0.42
1:C:292:ARG:HD2	1:C:292:ARG:HA	1.68	0.42
1:C:490:PRO:O	1:C:491:LEU:HD23	2.20	0.42
1:D:43:ASP:HA	1:D:47:PHE:O	2.19	0.42
1:E:156:GLN:NE2	1:F:712:PRO:O	2.53	0.42
1:E:279:MET:HE1	1:E:285:ASN:C	2.45	0.42
1:E:617:LEU:HD12	1:E:639:PRO:HG2	2.02	0.42
1:F:220:ARG:O	1:F:224:GLY:N	2.53	0.42
1:C:71:THR:O	1:C:75:GLN:N	2.52	0.42
1:C:343:CYS:HB3	1:C:346:TYR:HE1	1.83	0.42
1:D:82:ARG:HB3	1:D:345:ARG:HH12	1.84	0.42
1:D:262:PHE:CD1	1:D:268:LYS:HE2	2.55	0.42
1:D:357:LEU:O	1:D:361:ASP:N	2.32	0.42
1:E:89:TRP:CH2	1:E:350:LEU:HB3	2.55	0.42
1:F:165:LEU:HD21	1:F:173:ALA:HB1	2.02	0.42
1:A:683:SER:OG	1:A:684:ILE:N	2.52	0.42
1:B:248:LEU:HA	1:B:251:ASP:HB2	2.01	0.42
1:B:564:LEU:HD23	1:B:567:ILE:HD11	2.02	0.42
1:C:227:LEU:HD22	1:C:231:GLU:HG3	2.00	0.42
1:C:486:GLU:HB3	1:D:505:GLU:HG3	2.02	0.42
1:D:280:GLN:HE21	1:D:280:GLN:HB2	1.65	0.42
1:E:157:ILE:O	1:E:160:LYS:HB3	2.20	0.42
1:E:216:ASP:OD2	1:E:325:TYR:OH	2.36	0.42
1:F:262:PHE:O	1:F:266:SER:HA	2.19	0.42
1:F:588:VAL:HG12	1:F:591:LYS:HD3	2.02	0.42
1:A:495:ARG:HE	1:A:495:ARG:HB3	1.65	0.42
1:A:525:LEU:HD22	1:A:585:ILE:HD13	2.02	0.42
1:B:227:LEU:HD11	1:B:325:TYR:CE2	2.54	0.42
1:C:458:LEU:HA	1:C:590:GLN:CD	2.45	0.42
1:D:214:PHE:CG	1:D:218:LEU:HD11	2.55	0.42
1:E:56:HIS:CE1	1:E:101:CYS:HB2	2.55	0.42
1:F:35:SER:OG	1:F:55:ARG:NH2	2.53	0.42
1:F:47:PHE:HE1	1:F:337:VAL:HG13	1.85	0.42
1:A:247:GLY:O	1:A:251:ASP:N	2.42	0.41
1:A:723:LEU:HD12	1:A:723:LEU:HA	1.89	0.41
1:B:183:MET:SD	1:B:211:GLY:HA3	2.60	0.41
1:B:350:LEU:O	1:B:351:CYS:C	2.63	0.41
1:B:515:LEU:HD22	1:B:538:MET:HE1	2.02	0.41
1:C:48:CYS:HB2	1:C:301:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:PRO:HA	1:C:216:ASP:HB3	2.02	0.41
1:D:235:ILE:HA	1:D:238:ILE:HD12	2.01	0.41
1:E:220:ARG:O	1:E:225:ILE:N	2.41	0.41
1:F:301:GLU:O	1:F:305:LEU:N	2.34	0.41
1:A:182:GLU:O	1:A:186:THR:OG1	2.26	0.41
1:A:262:PHE:CD1	1:A:271:MET:HG3	2.55	0.41
1:A:301:GLU:HA	1:A:304:TYR:CE2	2.55	0.41
1:C:143:THR:HG23	1:C:146:ARG:HH21	1.86	0.41
1:C:495:ARG:HE	1:C:495:ARG:HB3	1.63	0.41
1:E:519:MET:HE2	1:E:534:TYR:CE2	2.55	0.41
1:E:588:VAL:CG1	1:E:589:GLN:H	2.21	0.41
1:F:358:LEU:O	1:F:362:THR:N	2.42	0.41
1:A:552:THR:HG21	1:A:635:LYS:HE2	2.02	0.41
1:D:253:PHE:CE1	1:D:340:SER:HB3	2.55	0.41
1:E:282:GLU:HG3	1:E:292:ARG:NH1	2.36	0.41
1:E:356:SER:HA	1:E:359:HIS:CE1	2.55	0.41
1:E:557:CYS:HA	1:E:558:PRO:HD3	1.95	0.41
1:F:114:GLU:O	1:F:118:LEU:HG	2.19	0.41
1:F:519:MET:HE2	1:F:534:TYR:CE2	2.49	0.41
1:F:607:PHE:CE2	1:F:723:LEU:HD13	2.55	0.41
1:A:152:LEU:HD12	1:B:459:VAL:HG13	2.02	0.41
1:A:352:LYS:HD3	1:A:352:LYS:H	1.84	0.41
1:B:31:SER:O	1:B:33:LEU:N	2.53	0.41
1:B:88:PRO:HD2	1:B:89:TRP:CZ3	2.56	0.41
1:B:319:ASN:O	1:B:323:GLN:N	2.53	0.41
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.84	0.41
1:C:298:LYS:O	1:C:299:GLN:C	2.63	0.41
1:C:350:LEU:HD22	1:C:353:GLU:OE1	2.21	0.41
1:C:457:TRP:HH2	1:C:702:VAL:HG23	1.85	0.41
1:C:582:MET:HE3	1:C:582:MET:HB3	1.89	0.41
1:D:291:ARG:O	1:D:294:GLN:HG2	2.20	0.41
1:E:104:GLU:HG2	1:E:105:ARG:HD2	2.02	0.41
1:E:614:TYR:HB2	1:E:687:THR:HG21	2.03	0.41
1:A:262:PHE:HE2	1:A:268:LYS:O	2.04	0.41
1:B:258:GLU:HA	1:B:261:GLU:HB3	2.03	0.41
1:B:321:LYS:H	1:B:321:LYS:HG3	1.63	0.41
1:D:271:MET:HE3	1:D:276:TRP:CB	2.51	0.41
1:F:89:TRP:HH2	1:F:350:LEU:HD13	1.86	0.41
1:F:206:ARG:NH2	1:F:244:ALA:O	2.54	0.41
1:B:70:ARG:O	1:B:74:GLU:HG2	2.21	0.41
1:B:93:PHE:HB2	1:B:339:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ARG:HG3	1:D:225:ILE:HB	2.01	0.41
1:D:334:PRO:HA	1:D:337:VAL:HG22	2.02	0.41
1:D:600:LEU:HD11	1:D:698:ILE:HG23	2.02	0.41
1:E:588:VAL:HG12	1:E:589:GLN:N	2.23	0.41
1:F:202:TYR:CE2	1:F:206:ARG:HD2	2.55	0.41
1:F:220:ARG:HH22	1:F:321:LYS:HZ3	1.69	0.41
1:A:105:ARG:NH1	1:A:221:PHE:O	2.54	0.41
1:A:175:VAL:HG11	1:A:226:MET:SD	2.60	0.41
1:A:199:LEU:HD21	1:A:300:TYR:OH	2.20	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.78	0.41
1:A:262:PHE:HE1	1:A:271:MET:HA	1.73	0.41
1:A:684:ILE:H	1:A:684:ILE:HG12	1.43	0.41
1:B:43:ASP:HA	1:B:47:PHE:O	2.21	0.41
1:C:143:THR:O	1:C:147:THR:OG1	2.37	0.41
1:F:355:ALA:O	1:F:359:HIS:N	2.45	0.41
1:A:256:ASP:OD1	1:A:256:ASP:N	2.54	0.41
1:B:667:ASP:OD1	1:B:667:ASP:N	2.53	0.41
1:C:98:LEU:HD23	1:C:98:LEU:HA	1.96	0.41
1:D:298:LYS:O	1:D:302:GLN:N	2.54	0.41
1:E:519:MET:HA	1:E:522:VAL:HB	2.03	0.41
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.83	0.41
1:A:196:PHE:HD2	1:A:277:LEU:HD22	1.86	0.41
1:A:298:LYS:HG3	1:A:302:GLN:HG3	2.03	0.41
1:B:213:PRO:HA	1:B:216:ASP:HB3	2.01	0.41
1:B:691:MET:HB2	1:B:691:MET:HE2	1.80	0.41
1:C:141:ASP:HB3	1:C:144:GLU:HB2	2.02	0.41
1:C:292:ARG:HH11	1:C:295:GLU:HB3	1.86	0.41
1:C:448:GLU:HB3	1:C:469:LYS:HD3	2.02	0.41
1:D:85:SER:HA	1:D:339:TRP:CZ2	2.56	0.41
1:E:56:HIS:HA	1:E:99:PRO:O	2.20	0.41
1:E:285:ASN:OD1	1:E:287:GLU:N	2.54	0.41
1:E:287:GLU:HA	1:E:290:LYS:HG2	2.03	0.41
1:E:438:ILE:HD12	1:E:438:ILE:HA	1.94	0.41
1:E:475:LEU:HD12	1:E:475:LEU:HA	1.81	0.41
1:F:146:ARG:HH11	1:F:146:ARG:HB3	1.86	0.41
1:F:241:PRO:HG2	1:F:304:TYR:CD2	2.56	0.41
1:F:451:ILE:HG23	1:F:582:MET:SD	2.61	0.41
1:F:519:MET:O	1:F:523:ARG:HB2	2.20	0.41
1:A:438:ILE:HD12	1:A:438:ILE:HA	1.92	0.41
1:B:62:ALA:O	1:B:92:HIS:NE2	2.54	0.41
1:D:216:ASP:OD1	1:D:220:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ALA:HB2	1:D:300:TYR:CB	2.51	0.41
1:D:285:ASN:O	1:D:286:ALA:C	2.64	0.41
1:A:44:ILE:O	1:A:47:PHE:HB2	2.20	0.40
1:B:206:ARG:HA	1:B:206:ARG:HD3	1.86	0.40
1:B:229:GLN:CD	1:B:229:GLN:H	2.29	0.40
1:B:258:GLU:HG3	1:B:271:MET:HB2	2.03	0.40
1:B:428:ASP:C	1:B:430:HIS:N	2.79	0.40
1:B:539:ARG:HG3	1:B:539:ARG:NH1	2.36	0.40
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.74	0.40
1:E:535:LEU:HD23	1:F:516:ILE:HG23	2.03	0.40
1:F:323:GLN:O	1:F:327:LYS:HB2	2.21	0.40
1:F:568:ARG:NH2	1:F:606:GLU:OE1	2.53	0.40
1:A:255:PHE:CD1	1:A:271:MET:HE1	2.56	0.40
1:D:36:VAL:HA	1:D:54:ARG:HA	2.03	0.40
1:E:249:ALA:CB	1:E:337:VAL:HG22	2.51	0.40
1:F:77:ILE:HD13	1:F:154:THR:HG22	2.02	0.40
1:F:268:LYS:HD3	1:F:271:MET:CE	2.47	0.40
1:A:183:MET:HE2	1:A:183:MET:HB3	1.83	0.40
1:A:486:GLU:HG2	1:B:505:GLU:HG3	2.03	0.40
1:D:238:ILE:HG23	1:D:311:PHE:CG	2.56	0.40
1:D:606:GLU:O	1:D:610:VAL:HG23	2.21	0.40
1:D:614:TYR:O	1:D:614:TYR:HD2	2.04	0.40
1:E:177:ILE:O	1:E:181:LYS:N	2.29	0.40
1:E:179:SER:C	1:E:183:MET:HE2	2.46	0.40
1:E:292:ARG:HG3	1:E:296:VAL:CG1	2.52	0.40
1:A:28:ILE:HA	1:A:324:THR:H	1.87	0.40
1:A:70:ARG:HH12	1:A:84:GLY:H	1.67	0.40
1:A:539:ARG:HH11	1:B:513:PHE:HZ	1.68	0.40
1:B:102:LYS:HE2	1:B:102:LYS:HB2	1.82	0.40
1:C:61:LEU:HA	1:C:64:GLU:HG3	2.03	0.40
1:E:616:ASN:OD1	1:E:621:TYR:HB3	2.21	0.40
1:F:281:TRP:HB2	1:F:282:GLU:OE2	2.21	0.40
1:A:49:SER:C	1:A:305:LEU:HB3	2.46	0.40
1:A:89:TRP:CH2	1:A:350:LEU:HB3	2.56	0.40
1:A:297:THR:HA	1:A:300:TYR:HB2	2.04	0.40
1:C:559:SER:OG	1:C:562:GLN:HG3	2.22	0.40
1:D:98:LEU:HB2	1:D:101:CYS:SG	2.61	0.40
1:E:56:HIS:NE2	1:E:101:CYS:HB2	2.36	0.40
1:E:172:ARG:HD2	1:E:221:PHE:HD1	1.87	0.40
1:E:214:PHE:O	1:E:218:LEU:HG	2.21	0.40
1:F:718:LEU:O	1:F:718:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	556/725 (77%)	519 (93%)	32 (6%)	5 (1%)	14	47
1	B	585/725 (81%)	532 (91%)	47 (8%)	6 (1%)	13	45
1	C	559/725 (77%)	521 (93%)	35 (6%)	3 (0%)	25	58
1	D	575/725 (79%)	532 (92%)	42 (7%)	1 (0%)	44	73
1	E	577/725 (80%)	540 (94%)	28 (5%)	9 (2%)	8	35
1	F	592/725 (82%)	552 (93%)	34 (6%)	6 (1%)	13	45
All	All	3444/4350 (79%)	3196 (93%)	218 (6%)	30 (1%)	17	47

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ASP
1	A	459	VAL
1	C	459	VAL
1	E	619	GLU
1	F	32	THR
1	F	266	SER
1	F	351	CYS
1	F	589	GLN
1	A	588	VAL
1	A	683	SER
1	B	32	THR
1	B	266	SER
1	D	316	GLY
1	E	588	VAL
1	E	589	GLN
1	E	620	GLU
1	F	301	GLU

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Mol	Chain	Res	Type
1	F	588	VAL
1	A	29	LEU
1	B	31	SER
1	B	351	CYS
1	C	58	HIS
1	C	60	HIS
1	E	43	ASP
1	E	318	GLU
1	B	33	LEU
1	E	44	ILE
1	E	317	LYS
1	E	320	ILE
1	B	459	VAL

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	A	503/638 (79%)	468 (93%)	35 (7%)	12	39
1	B	524/638 (82%)	484 (92%)	40 (8%)	11	36
1	C	505/638 (79%)	463 (92%)	42 (8%)	9	32
1	D	519/638 (81%)	476 (92%)	43 (8%)	9	32
1	E	518/638 (81%)	479 (92%)	39 (8%)	11	37
1	F	532/638 (83%)	482 (91%)	50 (9%)	7	26
All	All	3101/3828 (81%)	2852 (92%)	249 (8%)	12	34

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	80	ILE
1	A	96	VAL
1	A	102	LYS
1	A	110	CYS

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Mol	Chain	Res	Type
1	A	154	THR
1	A	158	GLN
1	A	166	LEU
1	A	172	ARG
1	A	216	ASP
1	A	217	MET
1	A	225	ILE
1	A	226	MET
1	A	256	ASP
1	A	268	LYS
1	A	280	GLN
1	A	296	VAL
1	A	305	LEU
1	A	322	LEU
1	A	323	GLN
1	A	326	LEU
1	A	341	LEU
1	A	358	LEU
1	A	426	LEU
1	A	447	ARG
1	A	475	LEU
1	A	495	ARG
1	A	556	GLU
1	A	588	VAL
1	A	631	LEU
1	A	640	LEU
1	A	649	LYS
1	A	675	LEU
1	A	683	SER
1	A	684	ILE
1	B	30	ASN
1	B	33	LEU
1	B	48	CYS
1	B	60	HIS
1	B	98	LEU
1	B	161	MET
1	B	166	LEU
1	B	172	ARG
1	B	183	MET
1	B	216	ASP
1	B	228	THR
1	B	230	GLU

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Mol	Chain	Res	Type
1	B	239	VAL
1	B	253	PHE
1	B	290	LYS
1	B	295	GLU
1	B	303	GLN
1	B	304	TYR
1	B	310	ASP
1	B	327	LYS
1	B	336	ASN
1	B	352	LYS
1	B	459	VAL
1	B	460	LEU
1	B	475	LEU
1	B	530	CYS
1	B	541	LEU
1	B	590	GLN
1	B	621	TYR
1	B	625	LYS
1	B	629	GLU
1	B	649	LYS
1	B	690	LYS
1	B	691	MET
1	B	693	GLU
1	B	695	MET
1	B	696	GLU
1	B	697	LYS
1	B	700	ASP
1	B	701	SER
1	C	56	HIS
1	C	57	HIS
1	C	58	HIS
1	C	60	HIS
1	C	80	ILE
1	C	97	VAL
1	C	140	LEU
1	C	155	LYS
1	C	162	LEU
1	C	182	GLU
1	C	208	ILE
1	C	226	MET
1	C	250	ASN
1	C	290	LYS

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Mol	Chain	Res	Type
1	C	292	ARG
1	C	293	VAL
1	C	295	GLU
1	C	296	VAL
1	C	297	THR
1	C	300	TYR
1	C	302	GLN
1	C	303	GLN
1	C	305	LEU
1	C	311	PHE
1	C	317	LYS
1	C	333	VAL
1	C	340	SER
1	C	341	LEU
1	C	441	LEU
1	C	459	VAL
1	C	460	LEU
1	C	468	LEU
1	C	486	GLU
1	C	541	LEU
1	C	559	SER
1	C	589	GLN
1	C	591	LYS
1	C	611	ARG
1	C	617	LEU
1	C	633	GLU
1	C	649	LYS
1	C	684	ILE
1	D	33	LEU
1	D	60	HIS
1	D	63	ASN
1	D	69	CYS
1	D	72	ASP
1	D	73	TRP
1	D	75	GLN
1	D	77	ILE
1	D	89	TRP
1	D	98	LEU
1	D	120	ASP
1	D	146	ARG
1	D	154	THR
1	D	174	GLU

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Mol	Chain	Res	Type
1	D	197	ASN
1	D	219	MET
1	D	226	MET
1	D	228	THR
1	D	239	VAL
1	D	256	ASP
1	D	280	GLN
1	D	285	ASN
1	D	290	LYS
1	D	295	GLU
1	D	298	LYS
1	D	302	GLN
1	D	305	LEU
1	D	308	ILE
1	D	310	ASP
1	D	315	GLU
1	D	317	LYS
1	D	342	ARG
1	D	359	HIS
1	D	428	ASP
1	D	447	ARG
1	D	506	GLN
1	D	519	MET
1	D	601	SER
1	D	649	LYS
1	D	651	VAL
1	D	672	GLU
1	D	705	LEU
1	D	720	ILE
1	E	29	LEU
1	E	43	ASP
1	E	57	HIS
1	E	58	HIS
1	E	80	ILE
1	E	86	CYS
1	E	89	TRP
1	E	90	GLU
1	E	110	CYS
1	E	148	VAL
1	E	166	LEU
1	E	183	MET
1	E	205	TYR

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Mol	Chain	Res	Type
1	E	206	ARG
1	E	226	MET
1	E	234	ARG
1	E	261	GLU
1	E	282	GLU
1	E	317	LYS
1	E	319	ASN
1	E	320	ILE
1	E	342	ARG
1	E	346	TYR
1	E	447	ARG
1	E	454	LEU
1	E	459	VAL
1	E	463	HIS
1	E	475	LEU
1	E	479	SER
1	E	531	MET
1	E	570	LYS
1	E	571	THR
1	E	593	LEU
1	E	625	LYS
1	E	631	LEU
1	E	651	VAL
1	E	671	LYS
1	E	675	LEU
1	E	720	ILE
1	F	26	ASP
1	F	33	LEU
1	F	36	VAL
1	F	61	LEU
1	F	66	SER
1	F	69	CYS
1	F	74	GLU
1	F	75	GLN
1	F	77	ILE
1	F	90	GLU
1	F	98	LEU
1	F	100	PHE
1	F	102	LYS
1	F	120	ASP
1	F	146	ARG
1	F	161	MET

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Mol	Chain	Res	Type
1	F	164	GLU
1	F	165	LEU
1	F	174	GLU
1	F	201	GLU
1	F	226	MET
1	F	227	LEU
1	F	228	THR
1	F	233	LYS
1	F	240	LYS
1	F	279	MET
1	F	292	ARG
1	F	298	LYS
1	F	301	GLU
1	F	302	GLN
1	F	303	GLN
1	F	305	LEU
1	F	307	ASN
1	F	308	ILE
1	F	317	LYS
1	F	321	LYS
1	F	324	THR
1	F	352	LYS
1	F	436	GLU
1	F	443	SER
1	F	527	ASP
1	F	530	CYS
1	F	574	LEU
1	F	584	GLN
1	F	647	GLN
1	F	667	ASP
1	F	672	GLU
1	F	691	MET
1	F	719	LEU
1	F	720	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	280	GLN
1	A	285	ASN
1	A	329	GLN

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Mol	Chain	Res	Type
1	A	332	GLN
1	A	336	ASN
1	A	466	ASN
1	A	473	GLN
1	A	476	HIS
1	A	506	GLN
1	A	596	GLN
1	A	652	GLN
1	A	677	HIS
1	A	713	ASN
1	B	30	ASN
1	B	87	ASN
1	B	283	ASN
1	B	302	GLN
1	B	347	HIS
1	B	463	HIS
1	B	466	ASN
1	B	596	GLN
1	B	658	GLN
1	C	30	ASN
1	C	56	HIS
1	C	75	GLN
1	C	329	GLN
1	C	332	GLN
1	C	336	ASN
1	C	360	GLN
1	C	476	HIS
1	C	506	GLN
1	C	545	GLN
1	C	554	ASN
1	C	590	GLN
1	C	658	GLN
1	D	56	HIS
1	D	121	ASN
1	D	263	GLN
1	D	280	GLN
1	D	329	GLN
1	D	359	HIS
1	E	56	HIS
1	E	58	HIS
1	E	63	ASN
1	E	294	GLN

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Mol	Chain	Res	Type
1	E	303	GLN
1	E	307	ASN
1	E	319	ASN
1	E	336	ASN
1	E	347	HIS
1	E	360	GLN
1	E	467	GLN
1	E	473	GLN
1	E	476	HIS
1	E	545	GLN
1	E	554	ASN
1	E	713	ASN
1	F	56	HIS
1	F	58	HIS
1	F	121	ASN
1	F	263	GLN
1	F	280	GLN
1	F	307	ASN
1	F	336	ASN
1	F	499	HIS
1	F	545	GLN

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 ⓘ

There are no ligands in this entry.

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-47453. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ
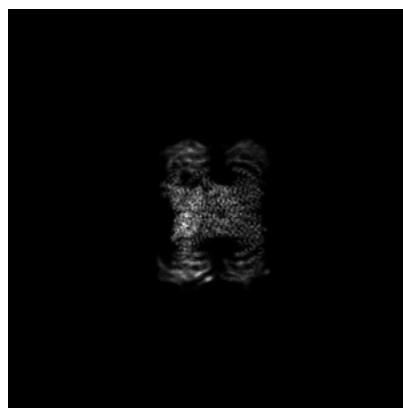
6.1.1 Primary map

X
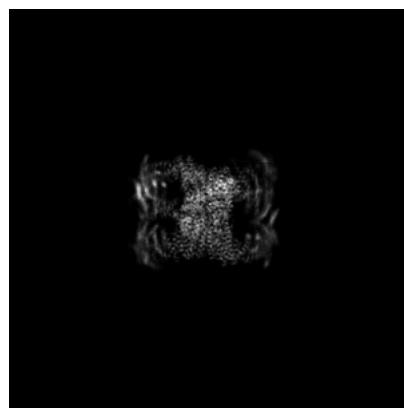
Y
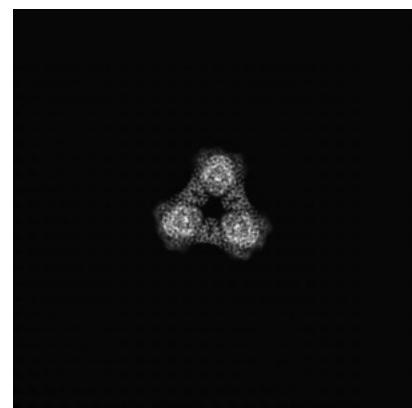
Z

6.1.2 Raw map

X

Y

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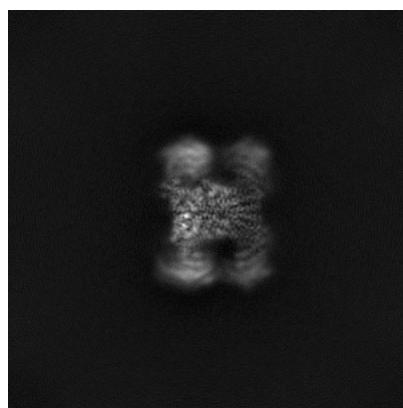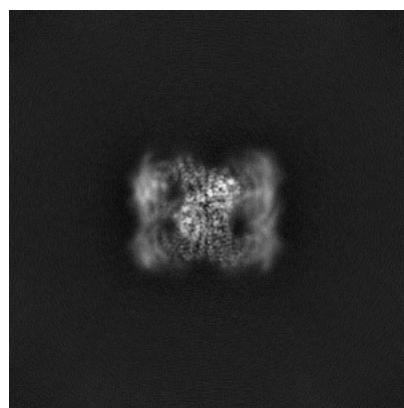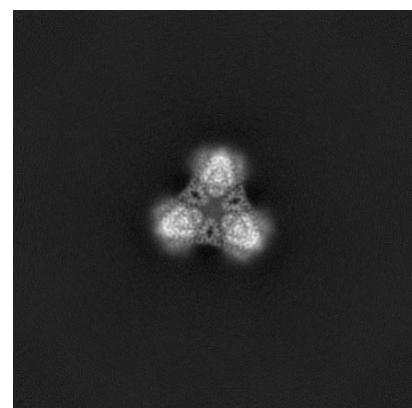
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

X Index: 192
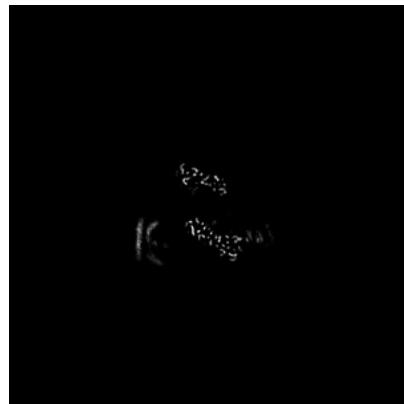
Y Index: 192
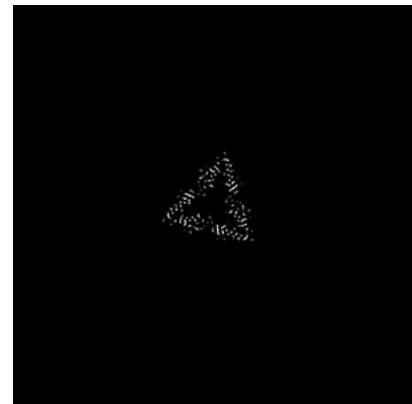
Z Index: 192

6.2.2 Raw map

X Index: 192
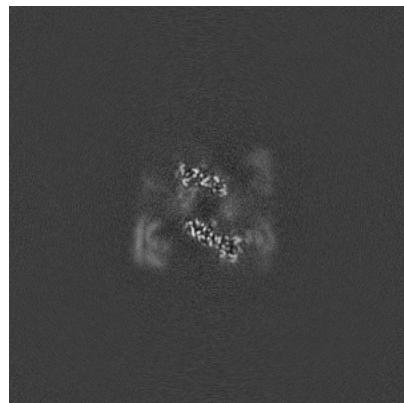
Y Index: 192
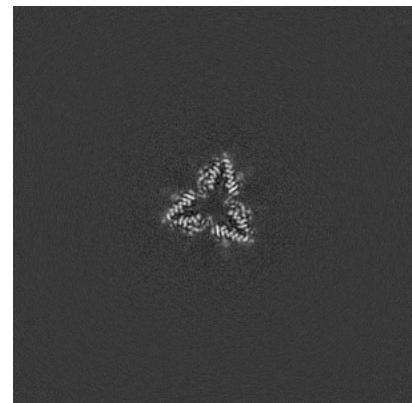
Z Index: 192

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
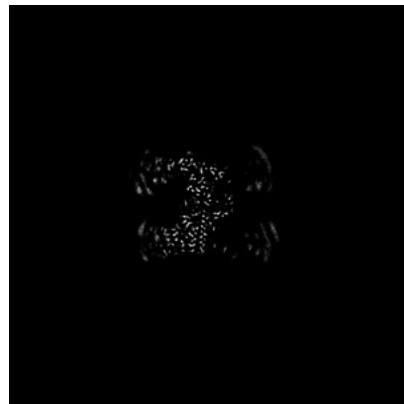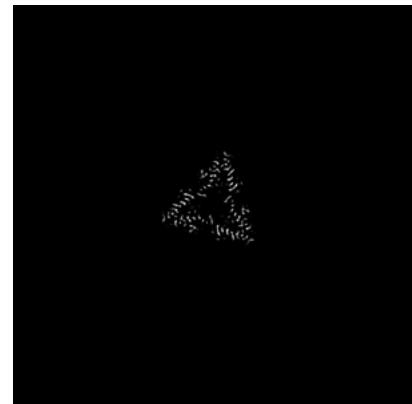
| X Index: 208 | Y Index: 170 | Z Index: 193 |

6.3.2 Raw map
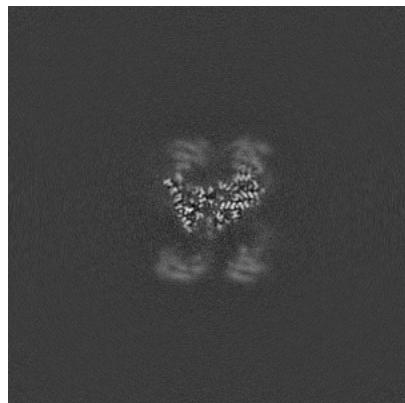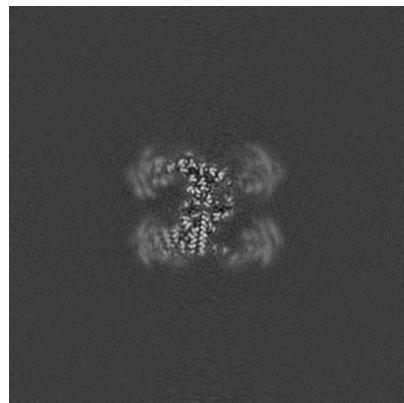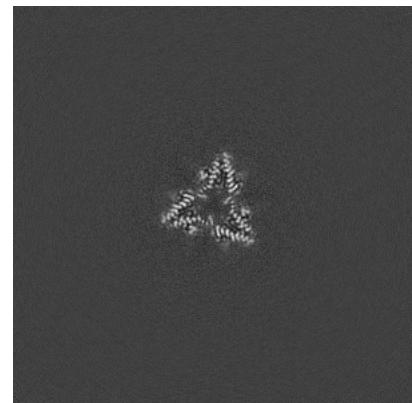
| X Index: 208 | Y Index: 170 | Z Index: 193 |

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

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

6.4.1 Primary map

| X | Y | Z |

6.4.2 Raw map

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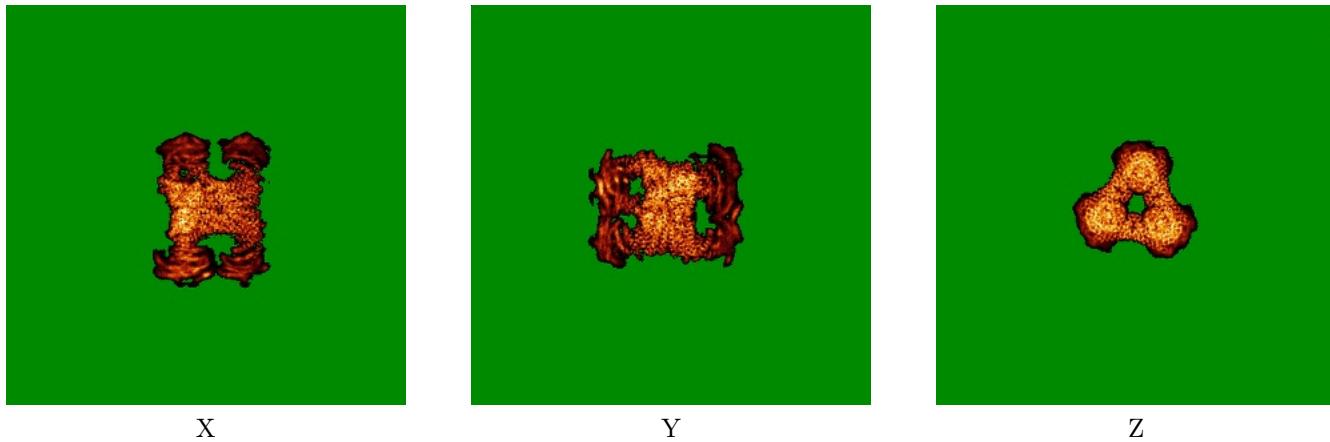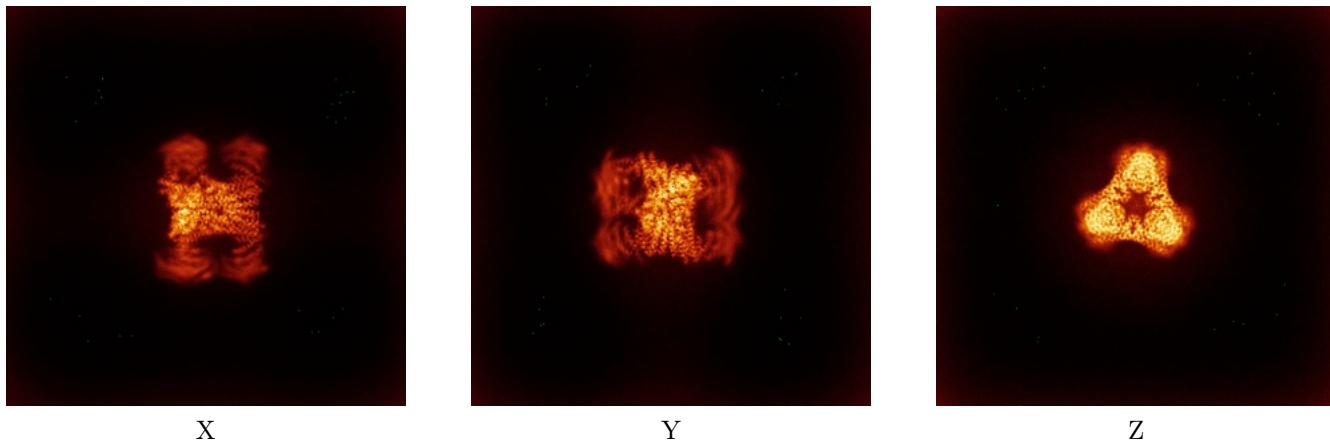
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views (i)

6.5.1   Primary map

| X | Y | Z |
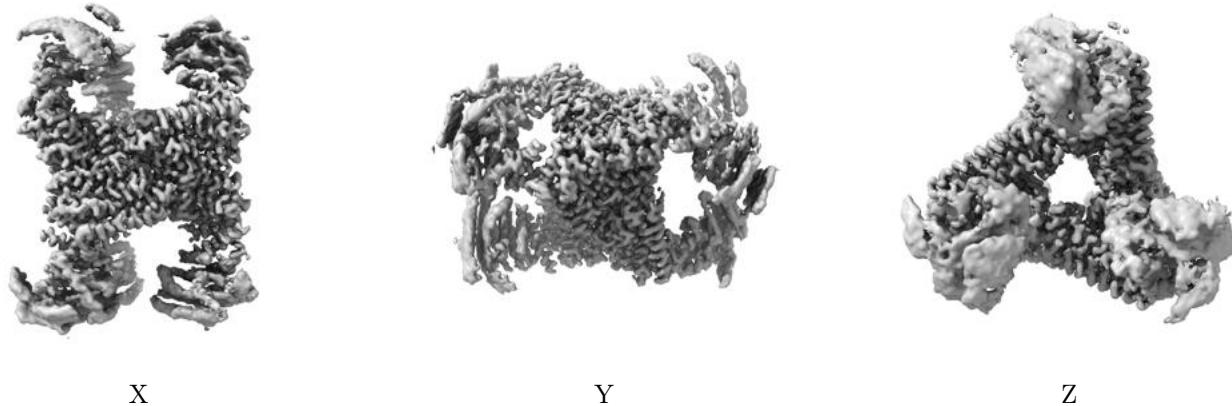
The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2   Raw map

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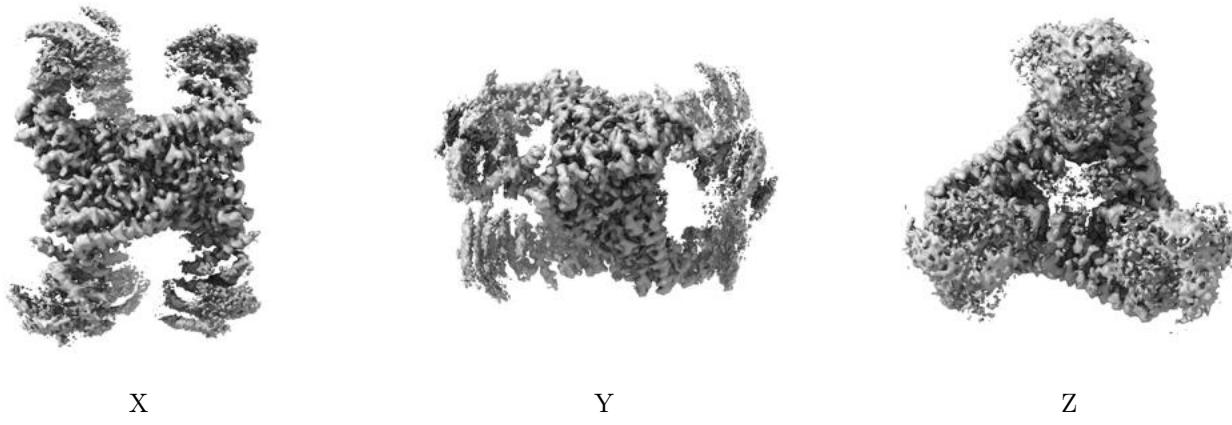
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6   Mask visualisation (i)

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

7   Map analysis ⓘ

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

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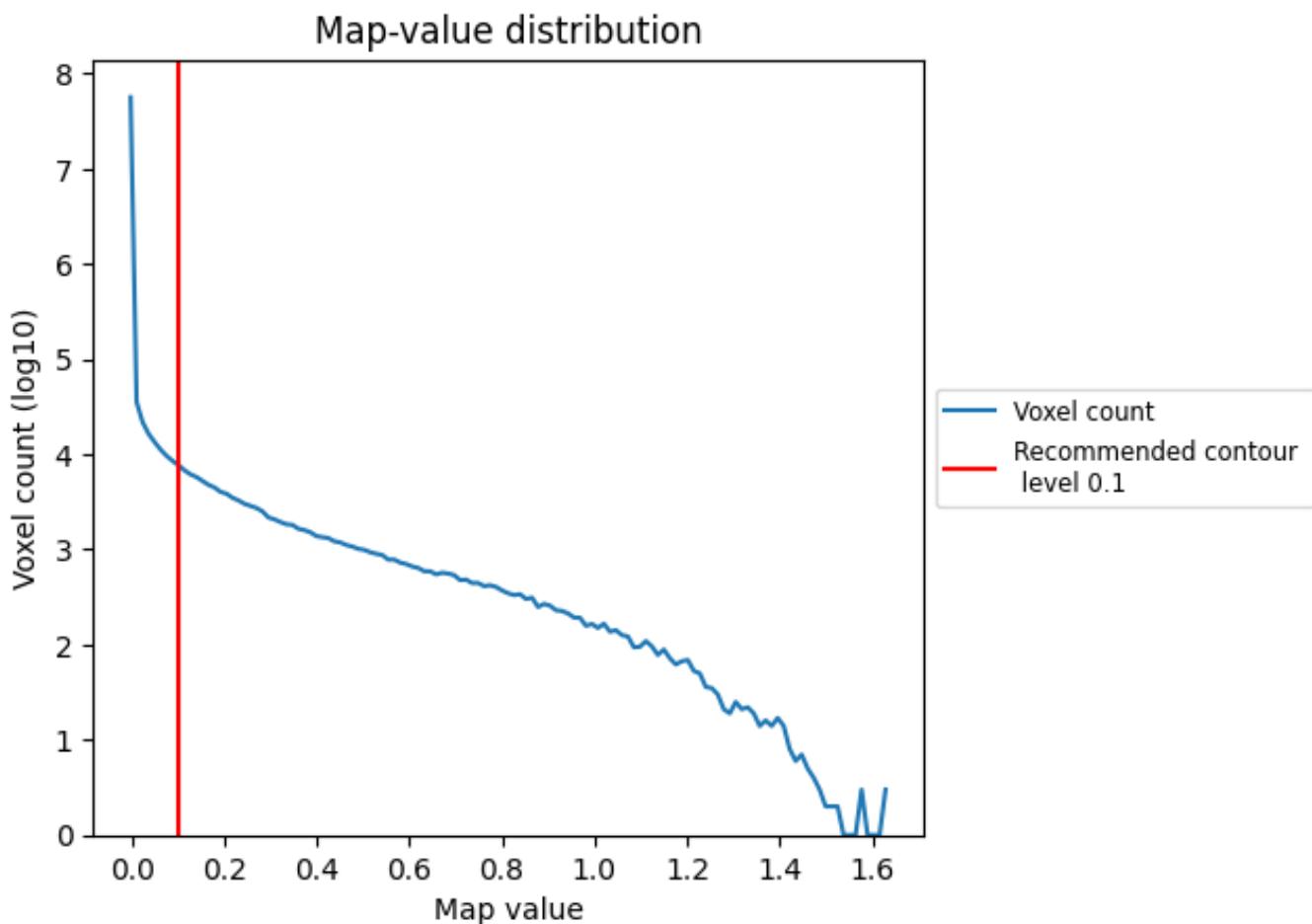
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
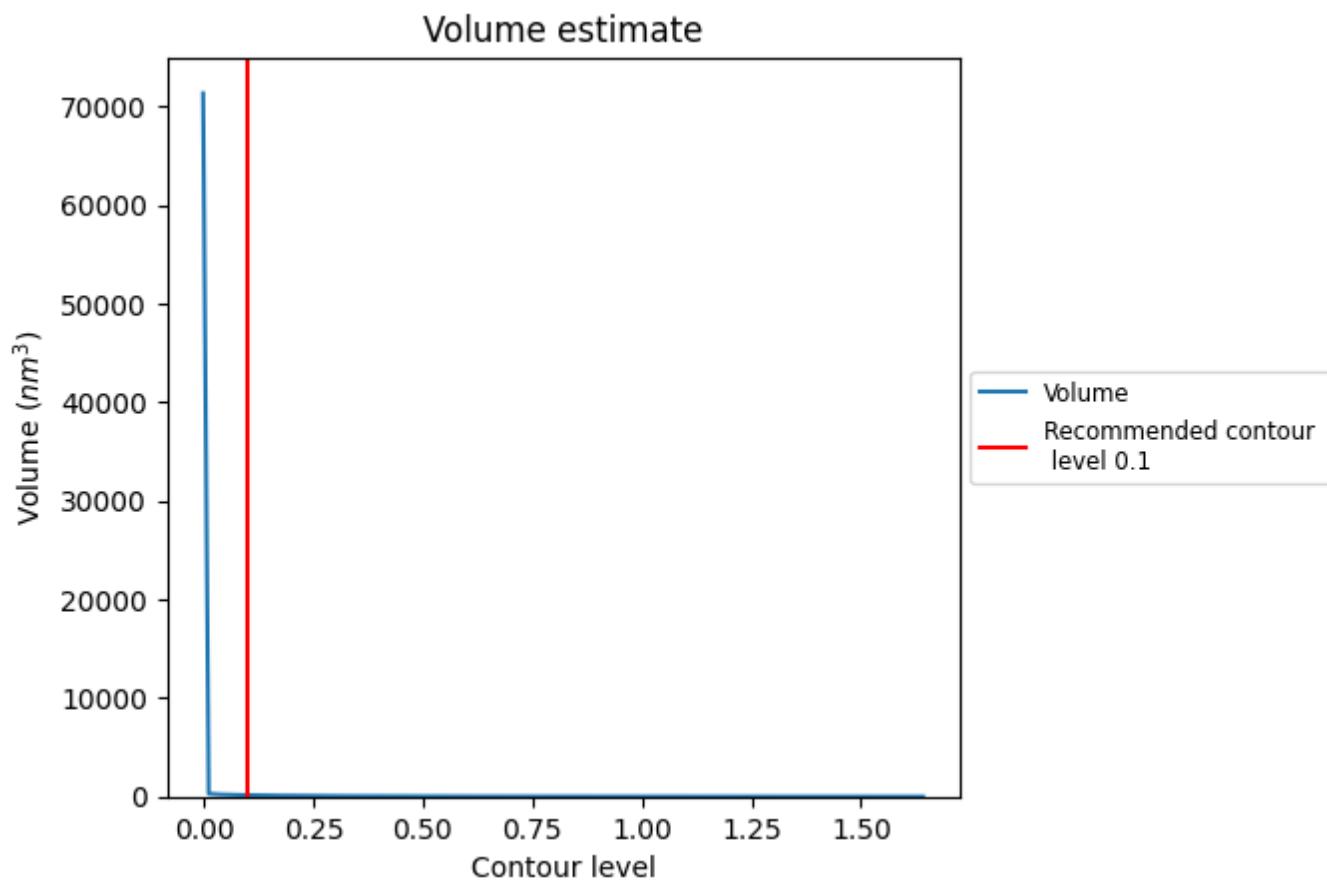
The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 129 kDa.

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 ⓘ
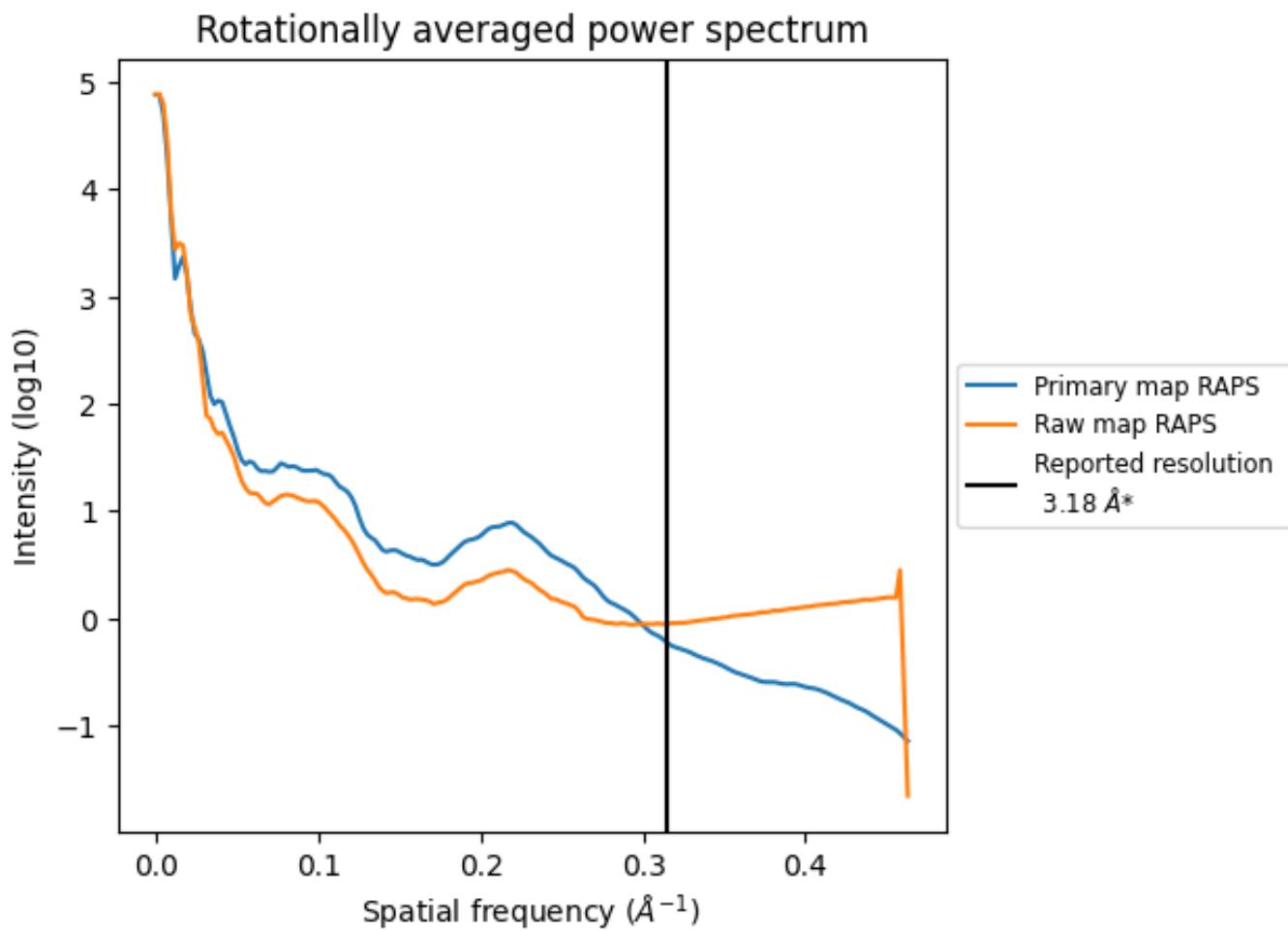
*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

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)
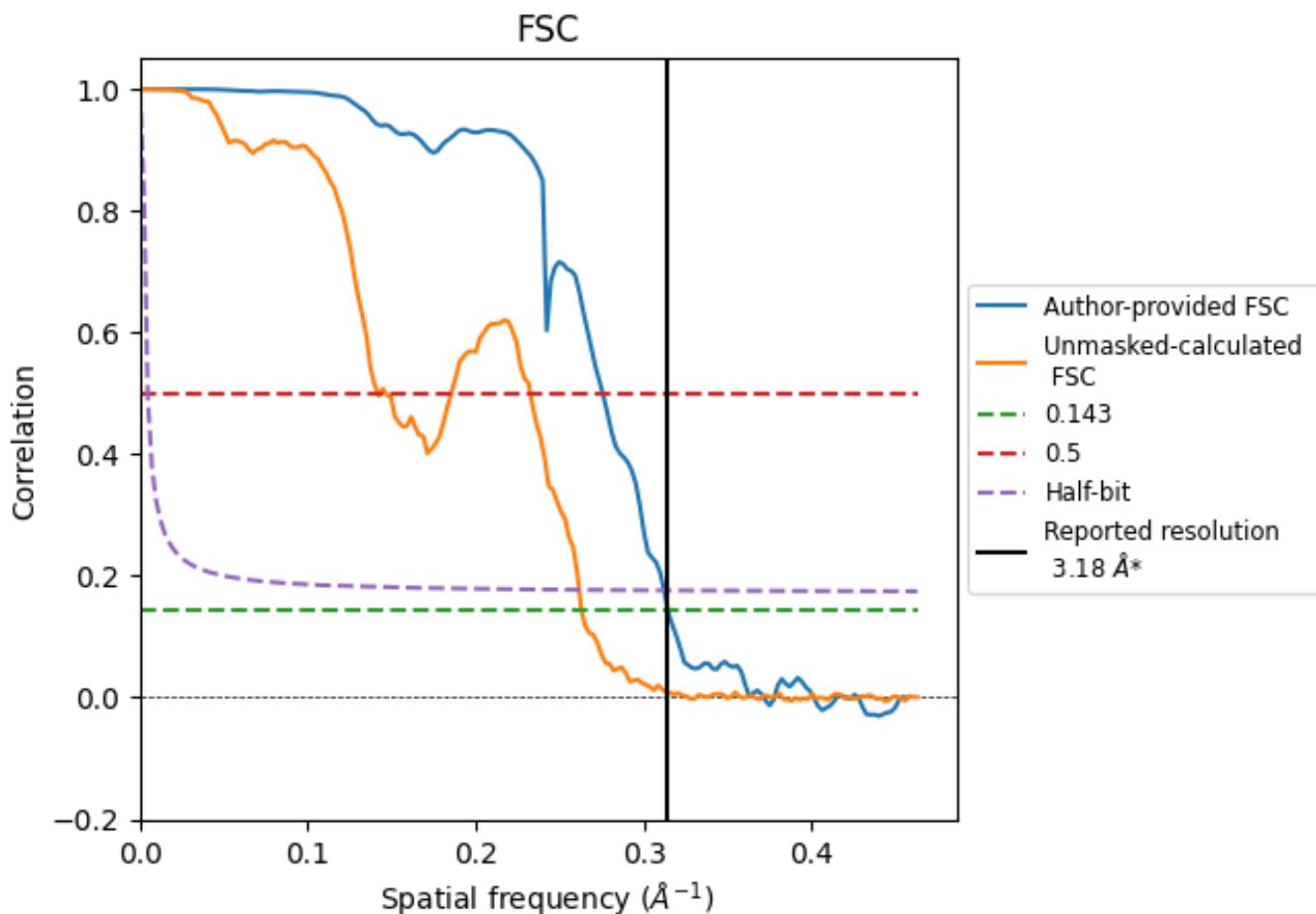
*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.63	3.20
Unmasked-calculated*	3.80	7.06	3.82

*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 3.80 differs from the reported value 3.18 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-47453 and PDB model 9E2I. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ
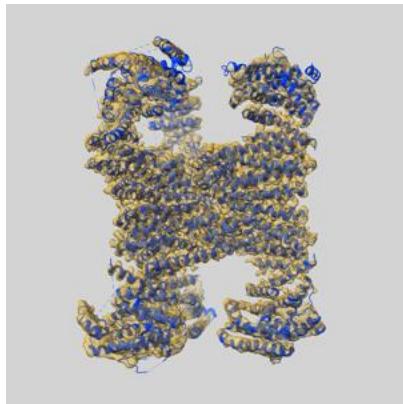
| X | Y | Z |
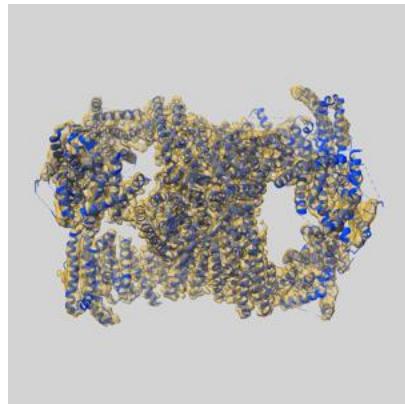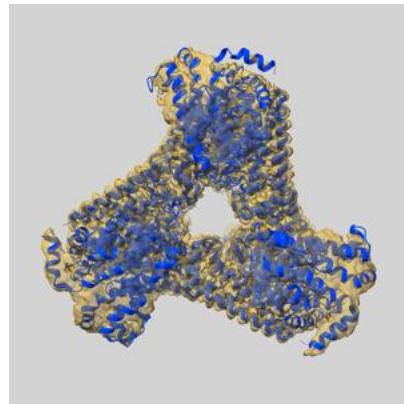
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model　ⓘ

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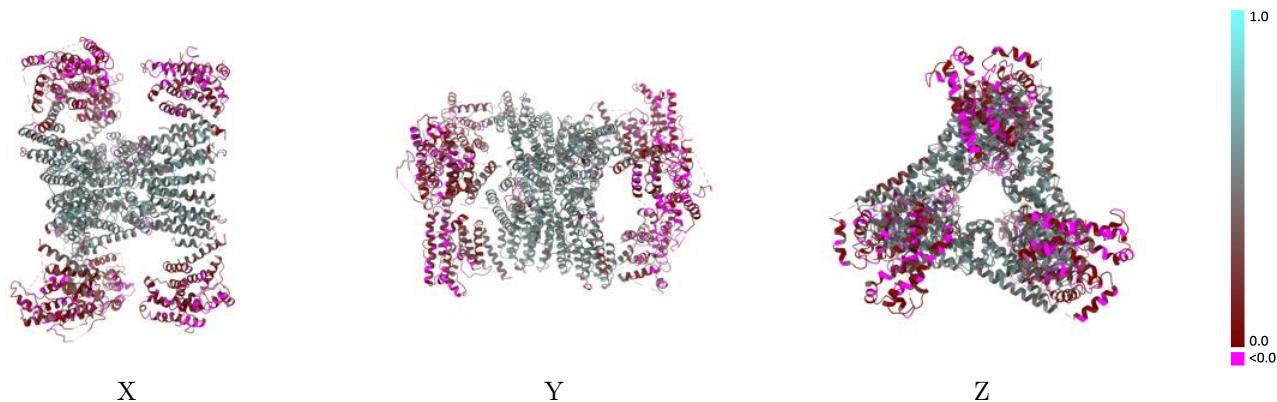
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3　Atom inclusion mapped to coordinate model　ⓘ

X　　　　　　　　　　　　Y　　　　　　　　　　　　Z
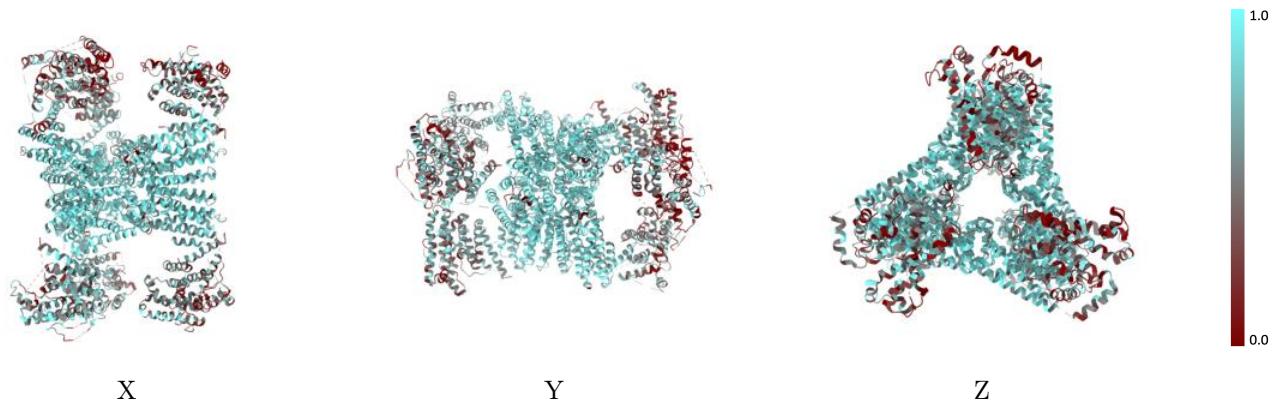
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion ⓘ
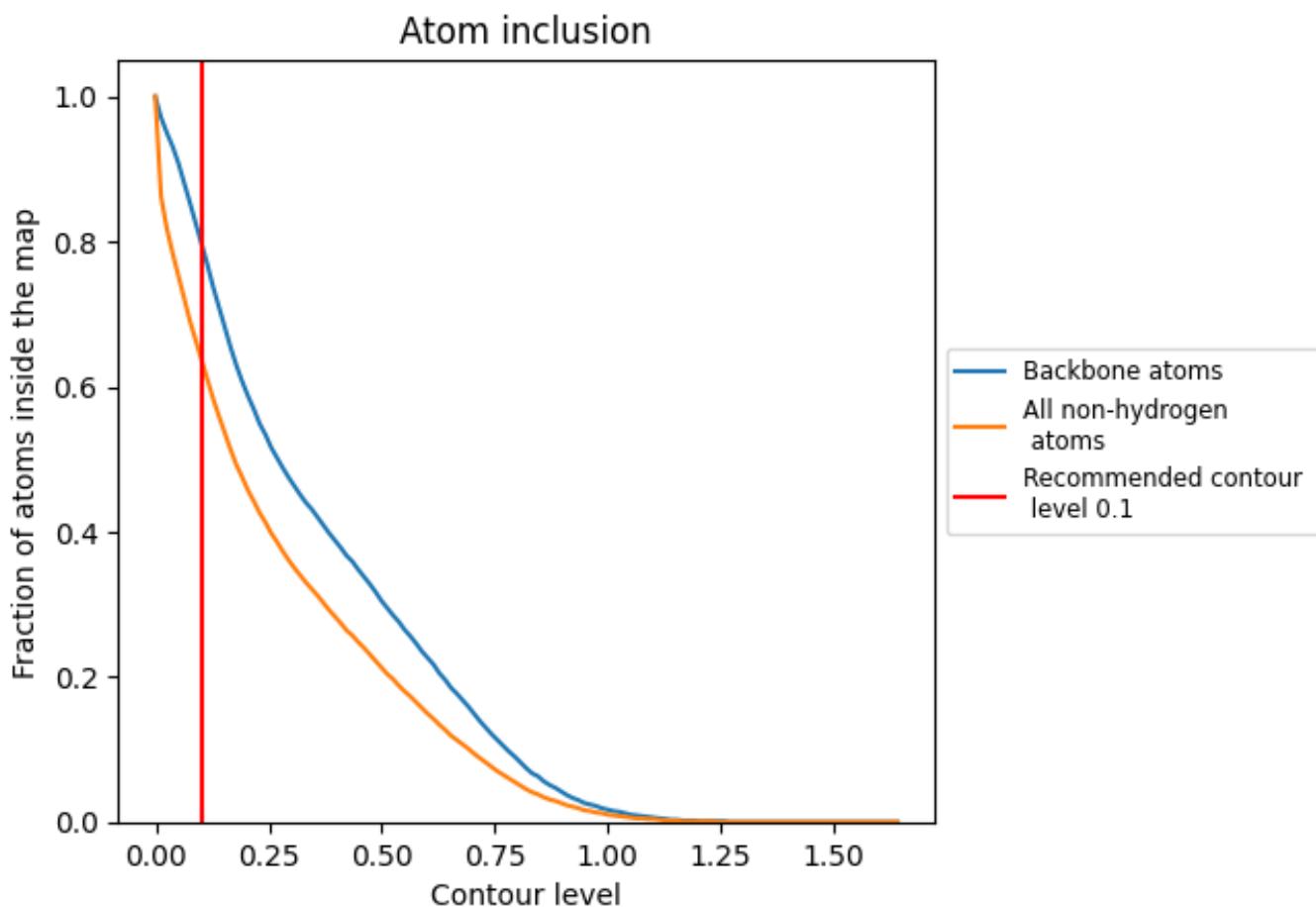
At the recommended contour level, 80% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6380	0.3190
A	0.6420	0.3250
B	0.6610	0.3190
C	0.6080	0.3150
D	0.6880	0.3310
E	0.5960	0.3040
F	0.6310	0.3180

1.0

0.0
<0.0