Full wwPDB EM Validation Report ⓘ

Nov 30, 2022 – 07:07 AM JST

PDB ID	:	7XOH
EMDB ID	:	EMD-33348
Title	:	Cystathionine beta-synthase of Mycobacterium tuberculosis in the presence of S-adenosylmethionine.
Authors	:	Bandyopadhyay, P.; Pramanick, I.; Biswas, R.; Sabarinath, P.S.; Sreedharan, S.; Singh, S.; Rajmani, R.; Laxman, S.; Dutta, S.; Singh, A.
Deposited on	:	2022-05-01
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:

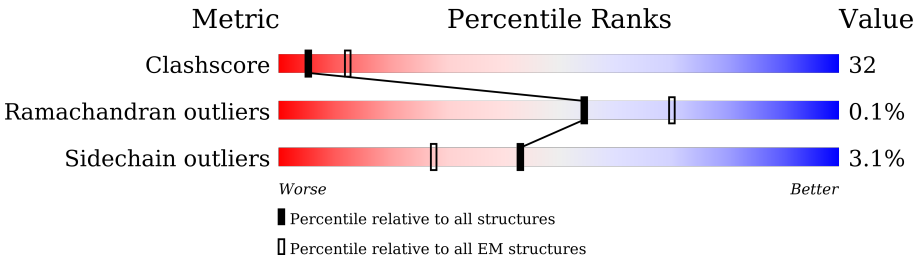
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	478	45% 50%
1	B	478	48% 46%
1	C	478	49% 45%
1	D	478	47% 48%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13528 atoms, of which 4 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 Putative cystathionine beta-synthase Rv1077.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	458	Total	C	N	O	S	0	0
			3366	2113	583	655	15		
1	A	458	Total	C	N	O	S	0	0
			3366	2113	583	655	15		
1	C	458	Total	C	N	O	S	0	0
			3366	2113	583	655	15		
1	D	458	Total	C	N	O	S	0	0
			3366	2113	583	655	15		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	insertion	UNP P9WP51
B	465	LYS	-	expression tag	UNP P9WP51
B	466	LEU	-	expression tag	UNP P9WP51
B	467	ALA	-	expression tag	UNP P9WP51
B	468	ALA	-	expression tag	UNP P9WP51
B	469	ALA	-	expression tag	UNP P9WP51
B	470	LEU	-	expression tag	UNP P9WP51
B	471	GLU	-	expression tag	UNP P9WP51
B	472	HIS	-	expression tag	UNP P9WP51
B	473	HIS	-	expression tag	UNP P9WP51
B	474	HIS	-	expression tag	UNP P9WP51
B	475	HIS	-	expression tag	UNP P9WP51
B	476	HIS	-	expression tag	UNP P9WP51
B	477	HIS	-	expression tag	UNP P9WP51
A	1	ALA	-	insertion	UNP P9WP51
A	465	LYS	-	expression tag	UNP P9WP51
A	466	LEU	-	expression tag	UNP P9WP51
A	467	ALA	-	expression tag	UNP P9WP51
A	468	ALA	-	expression tag	UNP P9WP51
A	469	ALA	-	expression tag	UNP P9WP51
A	470	LEU	-	expression tag	UNP P9WP51
A	471	GLU	-	expression tag	UNP P9WP51

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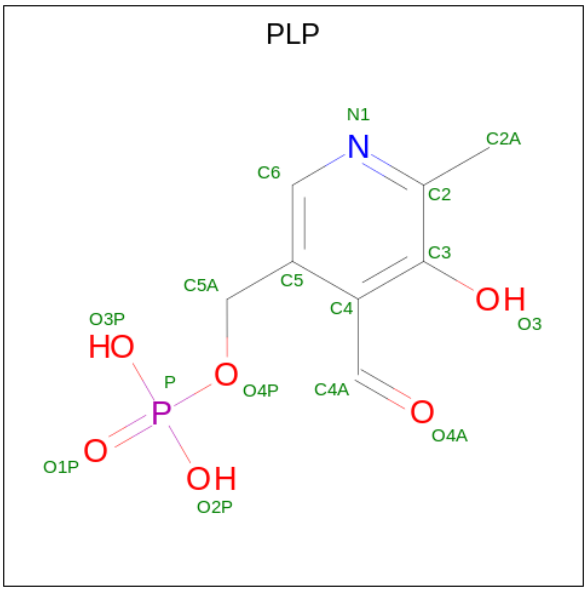
Chain	Residue	Modelled	Actual	Comment	Reference
A	472	HIS	-	expression tag	UNP P9WP51
A	473	HIS	-	expression tag	UNP P9WP51
A	474	HIS	-	expression tag	UNP P9WP51
A	475	HIS	-	expression tag	UNP P9WP51
A	476	HIS	-	expression tag	UNP P9WP51
A	477	HIS	-	expression tag	UNP P9WP51
C	1	ALA	-	insertion	UNP P9WP51
C	465	LYS	-	expression tag	UNP P9WP51
C	466	LEU	-	expression tag	UNP P9WP51
C	467	ALA	-	expression tag	UNP P9WP51
C	468	ALA	-	expression tag	UNP P9WP51
C	469	ALA	-	expression tag	UNP P9WP51
C	470	LEU	-	expression tag	UNP P9WP51
C	471	GLU	-	expression tag	UNP P9WP51
C	472	HIS	-	expression tag	UNP P9WP51
C	473	HIS	-	expression tag	UNP P9WP51
C	474	HIS	-	expression tag	UNP P9WP51
C	475	HIS	-	expression tag	UNP P9WP51
C	476	HIS	-	expression tag	UNP P9WP51
C	477	HIS	-	expression tag	UNP P9WP51
D	1	ALA	-	insertion	UNP P9WP51
D	465	LYS	-	expression tag	UNP P9WP51
D	466	LEU	-	expression tag	UNP P9WP51
D	467	ALA	-	expression tag	UNP P9WP51
D	468	ALA	-	expression tag	UNP P9WP51
D	469	ALA	-	expression tag	UNP P9WP51
D	470	LEU	-	expression tag	UNP P9WP51
D	471	GLU	-	expression tag	UNP P9WP51
D	472	HIS	-	expression tag	UNP P9WP51
D	473	HIS	-	expression tag	UNP P9WP51
D	474	HIS	-	expression tag	UNP P9WP51
D	475	HIS	-	expression tag	UNP P9WP51
D	476	HIS	-	expression tag	UNP P9WP51
D	477	HIS	-	expression tag	UNP P9WP51

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



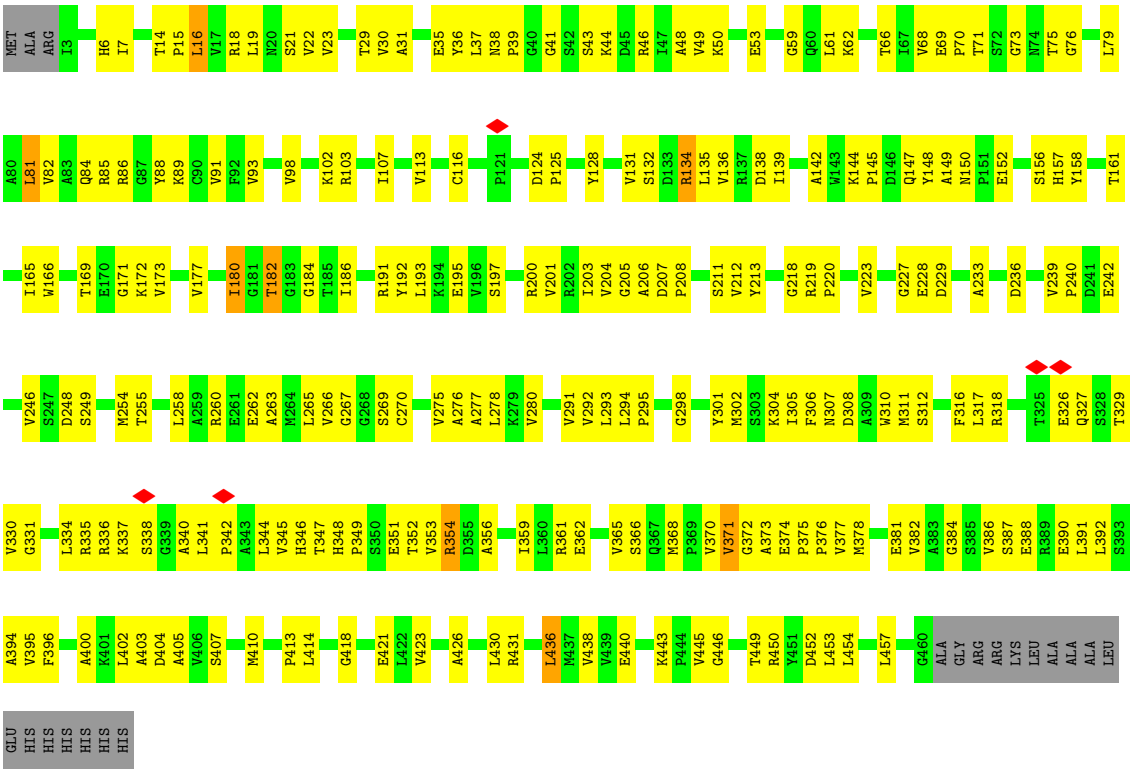
Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H	N	O	P	0
			16	8	1	1	5	1	
2	A	1	Total	C	H	N	O	P	0
			16	8	1	1	5	1	
2	C	1	Total	C	H	N	O	P	0
			16	8	1	1	5	1	
2	D	1	Total	C	H	N	O	P	0
			16	8	1	1	5	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

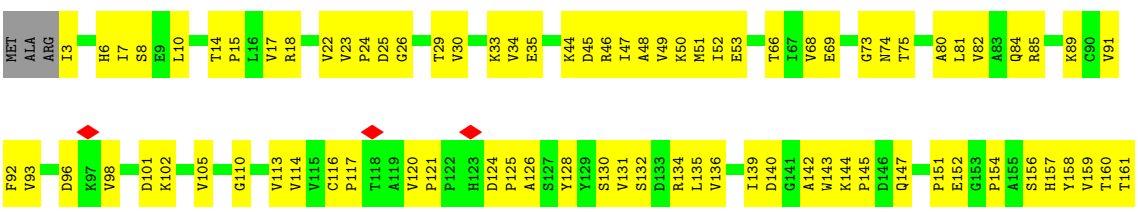
• Molecule 1: Putative cystathionine beta-synthase Rv1077

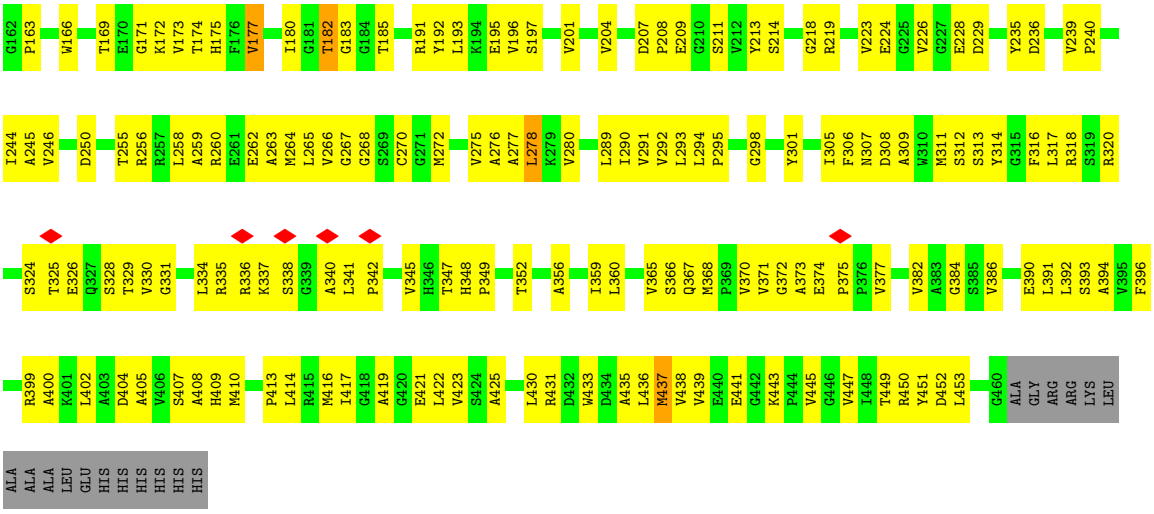
Chain B:



• Molecule 1: Putative cystathionine beta-synthase Rv1077

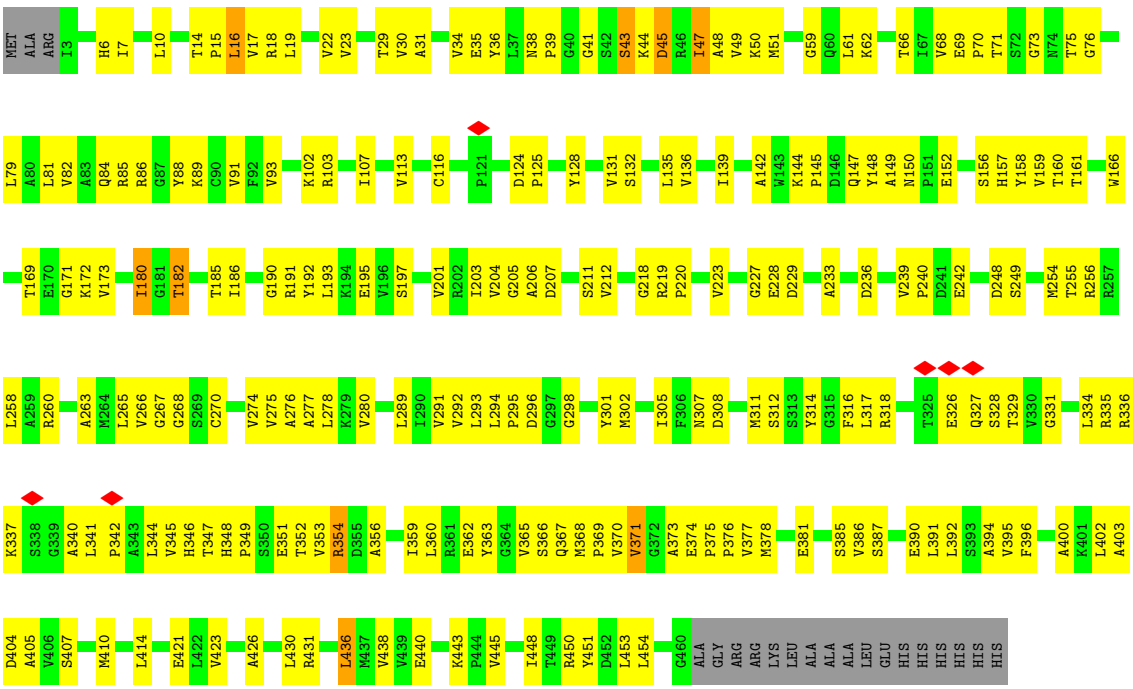
Chain A:





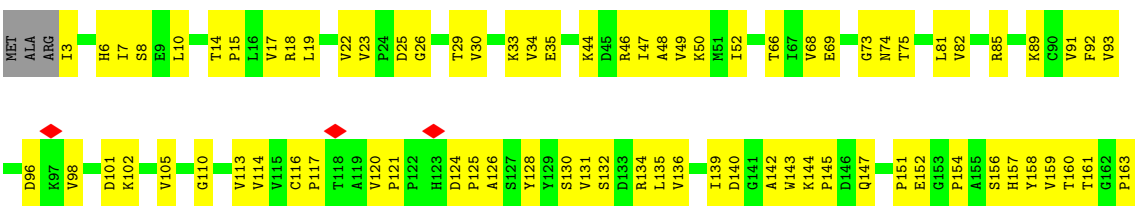
• Molecule 1: Putative cystathionine beta-synthase Rv1077

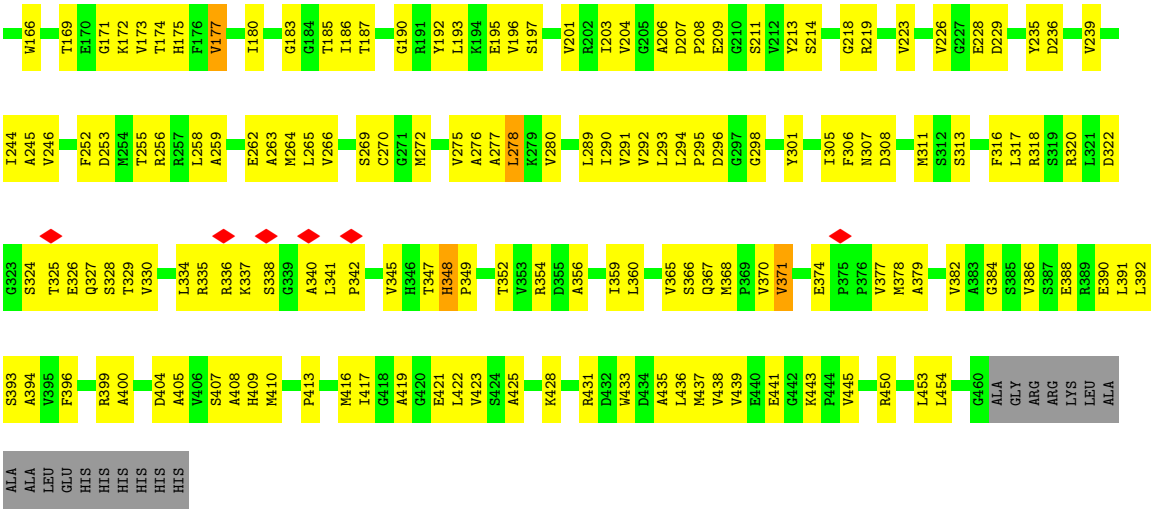
Chain C:



• Molecule 1: Putative cystathionine beta-synthase Rv1077

Chain D:




W166 T169 E170 G171 K172 V173 T174 H175 F176 V177 I180 G183 G184 T185 I186 T187 G190 R191 Y192 L193 K194 E195 V196 S197 V201 R202 I203 V204 G205 A206 D207 P208 E209 G210 S211 V212 Y213 S214 G218 R219 V223 V226 G227 E228 D229 Y235 D236 V239
I244 A245 V246 F252 D253 M254 T255 R256 R257 L258 A259 E262 A263 M264 L265 V266 S269 C270 G271 M272 V275 A276 A277 L278 K279 V280 L289 I290 V291 V292 L293 L294 P295 D296 G297 G298 Y301 I305 F306 N307 D308 M311 S312 S313 F316 L317 R318 S319 R320 L321 D322
G323 S324 T325 E326 Q327 S328 T329 V330 L334 R335 R336 K337 S338 G339 A340 L341 P342 V345 H346 T347 H348 P349 T352 V353 R354 D355 A356 I359 L360 V365 S366 Q367 M368 P369 V370 V371 E374 P375 P376 V377 M378 A379 V382 A383 G384 S385 V386 S387 E388 R389 E390 L391 L392
S393 A394 V395 F396 R399 A400 D404 A405 V406 S407 A408 H409 M410 P413 M416 I417 G418 A419 G420 E421 L422 V423 S424 A425 K428 R431 D432 W433 D434 A435 L436 M437 V438 V439 E440 E441 G442 K443 P444 V445 R450 L453 L454 G460 ALA GLY ARG ARG LYS LEU ALA
ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146444	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.219	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0348	Depositor
Map size (Å)	256.80002, 256.80002, 256.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.28	0/3434	0.50	0/4670
1	B	0.26	0/3434	0.49	0/4670
1	C	0.29	0/3434	0.51	0/4670
1	D	0.27	0/3434	0.50	0/4670
All	All	0.28	0/13736	0.50	0/18680

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3366	0	3337	233	0
1	B	3366	0	3339	224	0
1	C	3366	0	3338	211	0
1	D	3366	0	3338	227	0
2	A	15	1	7	5	0
2	B	15	1	7	5	0
2	C	15	1	7	3	0
2	D	15	1	7	5	0
All	All	13524	4	13380	853	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 32.

All (853) 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:173:VAL:HG12	1:D:289:LEU:HD22	1.37	1.06
1:A:173:VAL:HG12	1:A:289:LEU:HD22	1.38	1.00
1:B:180:ILE:HD11	1:B:205:GLY:HA3	1.42	0.99
1:C:345:VAL:HG22	1:C:368:MET:HE3	1.41	0.98
1:B:345:VAL:HG22	1:B:368:MET:HE3	1.45	0.97
1:A:131:VAL:HG23	1:A:134:ARG:HH21	1.37	0.90
1:D:131:VAL:HG23	1:D:134:ARG:HH21	1.35	0.90
1:A:246:VAL:HG11	1:A:275:VAL:HG11	1.57	0.86
1:D:183:GLY:HA3	1:D:235:TYR:HB2	1.55	0.86
1:D:246:VAL:HG11	1:D:275:VAL:HG11	1.58	0.85
1:B:66:THR:HG22	1:B:89:LYS:HE3	1.58	0.84
1:C:265:LEU:O	1:C:298:GLY:N	2.10	0.83
1:B:255:THR:HG21	1:B:305:ILE:HD12	1.62	0.82
1:B:249:SER:OG	1:B:318:ARG:NH1	2.12	0.82
1:C:249:SER:OG	1:C:318:ARG:NH1	2.12	0.82
1:B:337:LYS:HB2	1:B:340:ALA:HB2	1.63	0.81
1:B:265:LEU:O	1:B:298:GLY:N	2.12	0.80
1:B:258:LEU:HD23	1:B:266:VAL:HG21	1.63	0.80
1:C:66:THR:HG22	1:C:89:LYS:HE3	1.61	0.80
1:D:46:ARG:HD3	1:D:160:THR:HG23	1.62	0.80
1:C:337:LYS:HB2	1:C:340:ALA:HB2	1.63	0.79
1:D:193:LEU:O	1:D:197:SER:OG	2.01	0.79
1:B:219:ARG:HG2	1:B:220:PRO:HD2	1.65	0.78
1:D:158:TYR:OH	1:D:195:GLU:OE1	2.01	0.78
1:D:185:THR:HG21	1:D:293:LEU:CD2	2.16	0.76
1:B:345:VAL:HG22	1:B:368:MET:CE	2.16	0.76
1:C:345:VAL:HG22	1:C:368:MET:CE	2.15	0.76
1:A:307:ASN:OD1	1:A:308:ASP:N	2.19	0.75
1:B:335:ARG:O	1:B:340:ALA:HB3	1.85	0.75
1:D:307:ASN:OD1	1:D:308:ASP:N	2.20	0.75
1:B:135:LEU:O	1:B:139:ILE:HG22	1.85	0.75
1:B:423:VAL:HG13	1:B:453:LEU:HD11	1.66	0.75
1:C:191:ARG:NH2	1:C:236:ASP:OD2	2.16	0.75
1:B:344:LEU:HD23	1:B:376:PRO:HB3	1.69	0.75
1:A:345:VAL:HG22	1:A:368:MET:HE3	1.70	0.74
1:C:335:ARG:O	1:C:340:ALA:HB3	1.87	0.74
1:C:35:GLU:CD	1:C:43:SER:HB2	2.08	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:O	1:C:139:ILE:HG22	1.87	0.74
1:B:331:GLY:O	1:B:335:ARG:NE	2.19	0.74
1:D:185:THR:HG21	1:D:293:LEU:HD23	1.68	0.74
1:C:344:LEU:HD23	1:C:376:PRO:HB3	1.69	0.74
1:C:219:ARG:HG2	1:C:220:PRO:HD2	1.68	0.73
1:C:346:HIS:NE2	1:C:374:GLU:HG3	2.03	0.73
1:B:249:SER:HG	1:B:318:ARG:HH12	1.33	0.73
1:B:36:TYR:HA	1:B:41:GLY:O	1.88	0.73
1:D:265:LEU:O	1:D:298:GLY:N	2.18	0.73
1:D:334:LEU:CD1	1:D:438:VAL:HG21	2.18	0.73
1:D:325:THR:HG22	1:D:326:GLU:HG3	1.70	0.73
1:D:256:ARG:NH2	1:D:311:MET:HG3	2.04	0.72
1:C:255:THR:HG21	1:C:305:ILE:HD12	1.71	0.72
1:A:325:THR:HG23	1:A:326:GLU:H	1.54	0.72
1:C:331:GLY:O	1:C:335:ARG:NE	2.21	0.72
1:D:180:ILE:HG22	1:D:206:ALA:O	1.88	0.72
1:A:209:GLU:N	1:A:246:VAL:O	2.23	0.72
1:A:334:LEU:CD1	1:A:438:VAL:HG21	2.19	0.72
1:C:219:ARG:NH2	1:C:248:ASP:OD2	2.24	0.71
1:A:47:ILE:O	1:A:51:MET:HG3	1.91	0.71
1:A:256:ARG:NH2	1:A:311:MET:HG3	2.05	0.71
1:D:44:LYS:CE	2:D:501:PLP:H5A1	2.20	0.71
1:A:158:TYR:OH	1:A:195:GLU:OE1	2.08	0.71
1:B:22:VAL:HG12	1:B:278:LEU:HD11	1.71	0.71
1:C:249:SER:HG	1:C:318:ARG:HH12	1.36	0.71
1:C:258:LEU:HD23	1:C:266:VAL:HG21	1.71	0.71
1:B:219:ARG:NH2	1:B:248:ASP:OD2	2.24	0.71
1:D:14:THR:OG1	1:D:34:VAL:O	2.07	0.71
1:C:370:VAL:HG21	1:C:410:MET:SD	2.31	0.70
1:B:139:ILE:HG23	1:B:142:ALA:HB2	1.72	0.70
1:A:14:THR:CG2	1:A:33:LYS:HE2	2.22	0.70
1:A:265:LEU:O	1:A:298:GLY:N	2.18	0.70
1:C:139:ILE:HG23	1:C:142:ALA:HB2	1.72	0.70
1:D:209:GLU:N	1:D:246:VAL:O	2.23	0.70
1:D:6:HIS:CD2	1:D:85:ARG:HB2	2.26	0.70
1:D:404:ASP:OD1	1:D:405:ALA:N	2.25	0.69
1:A:14:THR:HG23	1:A:33:LYS:HE2	1.74	0.69
1:D:44:LYS:NZ	2:D:501:PLP:H5A1	2.08	0.69
1:D:266:VAL:HB	1:D:270:CYS:SG	2.33	0.69
1:C:22:VAL:HG12	1:C:278:LEU:HD11	1.74	0.69
1:C:124:ASP:HB2	1:C:125:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:VAL:HG21	1:D:277:ALA:HB2	1.75	0.69
1:B:354:ARG:HD2	1:A:314:TYR:HE1	1.58	0.69
1:D:14:THR:CG2	1:D:33:LYS:HE2	2.22	0.69
1:B:191:ARG:NH2	1:B:236:ASP:OD2	2.17	0.68
1:A:193:LEU:O	1:A:197:SER:OG	2.10	0.68
1:A:404:ASP:OD1	1:A:405:ALA:N	2.25	0.68
1:A:135:LEU:O	1:A:139:ILE:HG22	1.94	0.68
1:D:14:THR:HG23	1:D:33:LYS:HE2	1.73	0.68
1:A:10:LEU:HD13	1:C:15:PRO:HG3	1.76	0.68
1:B:128:TYR:HA	1:B:131:VAL:HG12	1.75	0.68
1:B:431:ARG:HG3	1:A:396:PHE:O	1.94	0.68
1:A:35:GLU:OE2	1:A:46:ARG:NE	2.25	0.68
1:A:14:THR:OG1	1:A:34:VAL:O	2.10	0.68
1:D:116:CYS:SG	1:D:131:VAL:HG11	2.34	0.68
1:A:125:PRO:HA	1:A:130:SER:CB	2.24	0.68
1:C:128:TYR:HA	1:C:131:VAL:HG12	1.75	0.67
1:A:116:CYS:SG	1:A:131:VAL:HG11	2.34	0.67
1:B:124:ASP:HB2	1:B:125:PRO:HD2	1.76	0.67
1:A:177:VAL:HG21	1:A:277:ALA:HB2	1.77	0.67
1:D:326:GLU:HB2	1:D:422:LEU:HD23	1.77	0.67
1:B:430:LEU:HD12	1:B:436:LEU:HD21	1.75	0.67
1:A:421:GLU:OE1	1:A:425:ALA:HB3	1.94	0.67
1:D:69:GLU:HG2	1:D:145:PRO:HG2	1.75	0.67
1:B:15:PRO:HG3	1:D:10:LEU:HD13	1.75	0.67
1:D:433:TRP:O	1:D:450:ARG:NH2	2.28	0.67
1:B:326:GLU:O	1:B:327:GLN:HG3	1.94	0.66
1:D:421:GLU:OE1	1:D:425:ALA:HB3	1.95	0.66
1:B:348:HIS:NE2	1:B:374:GLU:HB2	2.10	0.66
1:A:250:ASP:OD1	1:A:318:ARG:NH2	2.26	0.66
1:A:266:VAL:HB	1:A:270:CYS:SG	2.34	0.66
1:C:347:THR:HG21	1:C:356:ALA:HB2	1.76	0.66
1:A:366:SER:O	1:A:367:GLN:HG3	1.96	0.66
1:C:362:GLU:HG3	1:C:363:TYR:HD1	1.61	0.66
1:B:341:LEU:N	1:B:342:PRO:HD3	2.10	0.66
1:D:156:SER:O	1:D:160:THR:HG22	1.96	0.66
1:D:125:PRO:HA	1:D:130:SER:CB	2.26	0.66
1:D:128:TYR:HA	1:D:131:VAL:HG12	1.78	0.66
1:D:349:PRO:O	1:D:407:SER:HB2	1.96	0.66
1:C:387:SER:HB3	1:C:390:GLU:HG2	1.77	0.65
1:D:334:LEU:HD11	1:D:438:VAL:HG21	1.78	0.65
1:D:35:GLU:OE1	1:D:293:LEU:HD11	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:SER:N	1:B:262:GLU:OE2	2.29	0.65
1:A:156:SER:O	1:A:160:THR:HG22	1.95	0.65
1:A:50:LYS:HG2	1:A:156:SER:HB3	1.77	0.65
1:A:386:VAL:HG21	1:A:391:LEU:HD11	1.77	0.64
1:A:329:THR:OG1	1:A:421:GLU:N	2.30	0.64
1:D:22:VAL:HG21	1:D:258:LEU:HD12	1.80	0.64
1:A:334:LEU:HD11	1:A:438:VAL:HG21	1.78	0.64
1:C:266:VAL:HG11	1:C:294:LEU:HD13	1.79	0.64
1:B:347:THR:HG21	1:B:356:ALA:HB2	1.78	0.64
1:B:361:ARG:HG3	1:A:451:TYR:OH	1.96	0.64
1:D:423:VAL:HG13	1:D:453:LEU:HD11	1.80	0.64
1:A:124:ASP:HB2	1:A:125:PRO:HD2	1.81	0.63
1:A:158:TYR:HD1	1:A:192:TYR:HB2	1.63	0.63
1:A:6:HIS:CD2	1:A:85:ARG:HB2	2.32	0.63
1:B:386:VAL:HG21	1:B:391:LEU:HD11	1.80	0.63
1:D:266:VAL:HG11	1:D:294:LEU:HD13	1.81	0.63
1:A:128:TYR:HA	1:A:131:VAL:HG12	1.80	0.63
1:A:185:THR:HG21	1:A:293:LEU:HD23	1.81	0.63
1:A:423:VAL:HG13	1:A:453:LEU:HD11	1.79	0.63
1:C:82:VAL:O	1:C:85:ARG:HB3	1.99	0.63
1:D:366:SER:O	1:D:367:GLN:HG3	1.98	0.63
1:C:362:GLU:HG3	1:C:363:TYR:CD1	2.33	0.62
1:B:263:ALA:O	1:D:7:ILE:HG21	1.99	0.62
1:A:96:ASP:OD2	1:A:117:PRO:HA	1.99	0.62
1:C:256:ARG:NH2	1:C:311:MET:HG3	2.14	0.62
1:D:329:THR:OG1	1:D:421:GLU:N	2.32	0.62
1:D:386:VAL:HG21	1:D:391:LEU:HD11	1.81	0.62
1:B:334:LEU:HD11	1:B:438:VAL:HG11	1.81	0.62
1:A:325:THR:HG23	1:A:326:GLU:N	2.14	0.62
1:D:96:ASP:OD2	1:D:117:PRO:HA	1.99	0.62
1:C:71:THR:HG21	1:C:76:GLY:N	2.14	0.62
1:B:266:VAL:HB	1:B:270:CYS:CB	2.30	0.62
1:A:312:SER:HB2	1:A:317:LEU:HD22	1.82	0.62
1:C:334:LEU:HD11	1:C:438:VAL:HG11	1.82	0.62
1:D:132:SER:O	1:D:136:VAL:HG23	1.99	0.61
1:D:124:ASP:HB2	1:D:125:PRO:HD2	1.82	0.61
1:B:82:VAL:O	1:B:85:ARG:HB3	1.99	0.61
1:A:125:PRO:HA	1:A:130:SER:OG	2.01	0.61
1:D:35:GLU:OE2	1:D:46:ARG:NH2	2.30	0.61
1:A:22:VAL:HG23	1:A:262:GLU:OE2	1.99	0.61
1:A:44:LYS:HD2	1:A:47:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ARG:C	1:A:337:LYS:HD2	2.20	0.61
1:D:135:LEU:HD11	1:D:139:ILE:HD11	1.83	0.61
1:B:48:ALA:HB1	1:B:79:LEU:HD23	1.82	0.61
1:B:71:THR:HG21	1:B:76:GLY:N	2.15	0.61
1:A:356:ALA:O	1:A:359:ILE:HG22	2.01	0.61
1:B:396:PHE:O	1:A:431:ARG:HG3	2.00	0.61
1:A:191:ARG:NH2	1:A:236:ASP:OD2	2.21	0.61
1:B:6:HIS:CD2	1:B:85:ARG:HB2	2.36	0.61
1:A:73:GLY:O	1:A:102:LYS:HD2	1.99	0.61
1:C:256:ARG:HH22	1:C:311:MET:HG3	1.66	0.61
1:D:336:ARG:C	1:D:337:LYS:HD2	2.21	0.61
1:B:49:VAL:O	1:B:53:GLU:HG2	2.02	0.60
1:A:69:GLU:HG2	1:A:145:PRO:HG2	1.84	0.60
1:B:266:VAL:HG11	1:B:294:LEU:HD13	1.81	0.60
1:A:266:VAL:HB	1:A:270:CYS:CB	2.31	0.60
1:D:174:THR:O	1:D:201:VAL:HA	2.02	0.60
1:D:348:HIS:NE2	1:D:374:GLU:OE1	2.28	0.60
1:C:266:VAL:HB	1:C:270:CYS:CB	2.31	0.60
1:D:255:THR:HG21	1:D:305:ILE:HD12	1.83	0.60
1:B:404:ASP:OD1	1:B:405:ALA:N	2.34	0.60
1:B:19:LEU:HB2	1:B:30:VAL:HG13	1.82	0.60
1:C:396:PHE:O	1:D:431:ARG:HG3	2.00	0.60
1:C:50:LYS:HG2	1:C:156:SER:HB2	1.81	0.60
1:C:341:LEU:N	1:C:342:PRO:HD3	2.17	0.60
1:D:128:TYR:HA	1:D:131:VAL:CG1	2.31	0.60
1:A:69:GLU:CG	1:A:145:PRO:HG2	2.32	0.60
1:C:19:LEU:HB2	1:C:30:VAL:HG13	1.83	0.60
1:C:158:TYR:OH	1:C:195:GLU:OE1	2.18	0.60
1:D:69:GLU:CG	1:D:145:PRO:HG2	2.32	0.60
1:B:370:VAL:HG21	1:B:410:MET:SD	2.41	0.60
1:A:68:VAL:O	1:A:144:LYS:HA	2.02	0.60
1:B:336:ARG:O	1:B:337:LYS:HD2	2.02	0.59
1:C:159:VAL:HG12	1:C:160:THR:HG23	1.84	0.59
1:C:454:LEU:HD12	1:D:392:LEU:CD2	2.31	0.59
1:D:223:VAL:HG23	1:D:226:VAL:HG22	1.82	0.59
1:B:311:MET:HE3	1:B:317:LEU:H	1.66	0.59
1:A:128:TYR:HA	1:A:131:VAL:CG1	2.32	0.59
1:B:131:VAL:O	1:B:135:LEU:HD23	2.02	0.59
1:B:334:LEU:CD1	1:B:438:VAL:HG21	2.32	0.59
1:B:390:GLU:O	1:B:394:ALA:N	2.28	0.59
1:D:386:VAL:CG2	1:D:391:LEU:HD11	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ARG:NH1	1:A:393:SER:HA	2.18	0.59
1:C:44:LYS:HG2	1:C:75:THR:OG1	2.01	0.59
1:A:66:THR:HG22	1:A:89:LYS:HB2	1.84	0.59
1:C:73:GLY:O	1:C:102:LYS:HE3	2.01	0.59
1:A:174:THR:O	1:A:201:VAL:HA	2.01	0.59
1:D:125:PRO:HA	1:D:130:SER:OG	2.02	0.59
1:C:336:ARG:O	1:C:337:LYS:HD2	2.01	0.59
1:D:68:VAL:O	1:D:144:LYS:HA	2.03	0.59
1:D:272:MET:O	1:D:275:VAL:HG12	2.03	0.59
1:B:136:VAL:HG21	1:B:144:LYS:HB2	1.85	0.59
1:A:328:SER:O	1:A:422:LEU:HA	2.02	0.59
1:C:136:VAL:HG21	1:C:144:LYS:HB2	1.83	0.59
1:B:73:GLY:O	1:B:102:LYS:HE3	2.03	0.58
1:C:326:GLU:O	1:C:327:GLN:HG2	2.04	0.58
1:C:450:ARG:NH1	1:D:393:SER:HA	2.18	0.58
1:D:218:GLY:HA2	1:D:229:ASP:OD1	2.04	0.58
1:B:35:GLU:CG	1:B:43:SER:HB2	2.33	0.58
1:A:272:MET:O	1:A:275:VAL:HG12	2.03	0.58
1:D:50:LYS:HG2	1:D:156:SER:HB3	1.85	0.58
1:D:266:VAL:HB	1:D:270:CYS:CB	2.33	0.58
1:B:305:ILE:HG13	1:B:306:PHE:CD1	2.38	0.58
1:A:132:SER:O	1:A:136:VAL:HG23	2.02	0.58
1:A:158:TYR:CD1	1:A:192:TYR:HB2	2.39	0.58
1:B:184:GLY:N	2:B:501:PLP:O1P	2.35	0.58
1:D:370:VAL:HG21	1:D:410:MET:SD	2.43	0.58
1:D:73:GLY:O	1:D:102:LYS:HD2	2.04	0.58
1:C:6:HIS:CD2	1:C:85:ARG:HB2	2.38	0.58
1:C:131:VAL:O	1:C:135:LEU:HD23	2.02	0.58
1:A:7:ILE:HG21	1:C:263:ALA:O	2.04	0.58
1:A:44:LYS:HD2	1:A:47:ILE:CD1	2.34	0.58
1:C:193:LEU:O	1:C:197:SER:HB2	2.03	0.58
1:A:207:ASP:OD2	1:A:213:TYR:HB2	2.04	0.57
1:A:120:VAL:CG1	1:A:121:PRO:HD2	2.34	0.57
1:A:246:VAL:HG11	1:A:275:VAL:CG1	2.33	0.57
1:A:433:TRP:O	1:A:450:ARG:NH2	2.37	0.57
1:A:50:LYS:CB	1:A:156:SER:HB3	2.35	0.57
1:A:218:GLY:HA2	1:A:229:ASP:OD1	2.05	0.57
1:D:341:LEU:N	1:D:342:PRO:HD3	2.19	0.57
1:D:367:GLN:OE1	1:D:435:ALA:HB3	2.05	0.57
1:B:50:LYS:CB	1:B:156:SER:HB2	2.34	0.57
1:A:341:LEU:N	1:A:342:PRO:HD3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LYS:HB2	1:D:340:ALA:HB2	1.87	0.57
1:A:386:VAL:CG2	1:A:391:LEU:HD11	2.35	0.57
1:C:334:LEU:CD1	1:C:438:VAL:HG21	2.34	0.57
1:D:421:GLU:CD	1:D:425:ALA:HB3	2.25	0.57
1:B:44:LYS:HD3	2:B:501:PLP:C4	2.35	0.56
1:B:134:ARG:HG3	1:B:138:ASP:OD2	2.05	0.56
1:C:369:PRO:HA	1:C:385:SER:HA	1.87	0.56
1:B:35:GLU:HB3	1:B:43:SER:HB2	1.86	0.56
1:D:66:THR:HG22	1:D:89:LYS:HB2	1.86	0.56
1:D:120:VAL:CG1	1:D:121:PRO:HD2	2.35	0.56
1:C:172:LYS:HD2	1:C:172:LYS:O	2.05	0.56
1:D:438:VAL:O	1:D:445:VAL:HG12	2.05	0.56
1:B:356:ALA:O	1:B:359:ILE:HG22	2.06	0.56
1:A:101:ASP:OD1	1:C:302:MET:HB3	2.05	0.56
1:C:219:ARG:CG	1:C:220:PRO:HD2	2.36	0.56
1:A:438:VAL:HG23	1:A:438:VAL:O	2.06	0.56
1:C:66:THR:CG2	1:C:89:LYS:HE3	2.35	0.56
1:B:93:VAL:HG11	1:B:131:VAL:HG13	1.87	0.56
1:A:185:THR:HB	2:A:501:PLP:O1P	2.06	0.56
1:D:207:ASP:OD2	1:D:213:TYR:HB2	2.06	0.56
1:C:369:PRO:O	1:C:371:VAL:HG12	2.05	0.56
1:B:35:GLU:CB	1:B:43:SER:HB2	2.36	0.55
1:B:103:ARG:O	1:B:107:ILE:HG13	2.06	0.55
1:A:377:VAL:HG13	1:A:443:LYS:NZ	2.20	0.55
1:D:17:VAL:HG12	1:D:34:VAL:HG23	1.89	0.55
1:A:365:VAL:HG22	1:A:366:SER:H	1.71	0.55
1:D:190:GLY:HA2	1:D:203:ILE:CD1	2.36	0.55
1:B:311:MET:CE	1:B:316:PHE:HB3	2.37	0.55
1:B:14:THR:OG1	1:B:15:PRO:HD2	2.07	0.55
1:C:50:LYS:CB	1:C:156:SER:HB2	2.37	0.55
1:C:190:GLY:HA2	1:C:203:ILE:CD1	2.36	0.55
1:C:438:VAL:HG23	1:C:438:VAL:O	2.07	0.55
1:C:14:THR:OG1	1:C:15:PRO:HD2	2.06	0.55
1:D:328:SER:O	1:D:422:LEU:HA	2.06	0.55
1:A:45:ASP:O	1:A:49:VAL:HG23	2.07	0.55
1:C:307:ASN:OD1	1:C:308:ASP:N	2.40	0.55
1:D:438:VAL:O	1:D:438:VAL:HG23	2.07	0.55
1:B:66:THR:CG2	1:B:89:LYS:HE3	2.33	0.55
1:B:219:ARG:HG2	1:B:220:PRO:CD	2.37	0.55
1:A:349:PRO:O	1:A:407:SER:HB2	2.06	0.55
1:A:377:VAL:HG12	1:A:377:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:VAL:HB	1:A:382:VAL:HG12	1.87	0.55
1:A:421:GLU:CD	1:A:425:ALA:HB3	2.26	0.55
1:B:438:VAL:HG23	1:B:438:VAL:O	2.07	0.54
1:A:255:THR:HG21	1:A:305:ILE:HD12	1.88	0.54
1:A:348:HIS:CD2	1:A:372:GLY:HA2	2.42	0.54
1:C:93:VAL:HG11	1:C:131:VAL:CG1	2.37	0.54
1:D:246:VAL:HG11	1:D:275:VAL:CG1	2.33	0.54
1:D:360:LEU:HD22	1:D:365:VAL:HG13	1.89	0.54
1:B:93:VAL:HG11	1:B:131:VAL:CG1	2.37	0.54
1:C:103:ARG:O	1:C:107:ILE:HG13	2.06	0.54
1:B:219:ARG:CG	1:B:220:PRO:HD2	2.36	0.54
1:A:17:VAL:HG12	1:A:34:VAL:HG23	1.89	0.54
1:C:93:VAL:HG11	1:C:131:VAL:HG13	1.89	0.54
1:D:158:TYR:HD1	1:D:192:TYR:HB2	1.72	0.54
1:C:254:MET:HG2	1:C:275:VAL:HG23	1.89	0.54
1:B:59:GLY:O	1:B:62:LYS:NZ	2.41	0.54
1:B:150:ASN:OD1	1:B:152:GLU:HG2	2.08	0.54
1:A:120:VAL:HG13	1:A:121:PRO:HD2	1.89	0.54
1:A:159:VAL:O	1:A:163:PRO:HG2	2.08	0.54
1:A:367:GLN:OE1	1:A:435:ALA:HB3	2.07	0.54
1:D:337:LYS:O	1:D:338:SER:HB3	2.08	0.54
1:B:15:PRO:CG	1:D:10:LEU:HD13	2.38	0.54
1:A:337:LYS:O	1:A:338:SER:HB3	2.08	0.54
1:B:193:LEU:HB3	1:B:201:VAL:HG11	1.90	0.54
1:A:7:ILE:HD12	1:A:10:LEU:HD12	1.90	0.54
1:A:75:THR:HG21	1:A:147:GLN:OE1	2.08	0.54
1:A:438:VAL:O	1:A:445:VAL:HG12	2.07	0.54
1:C:30:VAL:HG13	1:C:30:VAL:O	2.08	0.54
1:C:59:GLY:O	1:C:62:LYS:NZ	2.41	0.54
1:C:223:VAL:O	1:C:223:VAL:HG13	2.08	0.54
1:C:353:VAL:HG23	1:C:404:ASP:O	2.06	0.54
1:D:370:VAL:HG23	1:D:370:VAL:O	2.07	0.54
1:B:128:TYR:HA	1:B:131:VAL:CG1	2.36	0.54
1:A:82:VAL:O	1:A:85:ARG:HB3	2.08	0.54
1:A:370:VAL:HG23	1:A:370:VAL:O	2.08	0.54
1:C:75:THR:HG21	1:C:147:GLN:OE1	2.07	0.54
1:C:430:LEU:HD12	1:C:436:LEU:HD21	1.90	0.54
1:B:30:VAL:HG13	1:B:30:VAL:O	2.08	0.54
1:B:346:HIS:HB2	1:B:371:VAL:HG13	1.90	0.54
1:A:370:VAL:HG21	1:A:410:MET:SD	2.48	0.54
1:C:347:THR:O	1:C:370:VAL:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ASP:OD1	1:C:405:ALA:N	2.41	0.54
1:A:337:LYS:HB2	1:A:340:ALA:HB2	1.90	0.53
1:D:441:GLU:O	1:D:441:GLU:HG2	2.08	0.53
1:A:223:VAL:HG23	1:A:268:GLY:HA3	1.90	0.53
1:A:276:ALA:O	1:A:280:VAL:HG23	2.08	0.53
1:A:441:GLU:O	1:A:441:GLU:HG2	2.08	0.53
1:C:219:ARG:HG2	1:C:220:PRO:CD	2.38	0.53
1:D:345:VAL:HG22	1:D:368:MET:HE3	1.89	0.53
1:A:44:LYS:CG	2:A:501:PLP:C4A	2.86	0.53
1:C:23:VAL:HB	1:C:30:VAL:HG11	1.90	0.53
1:C:365:VAL:HG22	1:C:366:SER:N	2.24	0.53
1:D:7:ILE:HD12	1:D:10:LEU:HD12	1.91	0.53
1:C:374:GLU:N	1:C:375:PRO:HD2	2.24	0.53
1:A:335:ARG:C	1:A:337:LYS:H	2.12	0.53
1:D:159:VAL:O	1:D:163:PRO:HG2	2.09	0.53
1:A:152:GLU:OE1	1:A:152:GLU:HA	2.08	0.53
1:D:120:VAL:HG13	1:D:121:PRO:HD2	1.90	0.53
1:A:10:LEU:HD13	1:C:15:PRO:CG	2.38	0.53
1:C:328:SER:O	1:C:423:VAL:HG23	2.09	0.53
1:C:371:VAL:HG21	1:C:378:MET:HG2	1.91	0.53
1:C:386:VAL:HG21	1:C:391:LEU:HD11	1.91	0.53
1:C:390:GLU:O	1:C:394:ALA:N	2.34	0.53
1:D:428:LYS:HD2	1:D:428:LYS:O	2.08	0.53
1:B:302:MET:HB3	1:D:101:ASP:OD1	2.08	0.53
1:A:49:VAL:O	1:A:53:GLU:HG2	2.09	0.53
1:C:47:ILE:HG13	1:C:48:ALA:N	2.24	0.53
1:D:75:THR:HG21	1:D:147:GLN:OE1	2.09	0.53
1:D:356:ALA:O	1:D:359:ILE:HG22	2.09	0.53
1:C:68:VAL:O	1:C:144:LYS:HA	2.09	0.53
1:B:15:PRO:HG3	1:B:37:LEU:HD12	1.89	0.53
1:C:392:LEU:CD2	1:D:454:LEU:HD22	2.39	0.53
1:D:218:GLY:O	1:D:219:ARG:HG3	2.09	0.53
1:B:353:VAL:HG23	1:B:404:ASP:O	2.09	0.52
1:C:150:ASN:OD1	1:C:152:GLU:HG2	2.08	0.52
1:C:431:ARG:HG3	1:D:396:PHE:O	2.08	0.52
1:D:30:VAL:HG13	1:D:30:VAL:O	2.10	0.52
1:B:191:ARG:O	1:B:195:GLU:HG3	2.10	0.52
1:B:349:PRO:O	1:B:407:SER:HB3	2.08	0.52
1:D:311:MET:HE3	1:D:317:LEU:H	1.75	0.52
1:B:35:GLU:HG3	1:B:43:SER:HB2	1.91	0.52
1:A:218:GLY:O	1:A:219:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:LYS:O	1:B:338:SER:HB2	2.09	0.52
1:A:92:PHE:O	1:A:114:VAL:HG22	2.09	0.52
1:C:317:LEU:O	1:C:317:LEU:HG	2.10	0.52
1:D:276:ALA:O	1:D:280:VAL:HG23	2.09	0.52
1:C:35:GLU:OE1	1:C:43:SER:HB2	2.09	0.52
1:D:92:PHE:O	1:D:114:VAL:HG22	2.10	0.52
1:D:378:MET:HE1	1:D:379:ALA:O	2.10	0.52
1:B:148:TYR:CD1	1:B:182:THR:HB	2.45	0.52
1:B:438:VAL:HG23	1:B:445:VAL:HG12	1.91	0.52
1:D:173:VAL:O	1:D:201:VAL:HG22	2.10	0.52
1:B:258:LEU:HD23	1:B:266:VAL:CG2	2.38	0.52
1:B:387:SER:HB3	1:B:390:GLU:HG2	1.91	0.52
1:C:44:LYS:HE3	1:C:75:THR:OG1	2.09	0.52
1:C:70:PRO:HB2	1:C:128:TYR:HD2	1.75	0.52
1:D:335:ARG:C	1:D:337:LYS:H	2.12	0.52
1:A:50:LYS:CG	1:A:156:SER:HB3	2.39	0.52
1:C:314:TYR:HE2	1:D:352:THR:HG21	1.75	0.51
1:D:365:VAL:HG22	1:D:366:SER:H	1.75	0.51
1:A:30:VAL:O	1:A:30:VAL:HG13	2.09	0.51
1:C:438:VAL:HG23	1:C:445:VAL:HG12	1.92	0.51
1:D:158:TYR:CD1	1:D:192:TYR:HB2	2.45	0.51
1:A:3:ILE:HD11	1:C:169:THR:HG22	1.92	0.51
1:C:128:TYR:HA	1:C:131:VAL:CG1	2.37	0.51
1:D:347:THR:O	1:D:370:VAL:HA	2.10	0.51
1:A:175:HIS:HB2	1:A:290:ILE:HG23	1.91	0.51
1:C:35:GLU:OE1	1:C:293:LEU:HD11	2.11	0.51
1:C:365:VAL:HG22	1:C:367:GLN:H	1.76	0.51
1:B:223:VAL:HG23	1:B:223:VAL:O	2.10	0.51
1:A:207:ASP:OD1	1:A:211:SER:HB3	2.11	0.51
1:A:317:LEU:O	1:A:317:LEU:HG	2.10	0.51
1:C:50:LYS:CG	1:C:156:SER:HB2	2.40	0.51
1:C:158:TYR:CD1	1:C:192:TYR:HB2	2.46	0.51
1:B:365:VAL:HG22	1:B:366:SER:H	1.76	0.51
1:C:266:VAL:HB	1:C:270:CYS:SG	2.51	0.51
1:D:417:ILE:O	1:D:438:VAL:HA	2.10	0.51
1:B:454:LEU:HD23	1:A:392:LEU:HD21	1.91	0.51
1:D:324:SER:OG	1:D:327:GLN:HG3	2.11	0.51
1:A:173:VAL:O	1:A:201:VAL:HG22	2.10	0.51
1:C:149:ALA:CB	1:C:233:ALA:HB3	2.41	0.51
1:A:29:THR:HG23	1:A:289:LEU:HG	1.92	0.51
1:C:212:VAL:HG23	1:C:228:GLU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:VAL:HG23	1:D:262:GLU:OE2	2.10	0.51
1:D:151:PRO:O	1:D:154:PRO:HG2	2.10	0.51
1:B:212:VAL:HG23	1:B:228:GLU:O	2.11	0.51
1:A:151:PRO:O	1:A:154:PRO:HG2	2.11	0.51
1:C:180:ILE:HG22	1:C:206:ALA:O	2.11	0.51
1:C:204:VAL:HG13	1:C:242:GLU:O	2.11	0.51
1:D:207:ASP:OD1	1:D:211:SER:HB3	2.10	0.51
1:B:70:PRO:HB2	1:B:128:TYR:HD2	1.75	0.50
1:B:307:ASN:OD1	1:B:308:ASP:N	2.44	0.50
1:A:417:ILE:O	1:A:438:VAL:HA	2.11	0.50
1:C:365:VAL:HG22	1:C:366:SER:H	1.76	0.50
1:D:256:ARG:HH22	1:D:311:MET:HG3	1.74	0.50
1:C:173:VAL:HG12	1:C:289:LEU:CD2	2.42	0.50
1:A:347:THR:O	1:A:370:VAL:HA	2.12	0.50
1:A:3:ILE:HG12	1:C:16:LEU:HD22	1.93	0.50
1:D:44:LYS:HE2	2:D:501:PLP:O2P	2.11	0.50
1:D:337:LYS:HB2	1:D:340:ALA:CB	2.41	0.50
1:B:312:SER:HB2	1:B:317:LEU:HD22	1.92	0.50
1:B:75:THR:HG21	1:B:147:GLN:OE1	2.12	0.50
1:B:68:VAL:O	1:B:144:LYS:HA	2.11	0.50
1:C:335:ARG:C	1:C:337:LYS:H	2.15	0.50
1:D:46:ARG:HD3	1:D:160:THR:CG2	2.35	0.50
1:D:152:GLU:HA	1:D:152:GLU:OE1	2.12	0.50
1:D:175:HIS:HB2	1:D:290:ILE:HG23	1.93	0.50
1:D:180:ILE:O	1:D:180:ILE:HG23	2.12	0.50
1:D:277:ALA:HB2	1:D:292:VAL:HG22	1.92	0.50
1:A:311:MET:HE3	1:A:317:LEU:H	1.76	0.50
1:D:377:VAL:HG13	1:D:443:LYS:NZ	2.26	0.50
1:B:254:MET:HG2	1:B:275:VAL:HG23	1.93	0.50
1:B:335:ARG:C	1:B:337:LYS:H	2.14	0.50
1:C:386:VAL:CG2	1:C:391:LEU:HD11	2.41	0.50
1:A:360:LEU:HD23	1:A:365:VAL:HG13	1.93	0.49
1:C:352:THR:CG2	1:C:403:ALA:HA	2.42	0.49
1:C:445:VAL:HG22	1:C:445:VAL:O	2.12	0.49
1:D:29:THR:HG23	1:D:289:LEU:HG	1.92	0.49
1:C:349:PRO:O	1:C:407:SER:HB3	2.11	0.49
1:A:320:ARG:HD3	1:A:324:SER:O	2.12	0.49
1:A:331:GLY:O	1:A:335:ARG:NE	2.23	0.49
1:C:132:SER:O	1:C:136:VAL:HG23	2.12	0.49
1:B:449:THR:HG23	1:B:452:ASP:H	1.77	0.49
1:A:371:VAL:HG22	1:A:372:GLY:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLU:HG2	1:C:70:PRO:HD2	1.94	0.49
1:D:438:VAL:HG23	1:D:445:VAL:CG1	2.42	0.49
1:B:386:VAL:CG2	1:B:391:LEU:HD11	2.40	0.49
1:A:223:VAL:HG13	1:A:226:VAL:HG22	1.94	0.49
1:A:336:ARG:NH1	1:A:336:ARG:HB2	2.28	0.49
1:C:370:VAL:HG23	1:C:370:VAL:O	2.13	0.49
1:B:329:THR:OG1	1:B:421:GLU:N	2.45	0.49
1:C:341:LEU:H	1:C:341:LEU:HD23	1.78	0.49
1:B:158:TYR:CD1	1:B:192:TYR:HB2	2.48	0.49
1:B:347:THR:HG23	1:B:351:GLU:OE1	2.13	0.49
1:C:296:ASP:OD2	2:C:501:PLP:H2A2	2.12	0.49
1:A:91:VAL:HG11	1:A:135:LEU:HD21	1.94	0.49
1:A:134:ARG:HD2	1:A:135:LEU:N	2.27	0.49
1:D:19:LEU:HB2	1:D:30:VAL:HG13	1.94	0.49
1:A:66:THR:HA	1:A:89:LYS:O	2.13	0.48
1:A:277:ALA:HB2	1:A:292:VAL:HG22	1.94	0.48
1:C:34:VAL:O	1:C:34:VAL:HG13	2.12	0.48
1:C:148:TYR:CD1	1:C:182:THR:OG1	2.66	0.48
1:B:132:SER:O	1:B:136:VAL:HG23	2.12	0.48
1:B:345:VAL:HG13	1:B:345:VAL:O	2.12	0.48
1:B:365:VAL:HG22	1:B:366:SER:N	2.28	0.48
1:A:345:VAL:HG22	1:A:368:MET:CE	2.43	0.48
1:A:408:ALA:O	1:A:409:HIS:ND1	2.47	0.48
1:D:223:VAL:HG23	1:D:223:VAL:O	2.14	0.48
1:D:317:LEU:HG	1:D:317:LEU:O	2.13	0.48
1:B:317:LEU:HG	1:B:317:LEU:O	2.12	0.48
1:A:263:ALA:HB3	1:C:7:ILE:HG21	1.96	0.48
1:A:377:VAL:HG13	1:A:443:LYS:HZ3	1.78	0.48
1:C:347:THR:HG23	1:C:351:GLU:OE1	2.13	0.48
1:D:345:VAL:HG13	1:D:345:VAL:O	2.14	0.48
1:C:334:LEU:CD1	1:C:438:VAL:HG11	2.42	0.48
1:D:377:VAL:HG12	1:D:377:VAL:O	2.13	0.48
1:B:377:VAL:HG12	1:B:377:VAL:O	2.14	0.48
1:B:204:VAL:HG11	1:B:280:VAL:HG21	1.96	0.48
1:B:438:VAL:HG23	1:B:445:VAL:CG1	2.44	0.48
1:A:48:ALA:O	1:A:52:ILE:HG12	2.14	0.48
1:A:337:LYS:HB2	1:A:340:ALA:CB	2.44	0.48
1:A:348:HIS:HB3	1:A:349:PRO:HD2	1.96	0.48
1:C:255:THR:HG21	1:C:305:ILE:CD1	2.42	0.48
1:C:377:VAL:HG12	1:C:377:VAL:O	2.13	0.48
1:B:15:PRO:CG	1:B:37:LEU:HD12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HA	1:B:31:ALA:HA	1.96	0.48
1:A:430:LEU:HD23	1:A:450:ARG:CG	2.43	0.48
1:A:438:VAL:HG23	1:A:445:VAL:CG1	2.44	0.48
1:C:192:TYR:HD1	1:C:193:LEU:HD23	1.78	0.48
1:C:345:VAL:HG13	1:C:345:VAL:O	2.14	0.48
1:B:172:LYS:O	1:B:172:LYS:HG2	2.14	0.47
1:D:336:ARG:HB2	1:D:336:ARG:NH1	2.28	0.47
1:B:334:LEU:HD13	1:B:438:VAL:HG21	1.96	0.47
1:B:341:LEU:HD23	1:B:341:LEU:H	1.79	0.47
1:C:51:MET:HG2	1:C:152:GLU:HB2	1.95	0.47
1:D:134:ARG:HD2	1:D:135:LEU:N	2.29	0.47
1:D:259:ALA:HA	1:D:264:MET:O	2.14	0.47
1:B:204:VAL:HG13	1:B:242:GLU:O	2.14	0.47
1:B:374:GLU:N	1:B:375:PRO:HD2	2.29	0.47
1:C:206:ALA:HB2	1:C:276:ALA:CB	2.44	0.47
1:D:371:VAL:HB	1:D:382:VAL:HG12	1.96	0.47
1:B:69:GLU:HB2	1:B:145:PRO:HD2	1.97	0.47
1:A:292:VAL:HG12	1:A:293:LEU:N	2.29	0.47
1:C:337:LYS:HB2	1:C:340:ALA:CB	2.41	0.47
1:D:223:VAL:HG12	1:D:252:PHE:HE1	1.78	0.47
1:B:370:VAL:O	1:B:370:VAL:HG23	2.14	0.47
1:A:223:VAL:HG13	1:A:223:VAL:O	2.14	0.47
1:B:157:HIS:O	1:B:161:THR:HB	2.15	0.47
1:B:266:VAL:HB	1:B:270:CYS:SG	2.55	0.47
1:B:329:THR:HA	1:B:421:GLU:O	2.14	0.47
1:B:359:ILE:HA	1:B:362:GLU:HG2	1.95	0.47
1:B:371:VAL:HG23	1:B:372:GLY:O	2.14	0.47
1:A:68:VAL:HA	1:A:91:VAL:O	2.15	0.47
1:A:258:LEU:HD23	1:A:266:VAL:HG21	1.96	0.47
1:D:416:MET:SD	1:D:439:VAL:HG11	2.54	0.47
1:B:148:TYR:CE1	1:B:182:THR:HB	2.49	0.47
1:B:218:GLY:HA2	1:B:229:ASP:OD1	2.15	0.47
1:B:341:LEU:N	1:B:342:PRO:CD	2.78	0.47
1:B:421:GLU:N	1:B:421:GLU:OE1	2.47	0.47
1:C:193:LEU:HB3	1:C:201:VAL:HG11	1.97	0.47
1:C:334:LEU:HD13	1:C:438:VAL:HG21	1.96	0.47
1:D:82:VAL:O	1:D:85:ARG:HB3	2.15	0.47
1:B:394:ALA:O	1:B:400:ALA:HB3	2.14	0.47
1:A:25:ASP:OD1	1:A:26:GLY:N	2.48	0.47
1:A:80:ALA:O	1:A:84:GLN:HG2	2.15	0.47
1:B:302:MET:HE1	1:D:105:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HB2	1:A:156:SER:HB3	1.97	0.47
1:A:384:GLY:HA2	1:A:413:PRO:HG3	1.97	0.47
1:D:386:VAL:HG13	1:D:386:VAL:O	2.15	0.47
1:D:408:ALA:O	1:D:409:HIS:ND1	2.47	0.47
1:B:169:THR:HG22	1:D:3:ILE:HD11	1.96	0.47
1:B:388:GLU:O	1:B:392:LEU:HG	2.15	0.47
1:A:309:ALA:O	1:A:313:SER:N	2.47	0.47
1:A:416:MET:SD	1:A:439:VAL:HG11	2.55	0.47
1:D:47:ILE:HG22	1:D:156:SER:OG	2.15	0.47
1:D:311:MET:CE	1:D:316:PHE:HB3	2.45	0.47
1:A:258:LEU:HD12	1:A:262:GLU:CG	2.44	0.46
1:A:301:TYR:HB3	1:A:305:ILE:HG12	1.96	0.46
1:C:346:HIS:HB2	1:C:371:VAL:HG13	1.97	0.46
1:D:69:GLU:HG2	1:D:145:PRO:CG	2.43	0.46
1:D:360:LEU:CD1	1:D:388:GLU:HB2	2.45	0.46
1:B:206:ALA:HB2	1:B:276:ALA:CB	2.46	0.46
1:B:346:HIS:NE2	1:B:374:GLU:HG3	2.30	0.46
1:A:311:MET:CE	1:A:316:PHE:HB3	2.45	0.46
1:D:66:THR:HA	1:D:89:LYS:O	2.15	0.46
1:D:68:VAL:HA	1:D:91:VAL:O	2.15	0.46
1:B:373:ALA:C	1:B:375:PRO:HD2	2.35	0.46
1:B:423:VAL:HG11	1:B:457:LEU:HD21	1.96	0.46
1:A:98:VAL:HG22	1:A:102:LYS:HB3	1.98	0.46
1:D:131:VAL:HG23	1:D:134:ARG:NH2	2.17	0.46
1:D:301:TYR:HB3	1:D:305:ILE:HG12	1.97	0.46
1:D:311:MET:O	1:D:316:PHE:HB2	2.16	0.46
1:C:69:GLU:HB2	1:C:145:PRO:HD2	1.96	0.46
1:D:337:LYS:HD3	1:D:340:ALA:CB	2.45	0.46
1:C:448:ILE:HD11	1:C:453:LEU:HD13	1.97	0.46
1:B:347:THR:OG1	1:B:368:MET:SD	2.69	0.46
1:A:259:ALA:HA	1:A:264:MET:O	2.16	0.46
1:C:207:ASP:OD1	1:C:211:SER:HB3	2.16	0.46
1:D:91:VAL:HG11	1:D:135:LEU:HD21	1.96	0.46
1:B:336:ARG:C	1:B:337:LYS:HD2	2.36	0.46
1:C:329:THR:OG1	1:C:421:GLU:N	2.48	0.46
1:D:113:VAL:O	1:D:113:VAL:HG13	2.16	0.46
1:D:423:VAL:HG12	1:D:423:VAL:O	2.16	0.46
1:B:180:ILE:HD11	1:B:205:GLY:CA	2.29	0.46
1:A:81:LEU:HG	1:C:263:ALA:HB1	1.98	0.46
1:D:186:ILE:HG23	1:D:187:THR:N	2.31	0.46
1:B:266:VAL:HB	1:B:270:CYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:CG1	1:B:426:ALA:HB2	2.46	0.46
1:B:445:VAL:HG22	1:B:445:VAL:O	2.15	0.46
1:C:394:ALA:O	1:C:400:ALA:HB3	2.16	0.46
1:D:74:ASN:HD21	1:D:296:ASP:CG	2.19	0.46
1:B:81:LEU:HG	1:D:263:ALA:HB1	1.98	0.46
1:A:22:VAL:HG12	1:A:278:LEU:HD11	1.98	0.46
1:A:345:VAL:HG13	1:A:345:VAL:O	2.15	0.46
1:B:207:ASP:OD1	1:B:211:SER:HB3	2.16	0.45
1:A:341:LEU:N	1:A:342:PRO:CD	2.79	0.45
1:A:347:THR:HG21	1:A:356:ALA:HB2	1.98	0.45
1:A:394:ALA:O	1:A:400:ALA:HB3	2.17	0.45
1:C:329:THR:HA	1:C:421:GLU:O	2.16	0.45
1:B:98:VAL:HG22	1:B:102:LYS:HB3	1.99	0.45
1:C:341:LEU:N	1:C:342:PRO:CD	2.78	0.45
1:D:186:ILE:HD11	1:D:203:ILE:HG22	1.98	0.45
1:D:269:SER:HB3	2:D:501:PLP:C2A	2.46	0.45
1:A:244:ILE:HD11	1:A:280:VAL:CG2	2.47	0.45
1:D:17:VAL:HG22	1:D:18:ARG:N	2.32	0.45
1:D:48:ALA:O	1:D:52:ILE:HG12	2.17	0.45
1:B:293:LEU:O	1:B:295:PRO:HD3	2.17	0.45
1:B:418:GLY:HA3	1:B:421:GLU:OE2	2.15	0.45
1:C:218:GLY:HA2	1:C:229:ASP:OD1	2.16	0.45
1:D:292:VAL:HG12	1:D:293:LEU:N	2.30	0.45
1:B:16:LEU:HD22	1:D:3:ILE:HG12	1.98	0.45
1:B:347:THR:O	1:B:370:VAL:HA	2.16	0.45
1:A:316:PHE:O	1:A:317:LEU:HB3	2.17	0.45
1:A:374:GLU:HB3	1:A:375:PRO:HD3	1.99	0.45
1:C:182:THR:HG22	2:C:501:PLP:O1P	2.15	0.45
1:C:426:ALA:O	1:C:430:LEU:HD13	2.17	0.45
1:D:394:ALA:O	1:D:400:ALA:HB3	2.16	0.45
1:C:18:ARG:HA	1:C:31:ALA:HA	1.97	0.45
1:C:354:ARG:HG3	1:D:313:SER:O	2.16	0.45
1:C:438:VAL:HG23	1:C:445:VAL:CG1	2.47	0.45
1:D:244:ILE:HD11	1:D:280:VAL:CG2	2.46	0.45
1:B:152:GLU:HA	1:B:152:GLU:OE1	2.16	0.45
1:B:334:LEU:CD1	1:B:438:VAL:HG11	2.45	0.45
1:B:395:VAL:HG11	1:B:402:LEU:HD13	1.99	0.45
1:A:365:VAL:HG22	1:A:366:SER:N	2.32	0.45
1:C:152:GLU:OE1	1:C:152:GLU:HA	2.17	0.45
1:B:227:GLY:O	1:B:228:GLU:HG2	2.16	0.45
1:A:449:THR:HG23	1:A:452:ASP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:LEU:O	1:D:295:PRO:HD3	2.17	0.45
1:D:316:PHE:O	1:D:317:LEU:HB3	2.17	0.45
1:B:165:ILE:HG23	1:B:291:VAL:HG11	1.99	0.45
1:C:360:LEU:HD23	1:C:365:VAL:HG13	1.99	0.45
1:B:23:VAL:HB	1:B:30:VAL:HG11	1.98	0.45
1:B:346:HIS:CE1	1:B:374:GLU:HG3	2.52	0.45
1:B:440:GLU:O	1:B:443:LYS:HG2	2.17	0.45
1:A:17:VAL:HG22	1:A:18:ARG:N	2.32	0.45
1:A:183:GLY:HA3	1:A:235:TYR:HB2	1.99	0.45
1:D:330:VAL:HG23	1:D:419:ALA:HA	1.99	0.45
1:D:341:LEU:N	1:D:342:PRO:CD	2.80	0.45
1:B:172:LYS:HE2	1:B:172:LYS:HB3	1.81	0.44
1:A:336:ARG:O	1:A:337:LYS:HD2	2.17	0.44
1:C:36:TYR:HA	1:C:41:GLY:O	2.17	0.44
1:C:191:ARG:O	1:C:195:GLU:HG3	2.17	0.44
1:C:277:ALA:HB2	1:C:292:VAL:HG22	2.00	0.44
1:B:260:ARG:NE	1:D:110:GLY:HA2	2.32	0.44
1:B:269:SER:OG	2:B:501:PLP:H2A3	2.17	0.44
1:A:6:HIS:CD2	1:A:85:ARG:HD2	2.53	0.44
1:A:15:PRO:HG3	1:C:10:LEU:HD13	1.98	0.44
1:A:69:GLU:HG3	1:A:145:PRO:HG2	1.99	0.44
1:C:348:HIS:NE2	1:C:374:GLU:HB2	2.33	0.44
1:B:44:LYS:HD3	2:B:501:PLP:C5	2.48	0.44
1:B:438:VAL:HG22	1:B:446:GLY:O	2.17	0.44
1:A:113:VAL:O	1:A:113:VAL:HG13	2.17	0.44
1:C:204:VAL:HG11	1:C:280:VAL:HG21	1.98	0.44
1:D:360:LEU:HD22	1:D:365:VAL:CG1	2.47	0.44
1:C:336:ARG:C	1:C:337:LYS:HD2	2.37	0.44
1:C:347:THR:HG21	1:C:356:ALA:CB	2.47	0.44
1:D:390:GLU:OE1	1:D:390:GLU:HA	2.18	0.44
1:A:224:GLU:O	2:A:501:PLP:H2A3	2.18	0.44
1:C:38:ASN:HB3	1:C:39:PRO:HD2	1.98	0.44
1:C:227:GLY:O	1:C:228:GLU:HG2	2.17	0.44
1:C:266:VAL:HB	1:C:270:CYS:HB2	1.98	0.44
1:D:25:ASP:OD1	1:D:26:GLY:N	2.51	0.44
1:A:66:THR:O	1:A:142:ALA:HA	2.17	0.44
1:C:293:LEU:O	1:C:295:PRO:HD3	2.17	0.44
1:A:110:GLY:HA2	1:C:260:ARG:NE	2.32	0.44
1:C:366:SER:O	1:C:367:GLN:HG2	2.18	0.44
1:D:253:ASP:HB2	1:D:318:ARG:NH1	2.33	0.44
1:A:120:VAL:HG11	1:A:126:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:THR:CG2	1:A:326:GLU:H	2.27	0.44
1:D:305:ILE:HG13	1:D:306:PHE:CD2	2.53	0.44
1:B:149:ALA:CB	1:B:233:ALA:HB3	2.48	0.43
1:B:304:LYS:O	1:B:310:TRP:CE3	2.71	0.43
1:A:258:LEU:HD12	1:A:262:GLU:HG2	1.99	0.43
1:B:69:GLU:CD	1:B:145:PRO:HG2	2.39	0.43
1:A:270:CYS:HB3	1:A:294:LEU:HD22	2.00	0.43
1:A:423:VAL:CG1	1:A:453:LEU:HD11	2.46	0.43
1:C:395:VAL:HG13	1:C:402:LEU:HD22	2.00	0.43
1:B:18:ARG:NH2	1:B:29:THR:HG21	2.32	0.43
1:B:166:TRP:NE1	1:B:171:GLY:HA2	2.33	0.43
1:B:177:VAL:HG21	1:B:277:ALA:HB2	2.00	0.43
1:B:193:LEU:O	1:B:197:SER:HB2	2.19	0.43
1:B:311:MET:HE1	1:B:316:PHE:HB3	2.01	0.43
1:B:392:LEU:O	1:A:450:ARG:HD3	2.19	0.43
1:C:356:ALA:O	1:C:359:ILE:HG22	2.18	0.43
1:C:421:GLU:N	1:C:421:GLU:OE1	2.51	0.43
1:D:98:VAL:HG22	1:D:102:LYS:HB3	2.01	0.43
1:D:120:VAL:HG11	1:D:126:ALA:CB	2.47	0.43
1:D:192:TYR:CE1	1:D:196:VAL:HG21	2.53	0.43
1:B:378:MET:HE3	1:B:382:VAL:HG12	2.00	0.43
1:A:120:VAL:HG11	1:A:126:ALA:HB1	2.01	0.43
1:A:143:TRP:CH2	1:A:145:PRO:HB3	2.54	0.43
1:A:320:ARG:HG3	1:A:325:THR:O	2.18	0.43
1:D:228:GLU:HG3	1:D:229:ASP:H	1.83	0.43
1:A:208:PRO:HG3	1:A:226:VAL:HG23	1.99	0.43
1:A:293:LEU:O	1:A:295:PRO:HD3	2.19	0.43
1:D:6:HIS:CD2	1:D:85:ARG:HD2	2.53	0.43
1:D:49:VAL:HA	1:D:82:VAL:HG11	2.01	0.43
1:C:316:PHE:O	1:C:317:LEU:HB3	2.18	0.43
1:D:158:TYR:CE1	1:D:192:TYR:HD2	2.36	0.43
1:A:256:ARG:HH22	1:A:311:MET:HG3	1.78	0.43
1:A:330:VAL:HG23	1:A:419:ALA:HA	1.99	0.43
1:C:149:ALA:HB1	1:C:233:ALA:HB3	1.99	0.43
1:D:336:ARG:O	1:D:337:LYS:HD2	2.18	0.43
1:B:50:LYS:HG2	1:B:156:SER:HB2	2.01	0.43
1:B:204:VAL:HG12	1:B:205:GLY:N	2.33	0.43
1:B:294:LEU:HA	1:B:295:PRO:HD3	1.86	0.43
1:B:341:LEU:O	1:B:341:LEU:HG	2.18	0.43
1:A:390:GLU:OE1	1:A:390:GLU:HA	2.18	0.43
1:C:312:SER:HB2	1:C:317:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:VAL:HG23	1:D:262:GLU:CD	2.39	0.43
1:D:431:ARG:O	1:D:431:ARG:HG2	2.18	0.43
1:A:158:TYR:CE1	1:A:192:TYR:HD2	2.37	0.43
1:A:390:GLU:O	1:A:394:ALA:N	2.48	0.43
1:C:69:GLU:CD	1:C:145:PRO:HG2	2.39	0.43
1:C:61:LEU:HD21	1:C:88:TYR:CD2	2.54	0.43
1:C:204:VAL:HG12	1:C:205:GLY:N	2.34	0.43
1:C:267:GLY:HA2	1:C:301:TYR:HD2	1.84	0.43
1:C:341:LEU:HG	1:C:341:LEU:O	2.18	0.43
1:C:359:ILE:HA	1:C:362:GLU:HG2	2.00	0.43
1:D:143:TRP:CH2	1:D:145:PRO:HB3	2.53	0.43
1:A:6:HIS:HD2	1:A:8:SER:HB3	1.84	0.42
1:A:256:ARG:HH21	1:A:311:MET:HG3	1.80	0.42
1:A:430:LEU:HD23	1:A:450:ARG:HG2	2.01	0.42
1:C:381:GLU:O	1:C:381:GLU:HG3	2.19	0.42
1:B:107:ILE:CG2	1:D:322:ASP:HB3	2.49	0.42
1:B:128:TYR:CA	1:B:131:VAL:HG12	2.48	0.42
1:B:277:ALA:HB2	1:B:292:VAL:HG22	2.01	0.42
1:A:44:LYS:HG2	2:A:501:PLP:C4A	2.48	0.42
1:A:236:ASP:HB2	1:A:239:VAL:HG23	2.01	0.42
1:C:373:ALA:C	1:C:375:PRO:HD2	2.40	0.42
1:D:22:VAL:HG12	1:D:278:LEU:HD11	2.01	0.42
1:B:44:LYS:HE3	2:B:501:PLP:H5A1	2.01	0.42
1:B:384:GLY:HA2	1:B:413:PRO:HG3	1.99	0.42
1:B:431:ARG:O	1:B:431:ARG:HG2	2.19	0.42
1:C:443:LYS:O	1:C:443:LYS:HG3	2.19	0.42
1:D:6:HIS:HD2	1:D:8:SER:HB3	1.85	0.42
1:B:22:VAL:HG23	1:B:262:GLU:HG2	2.01	0.42
1:B:173:VAL:O	1:B:201:VAL:HG22	2.20	0.42
1:B:426:ALA:O	1:B:430:LEU:HD13	2.19	0.42
1:A:329:THR:HA	1:A:421:GLU:O	2.19	0.42
1:D:185:THR:HG21	1:D:293:LEU:HD22	2.00	0.42
1:A:228:GLU:HG3	1:A:229:ASP:H	1.84	0.42
1:A:352:THR:HG22	1:A:402:LEU:O	2.20	0.42
1:C:48:ALA:HB1	1:C:79:LEU:HD23	2.01	0.42
1:B:61:LEU:HD21	1:B:88:TYR:CD2	2.54	0.42
1:B:430:LEU:CD1	1:B:436:LEU:HD21	2.48	0.42
1:A:157:HIS:O	1:A:161:THR:HB	2.20	0.42
1:A:192:TYR:CE1	1:A:196:VAL:HG21	2.54	0.42
1:A:399:ARG:NH1	1:A:399:ARG:HB2	2.35	0.42
1:C:182:THR:O	1:C:182:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:HD22	1:C:274:VAL:HG21	2.02	0.42
1:C:292:VAL:HG12	1:C:293:LEU:N	2.35	0.42
1:D:29:THR:CG2	1:D:289:LEU:HG	2.49	0.42
1:D:66:THR:HG22	1:D:89:LYS:HE3	2.01	0.42
1:D:66:THR:O	1:D:142:ALA:HA	2.19	0.42
1:D:360:LEU:HD12	1:D:388:GLU:HB2	2.01	0.42
1:C:128:TYR:CA	1:C:131:VAL:HG12	2.48	0.42
1:D:223:VAL:CG2	1:D:226:VAL:HG22	2.49	0.42
1:B:302:MET:CE	1:D:105:VAL:HA	2.50	0.42
1:B:352:THR:CG2	1:B:403:ALA:HA	2.50	0.42
1:C:223:VAL:HG23	1:C:268:GLY:HA3	2.01	0.42
1:D:236:ASP:HB2	1:D:239:VAL:HG23	2.02	0.42
1:D:256:ARG:HH21	1:D:311:MET:HG3	1.82	0.42
1:D:384:GLY:HA2	1:D:413:PRO:HG3	2.01	0.42
1:D:390:GLU:O	1:D:394:ALA:N	2.51	0.42
1:B:113:VAL:O	1:B:113:VAL:HG13	2.20	0.42
1:A:105:VAL:HA	1:C:302:MET:HE1	2.01	0.42
1:C:38:ASN:ND2	1:C:45:ASP:OD1	2.49	0.42
1:D:169:THR:O	1:D:172:LYS:HG2	2.20	0.42
1:B:14:THR:HG22	1:B:46:ARG:NH2	2.34	0.42
1:B:381:GLU:O	1:B:381:GLU:HG3	2.20	0.42
1:A:255:THR:OG1	1:A:267:GLY:O	2.28	0.42
1:A:266:VAL:HB	1:A:270:CYS:HB2	2.01	0.42
1:A:305:ILE:HG13	1:A:306:PHE:CD2	2.55	0.42
1:A:437:MET:HG3	1:A:447:VAL:HG22	2.01	0.42
1:B:387:SER:OG	1:B:388:GLU:N	2.53	0.41
1:A:169:THR:O	1:A:172:LYS:HG2	2.20	0.41
1:A:325:THR:CG2	1:A:326:GLU:N	2.82	0.41
1:A:414:LEU:H	1:A:414:LEU:HG	1.75	0.41
1:C:85:ARG:HG2	1:C:86:ARG:HG3	2.01	0.41
1:D:253:ASP:HB2	1:D:318:ARG:HH11	1.85	0.41
1:B:326:GLU:C	1:B:327:GLN:HG3	2.39	0.41
1:B:414:LEU:HD13	1:B:436:LEU:HA	2.02	0.41
1:C:185:THR:HG23	1:C:186:ILE:N	2.35	0.41
1:D:185:THR:HB	2:D:501:PLP:O1P	2.21	0.41
1:B:85:ARG:HG2	1:B:86:ARG:HG3	2.02	0.41
1:A:139:ILE:HD12	1:A:140:ASP:H	1.86	0.41
1:B:311:MET:HE3	1:B:317:LEU:N	2.35	0.41
1:B:337:LYS:HB2	1:B:340:ALA:CB	2.42	0.41
1:B:347:THR:HG21	1:B:356:ALA:CB	2.48	0.41
1:A:66:THR:HG22	1:A:89:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ARG:HD3	1:D:324:SER:O	2.21	0.41
1:D:378:MET:HE3	1:D:382:VAL:HG12	2.01	0.41
1:B:48:ALA:CB	1:B:79:LEU:HD23	2.49	0.41
1:B:71:THR:HG22	1:B:73:GLY:H	1.86	0.41
1:B:84:GLN:NE2	1:D:263:ALA:HA	2.36	0.41
1:C:17:VAL:HG12	1:C:18:ARG:N	2.35	0.41
1:D:120:VAL:HG11	1:D:126:ALA:HB1	2.03	0.41
1:D:166:TRP:CD1	1:D:171:GLY:HA2	2.56	0.41
1:D:214:SER:OG	1:D:245:ALA:HB2	2.21	0.41
1:D:399:ARG:NH1	1:D:399:ARG:HB2	2.35	0.41
1:B:207:ASP:OD2	1:B:213:TYR:HD2	2.02	0.41
1:A:44:LYS:NZ	2:A:501:PLP:H5A2	2.35	0.41
1:C:311:MET:CE	1:C:316:PHE:HB3	2.51	0.41
1:D:208:PRO:HD3	1:D:226:VAL:HG23	2.01	0.41
1:B:116:CYS:SG	1:B:131:VAL:HG11	2.60	0.41
1:B:139:ILE:HG23	1:B:139:ILE:O	2.21	0.41
1:A:24:PRO:HD3	1:A:278:LEU:HD13	2.01	0.41
1:D:157:HIS:O	1:D:161:THR:HB	2.21	0.41
1:D:265:LEU:HD23	1:D:265:LEU:HA	1.92	0.41
1:D:341:LEU:HG	1:D:341:LEU:O	2.21	0.41
1:D:438:VAL:HG23	1:D:445:VAL:HG12	2.03	0.41
1:B:35:GLU:HB2	1:B:294:LEU:O	2.21	0.41
1:A:166:TRP:CD1	1:A:171:GLY:HA2	2.56	0.41
1:A:263:ALA:HB2	1:C:84:GLN:HE21	1.85	0.41
1:C:113:VAL:O	1:C:113:VAL:HG13	2.20	0.41
1:C:139:ILE:HG23	1:C:139:ILE:O	2.20	0.41
1:B:50:LYS:CG	1:B:156:SER:HB2	2.51	0.41
1:B:68:VAL:HG22	1:B:91:VAL:HB	2.02	0.41
1:B:186:ILE:HD12	1:B:203:ILE:CG2	2.51	0.41
1:B:208:PRO:HA	1:B:246:VAL:O	2.21	0.41
1:B:267:GLY:HA2	1:B:301:TYR:HD2	1.85	0.41
1:B:301:TYR:HB3	1:B:305:ILE:HG12	2.03	0.41
1:A:14:THR:OG1	1:A:15:PRO:HD2	2.20	0.41
1:A:29:THR:CG2	1:A:289:LEU:HG	2.51	0.41
1:A:208:PRO:HD3	1:A:226:VAL:HG23	2.02	0.41
1:A:260:ARG:HD2	1:A:260:ARG:O	2.20	0.41
1:A:311:MET:O	1:A:316:PHE:HB2	2.21	0.41
1:C:102:LYS:HD2	1:C:102:LYS:HA	1.89	0.41
1:C:116:CYS:SG	1:C:131:VAL:HG11	2.61	0.41
1:C:166:TRP:NE1	1:C:171:GLY:HA2	2.36	0.41
1:C:311:MET:HE3	1:C:316:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:TYR:HB2	1:D:392:LEU:CD1	2.51	0.41
1:D:423:VAL:CG1	1:D:453:LEU:HD11	2.49	0.41
1:B:200:ARG:NH1	1:B:200:ARG:HB2	2.36	0.41
1:A:214:SER:OG	1:A:245:ALA:HB2	2.21	0.41
1:A:341:LEU:H	1:A:341:LEU:HD23	1.86	0.41
1:A:373:ALA:C	1:A:375:PRO:HD2	2.42	0.41
1:C:239:VAL:HB	1:C:240:PRO:CD	2.51	0.41
1:C:255:THR:OG1	1:C:267:GLY:O	2.20	0.41
1:D:139:ILE:HG22	1:D:140:ASP:N	2.35	0.41
1:B:7:ILE:HD12	1:D:264:MET:HG2	2.02	0.40
1:B:84:GLN:HE21	1:D:263:ALA:HB2	1.86	0.40
1:B:239:VAL:N	1:B:240:PRO:HD2	2.36	0.40
1:B:354:ARG:CD	1:A:314:TYR:HE1	2.30	0.40
1:A:239:VAL:HB	1:A:240:PRO:CD	2.52	0.40
1:C:18:ARG:NH2	1:C:29:THR:HG21	2.35	0.40
1:C:296:ASP:OD2	2:C:501:PLP:C2A	2.69	0.40
1:C:386:VAL:O	1:C:386:VAL:HG13	2.22	0.40
1:C:440:GLU:O	1:C:443:LYS:HG2	2.20	0.40
1:D:14:THR:OG1	1:D:15:PRO:HD2	2.21	0.40
1:D:50:LYS:CB	1:D:156:SER:HB3	2.50	0.40
1:A:185:THR:CG2	1:A:293:LEU:HD23	2.50	0.40
1:A:280:VAL:O	1:A:280:VAL:HG12	2.22	0.40
1:B:38:ASN:HB3	1:B:39:PRO:HD2	2.02	0.40
1:B:239:VAL:HB	1:B:240:PRO:CD	2.51	0.40
1:B:292:VAL:HG12	1:B:293:LEU:N	2.36	0.40
1:A:22:VAL:HG23	1:A:262:GLU:CD	2.42	0.40
1:C:157:HIS:O	1:C:161:THR:HB	2.21	0.40
1:C:239:VAL:N	1:C:240:PRO:HD2	2.37	0.40
1:C:311:MET:O	1:C:316:PHE:HB2	2.22	0.40
1:D:35:GLU:OE2	1:D:46:ARG:NE	2.54	0.40
1:D:266:VAL:HB	1:D:270:CYS:HB2	2.03	0.40
1:D:365:VAL:HG22	1:D:366:SER:N	2.35	0.40
1:A:7:ILE:HG13	1:A:7:ILE:O	2.22	0.40
1:A:437:MET:HE2	1:A:437:MET:HB2	1.97	0.40
1:C:68:VAL:HG22	1:C:91:VAL:HB	2.02	0.40
1:C:453:LEU:HD12	1:C:453:LEU:HA	1.73	0.40
1:D:341:LEU:H	1:D:341:LEU:HD23	1.86	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	456/478 (95%)	405 (89%)	50 (11%)	1 (0%)	47 79
1	B	456/478 (95%)	410 (90%)	46 (10%)	0	100 100
1	C	456/478 (95%)	410 (90%)	46 (10%)	0	100 100
1	D	456/478 (95%)	404 (89%)	52 (11%)	0	100 100
All	All	1824/1912 (95%)	1629 (89%)	194 (11%)	1 (0%)	54 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	THR

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	351/365 (96%)	340 (97%)	11 (3%)	40 71
1	B	351/365 (96%)	343 (98%)	8 (2%)	50 76
1	C	351/365 (96%)	338 (96%)	13 (4%)	34 66
1	D	351/365 (96%)	339 (97%)	12 (3%)	37 69
All	All	1404/1460 (96%)	1360 (97%)	44 (3%)	43 71

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	LEU
1	B	81	LEU
1	B	134	ARG
1	B	180	ILE
1	B	182	THR
1	B	354	ARG
1	B	371	VAL
1	B	436	LEU
1	A	23	VAL
1	A	74	ASN
1	A	93	VAL
1	A	177	VAL
1	A	180	ILE
1	A	182	THR
1	A	204	VAL
1	A	278	LEU
1	A	291	VAL
1	A	436	LEU
1	A	437	MET
1	C	16	LEU
1	C	43	SER
1	C	45	ASP
1	C	47	ILE
1	C	49	VAL
1	C	81	LEU
1	C	180	ILE
1	C	182	THR
1	C	291	VAL
1	C	354	ARG
1	C	371	VAL
1	C	414	LEU
1	C	436	LEU
1	D	23	VAL
1	D	81	LEU
1	D	93	VAL
1	D	177	VAL
1	D	204	VAL
1	D	278	LEU
1	D	291	VAL
1	D	348	HIS
1	D	354	ARG
1	D	371	VAL
1	D	436	LEU

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Mol	Chain	Res	Type
1	D	437	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	6	HIS
1	B	84	GLN
1	A	5	GLN
1	A	6	HIS
1	A	348	HIS
1	C	6	HIS
1	C	84	GLN
1	D	6	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PLP	A	501	1	15,15,16	1.76	3 (20%)	20,22,23	1.43	4 (20%)
2	PLP	D	501	1	15,15,16	1.60	3 (20%)	20,22,23	1.09	2 (10%)
2	PLP	B	501	1	15,15,16	1.72	3 (20%)	20,22,23	1.10	2 (10%)
2	PLP	C	501	1	15,15,16	1.54	2 (13%)	20,22,23	1.05	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	501	1	-	3/6/6/8	0/1/1/1
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1
2	PLP	B	501	1	-	3/6/6/8	0/1/1/1
2	PLP	C	501	1	-	2/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C5-C4	-4.76	1.35	1.40
2	B	501	PLP	C5-C4	-4.50	1.35	1.40
2	D	501	PLP	C5-C4	-4.20	1.35	1.40
2	C	501	PLP	C5-C4	-3.90	1.36	1.40
2	A	501	PLP	C3-C4	-2.58	1.34	1.40
2	B	501	PLP	C3-C2	-2.43	1.38	1.40
2	B	501	PLP	C3-C4	-2.36	1.35	1.40
2	A	501	PLP	C3-C2	-2.31	1.38	1.40
2	D	501	PLP	C3-C4	-2.10	1.35	1.40
2	D	501	PLP	C3-C2	-2.01	1.38	1.40
2	C	501	PLP	C3-C4	-2.01	1.35	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PLP	C2A-C2-C3	-2.50	117.80	120.89
2	D	501	PLP	C5-C6-N1	-2.45	119.74	123.82
2	B	501	PLP	C5-C6-N1	-2.45	119.75	123.82
2	A	501	PLP	O4P-C5A-C5	2.38	113.89	109.35
2	A	501	PLP	C6-C5-C4	2.36	120.01	118.16
2	C	501	PLP	O4P-C5A-C5	2.36	113.84	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	PLP	C6-C5-C4	2.31	119.98	118.16
2	A	501	PLP	C5-C6-N1	-2.26	120.05	123.82
2	B	501	PLP	C6-C5-C4	2.04	119.77	118.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

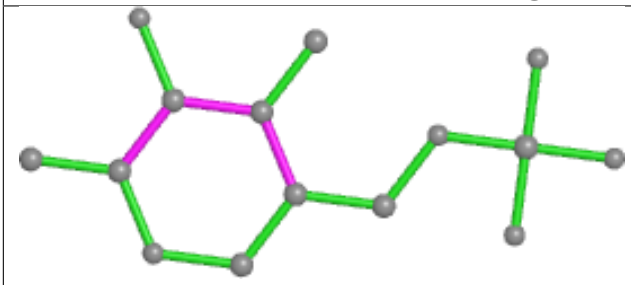
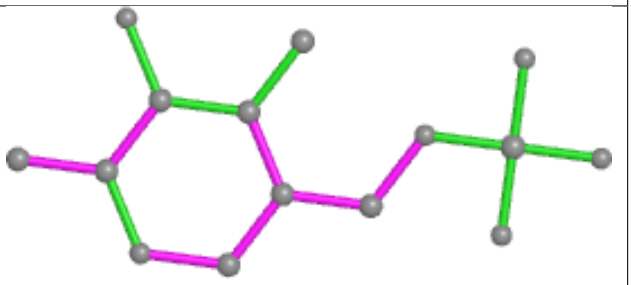
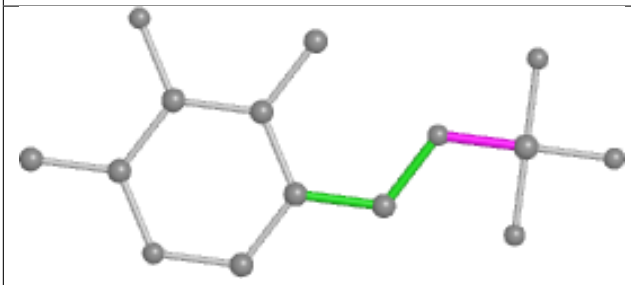
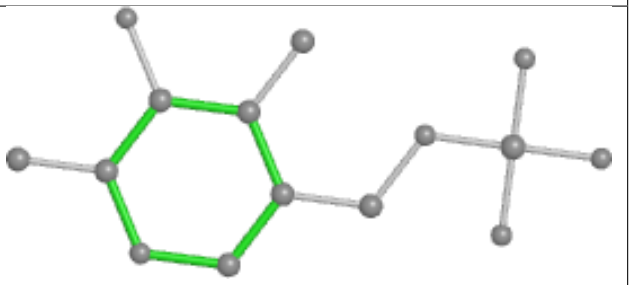
Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C5A-O4P-P-O2P
2	B	501	PLP	C5A-O4P-P-O3P
2	A	501	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C5A-O4P-P-O3P
2	C	501	PLP	C4-C5-C5A-O4P
2	C	501	PLP	C6-C5-C5A-O4P
2	B	501	PLP	C5A-O4P-P-O1P
2	A	501	PLP	C5A-O4P-P-O1P

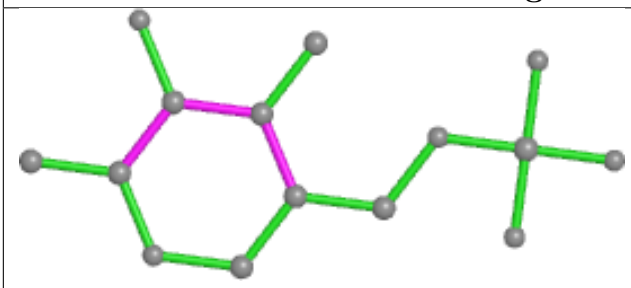
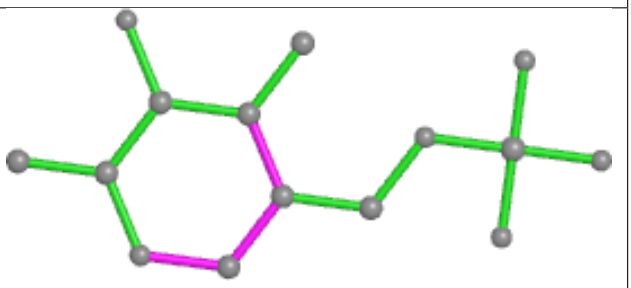
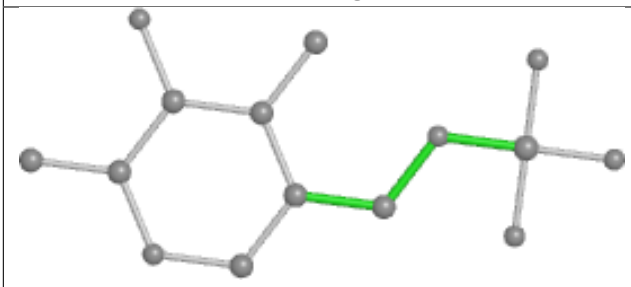
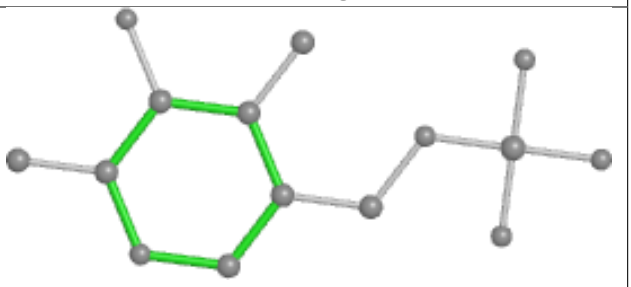
There are no ring outliers.

4 monomers are involved in 18 short contacts:

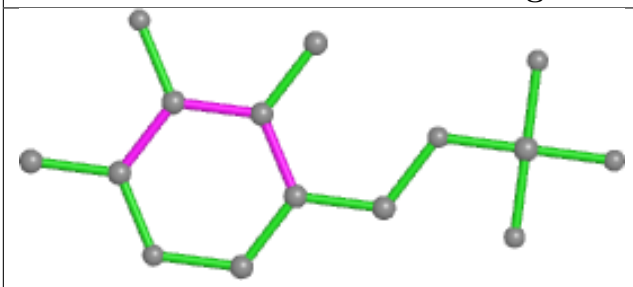
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	5	0
2	D	501	PLP	5	0
2	B	501	PLP	5	0
2	C	501	PLP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

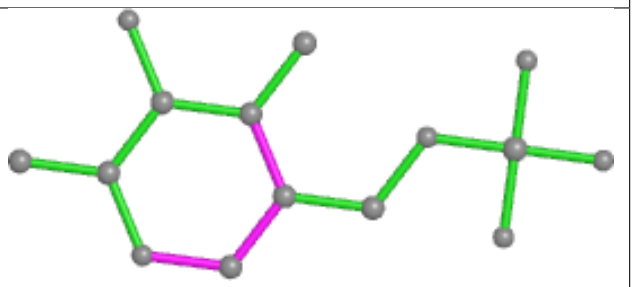
Ligand PLP A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

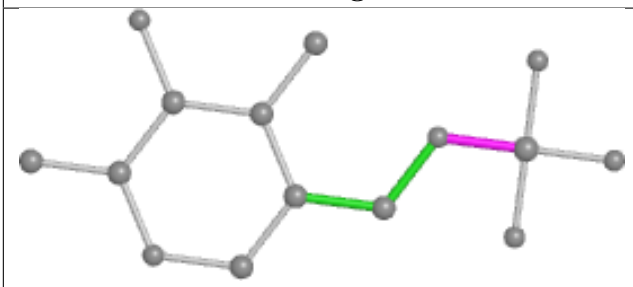
Ligand PLP B 501



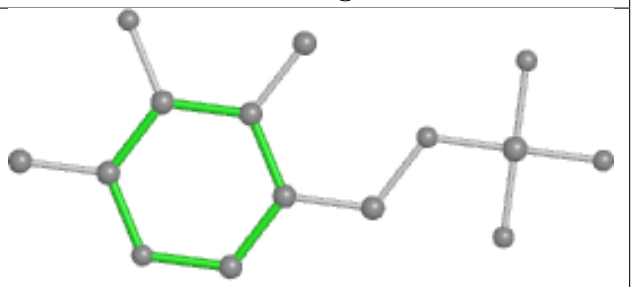
Bond lengths



Bond angles

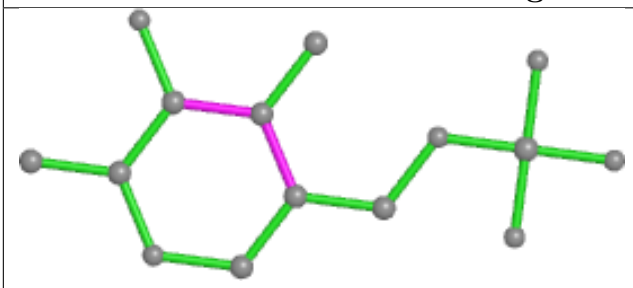


Torsions

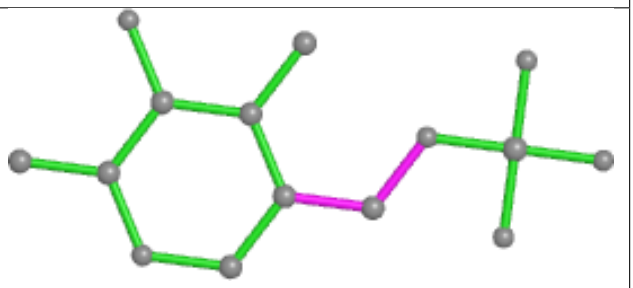


Rings

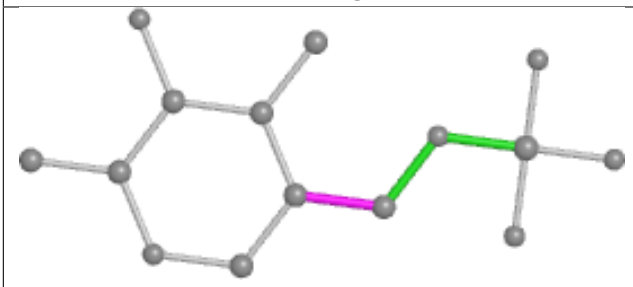
Ligand PLP C 501



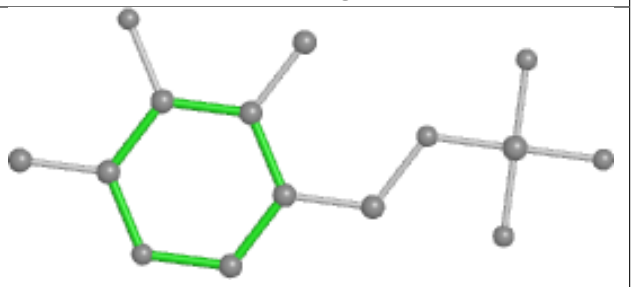
Bond lengths



Bond angles



Torsions



Rings

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.

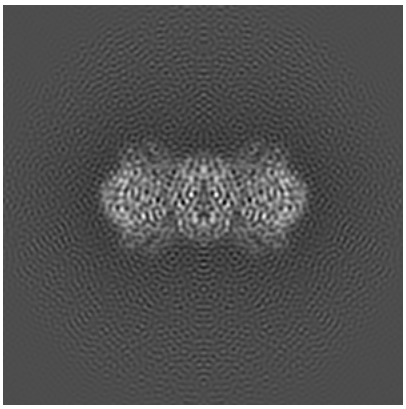
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33348. These allow visual inspection of the internal detail of the map and identification of artifacts.

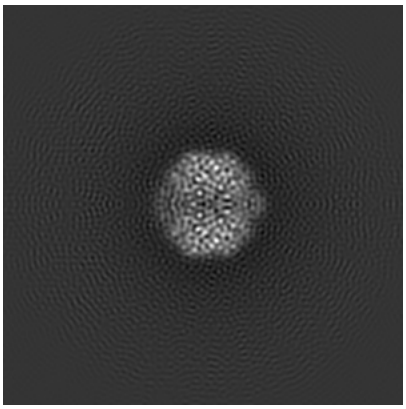
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

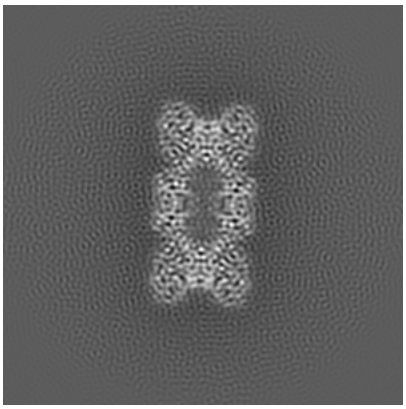
6.1.1 Primary map



X

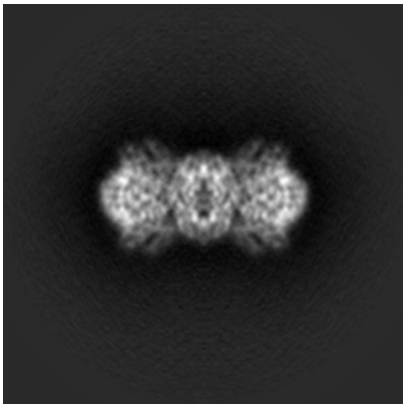


Y

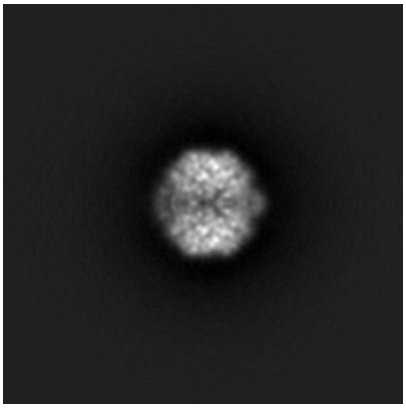


Z

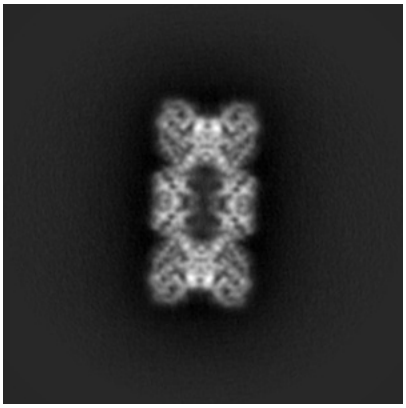
6.1.2 Raw map



X



Y

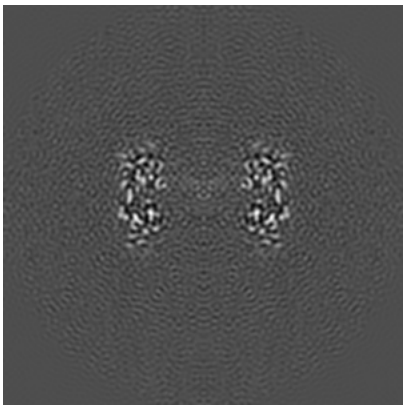


Z

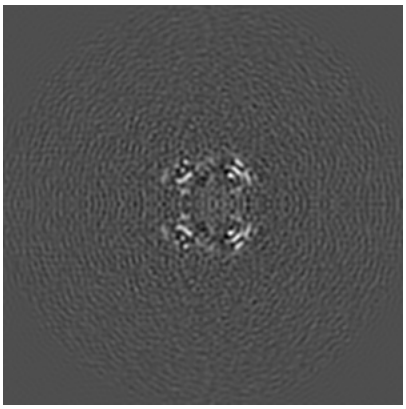
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

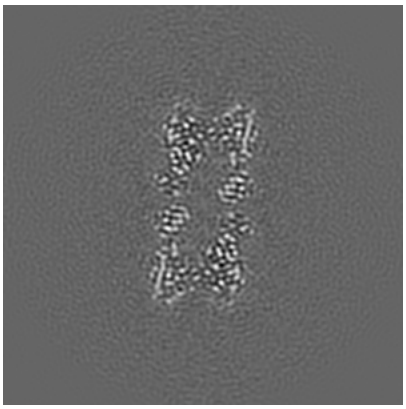
6.2.1 Primary map



X Index: 120

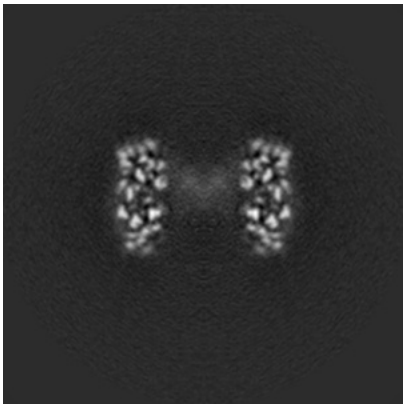


Y Index: 120

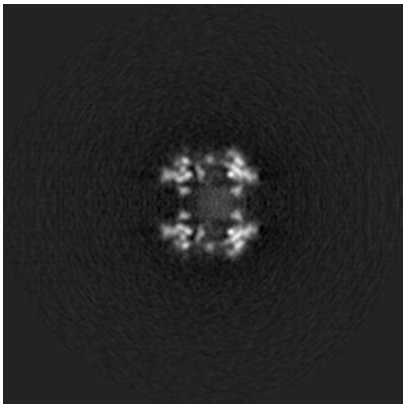


Z Index: 120

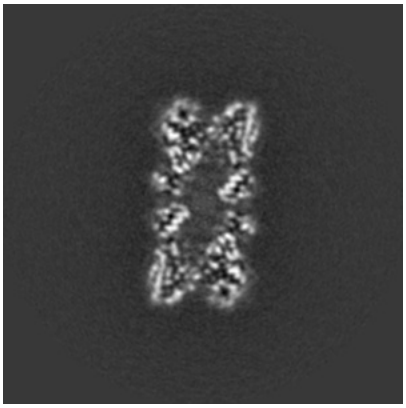
6.2.2 Raw map



X Index: 120



Y Index: 120

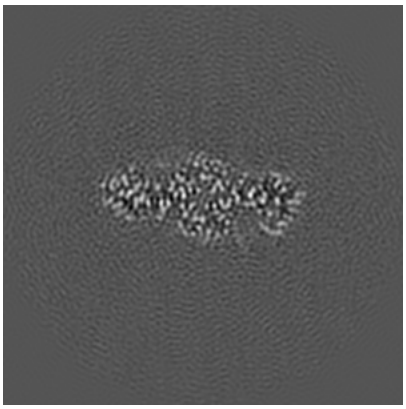


Z Index: 120

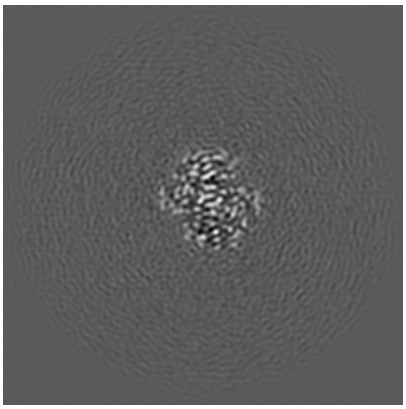
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

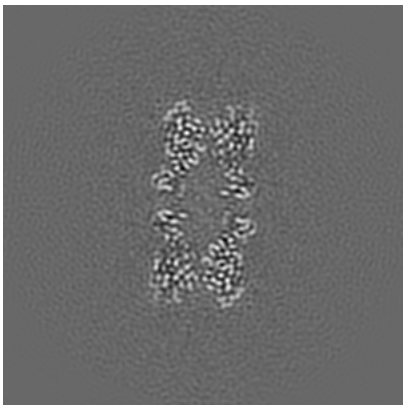
6.3.1 Primary map



X Index: 137

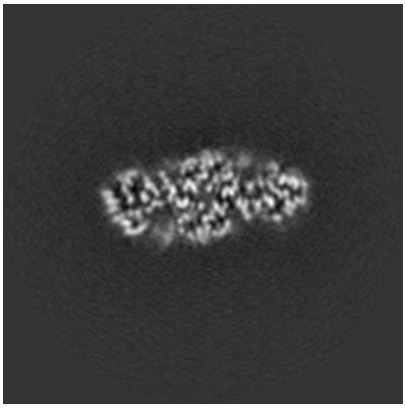


Y Index: 164

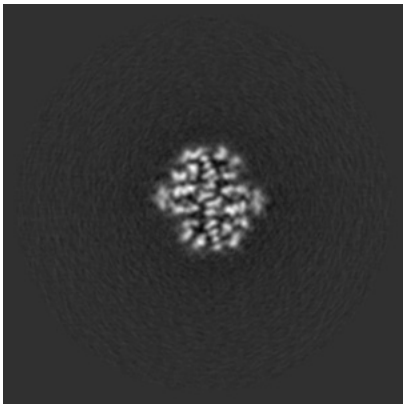


Z Index: 122

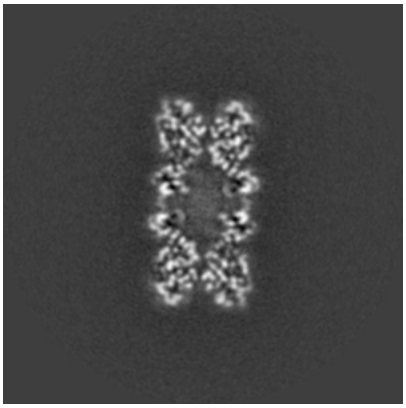
6.3.2 Raw map



X Index: 103



Y Index: 165



Z Index: 125

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

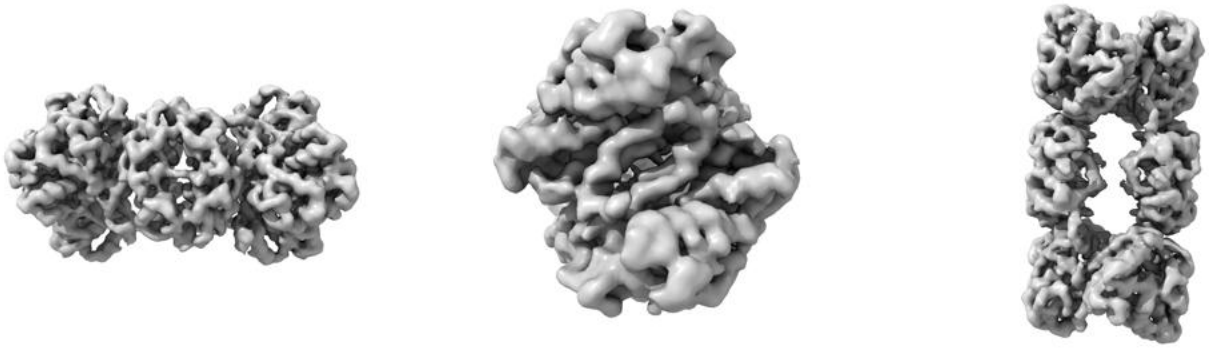
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0348. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

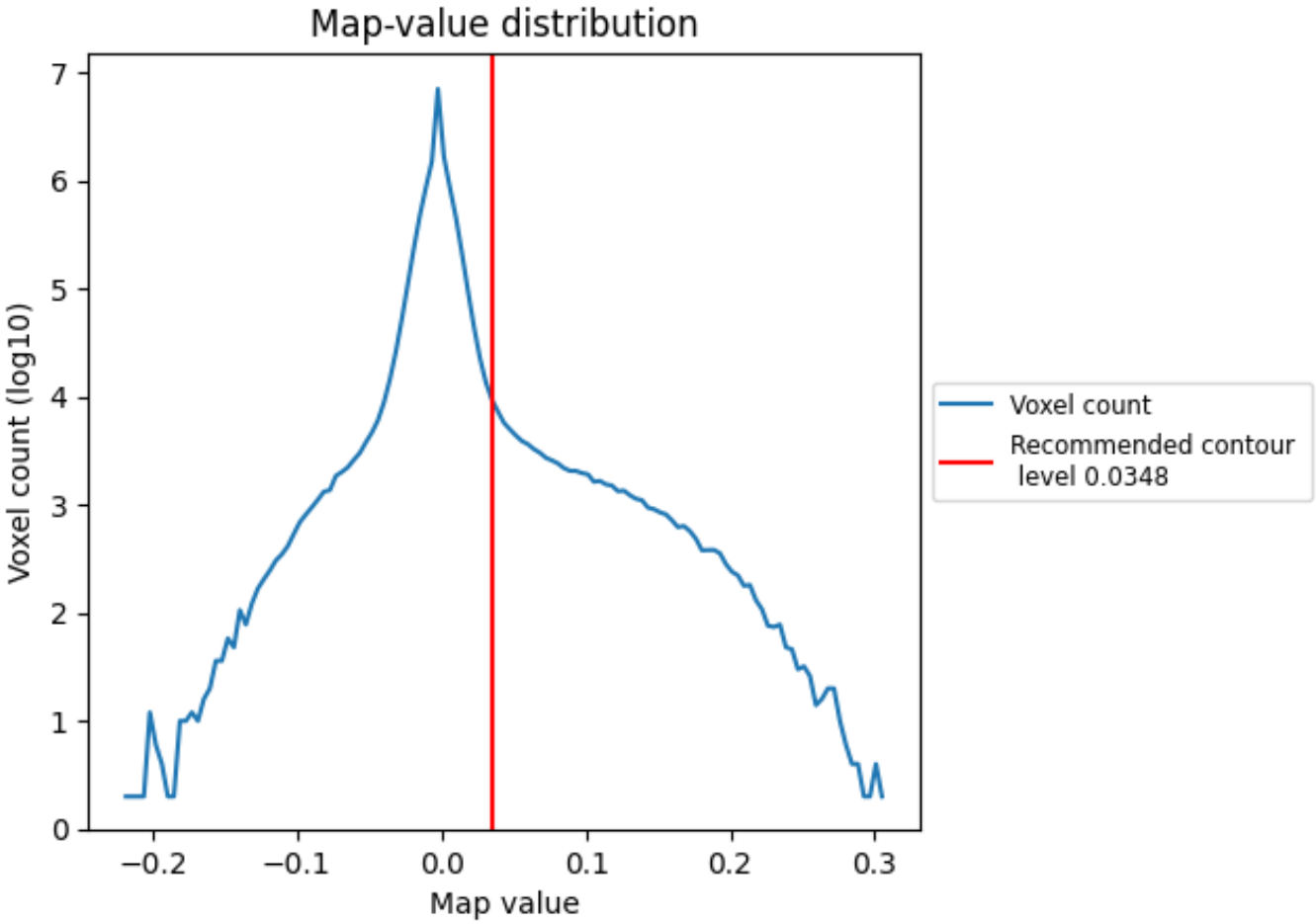
6.5 Mask visualisation (i)

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

7 Map analysis

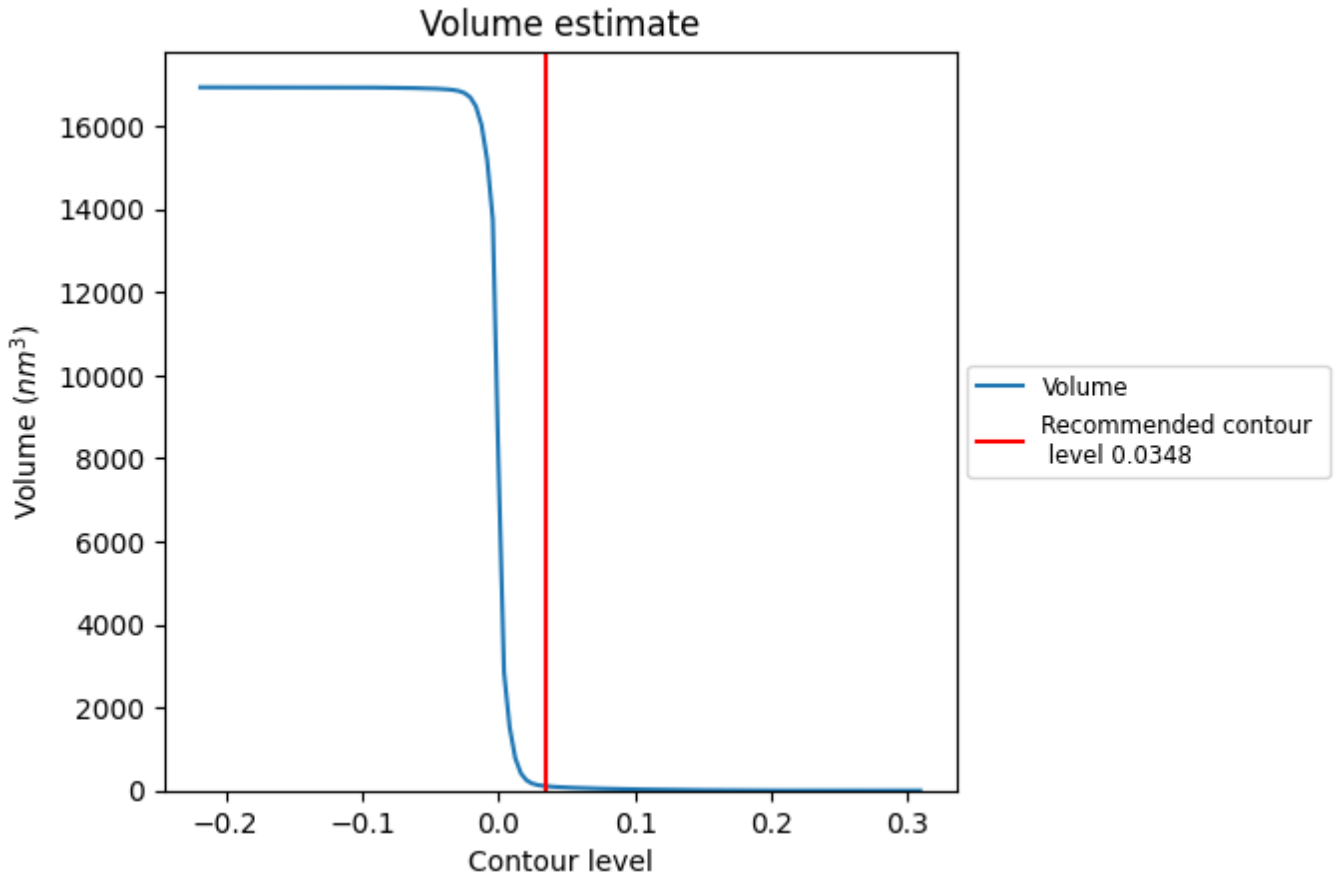
This section contains the results of statistical analysis of the map.

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.

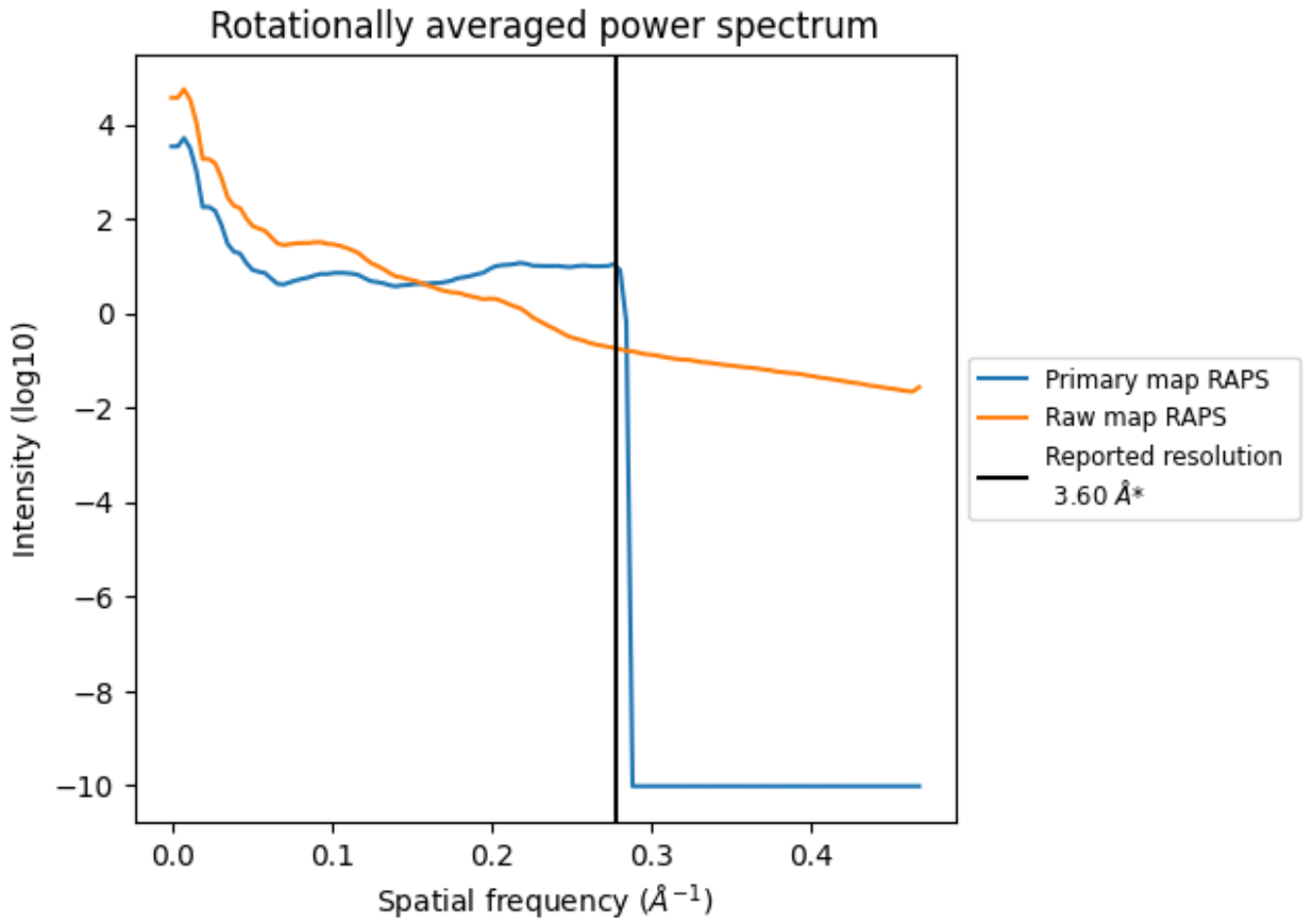
7.2 Volume estimate



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

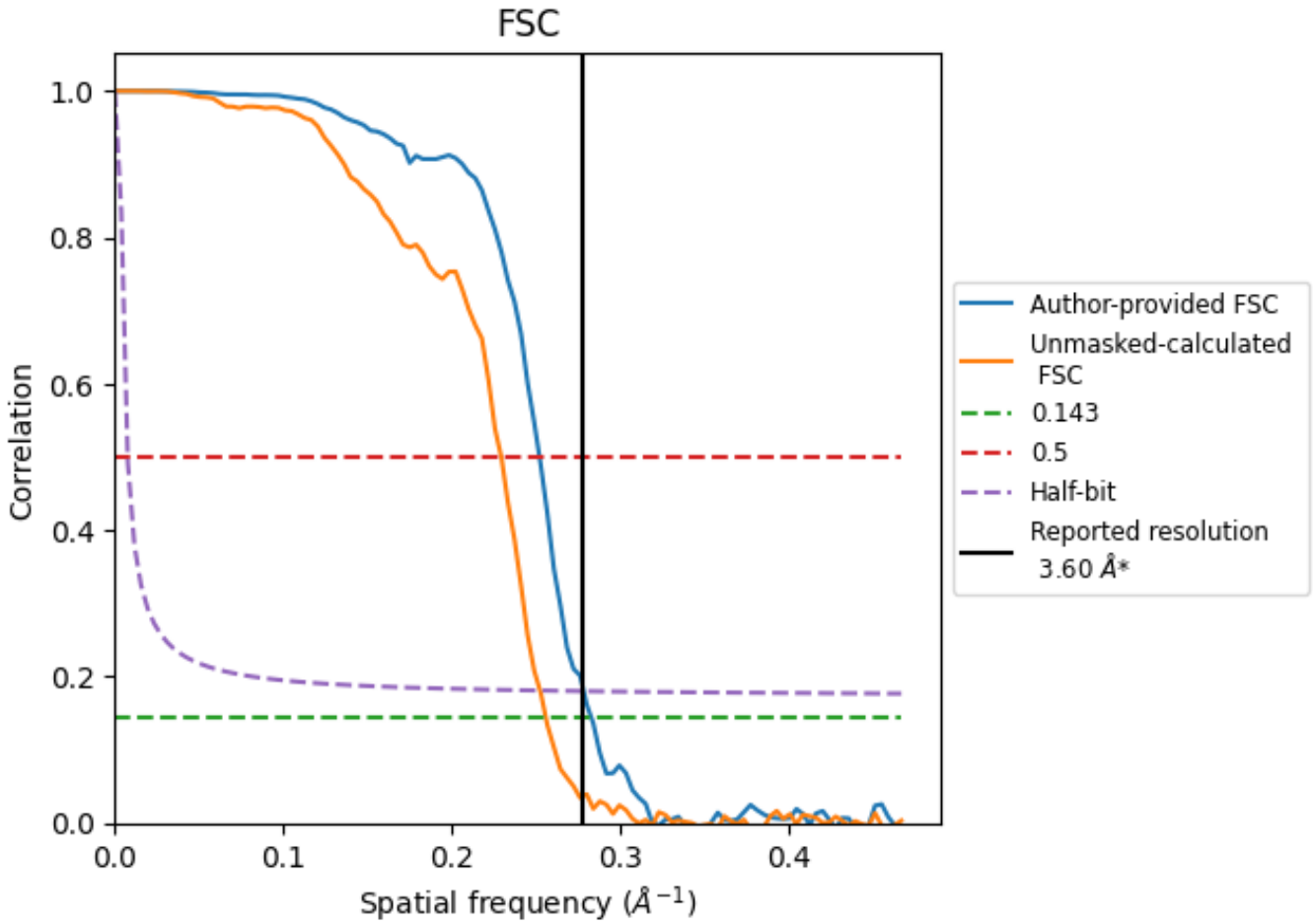


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

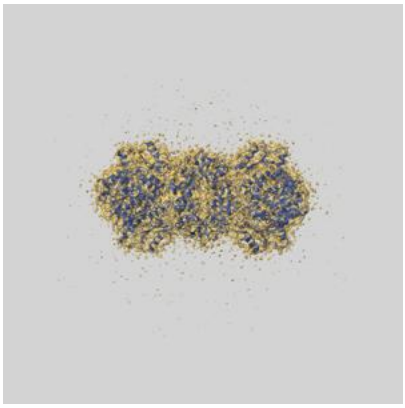
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	3.96	3.59
Unmasked-calculated*	3.90	4.36	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

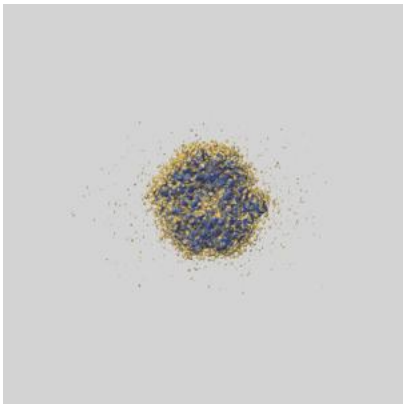
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33348 and PDB model 7XOH. Per-residue inclusion information can be found in section 3 on page 6.

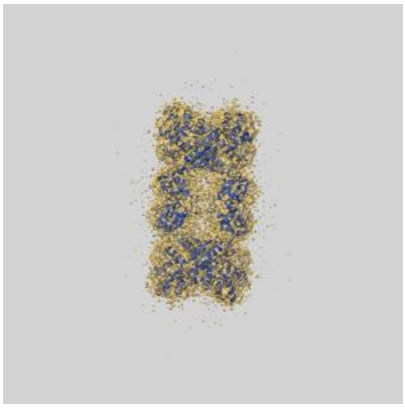
9.1 Map-model overlay



X



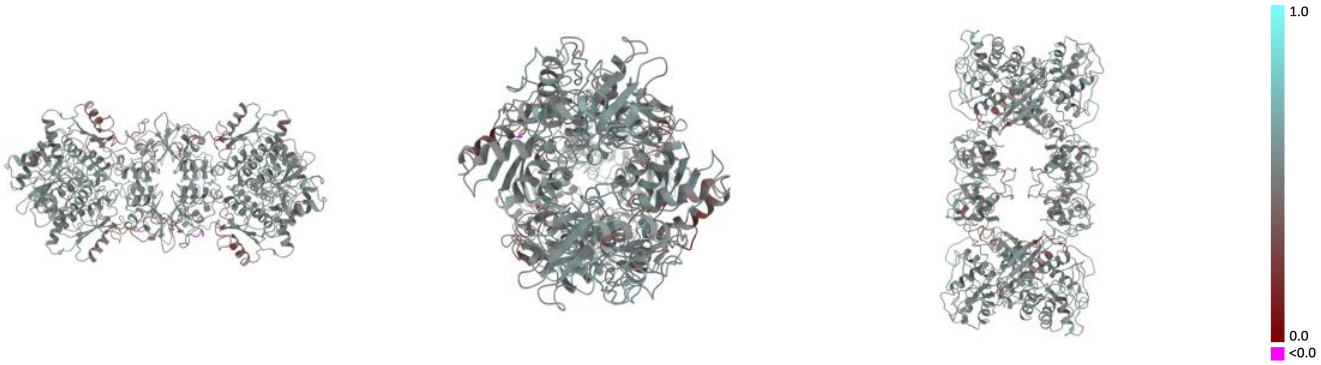
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0348 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

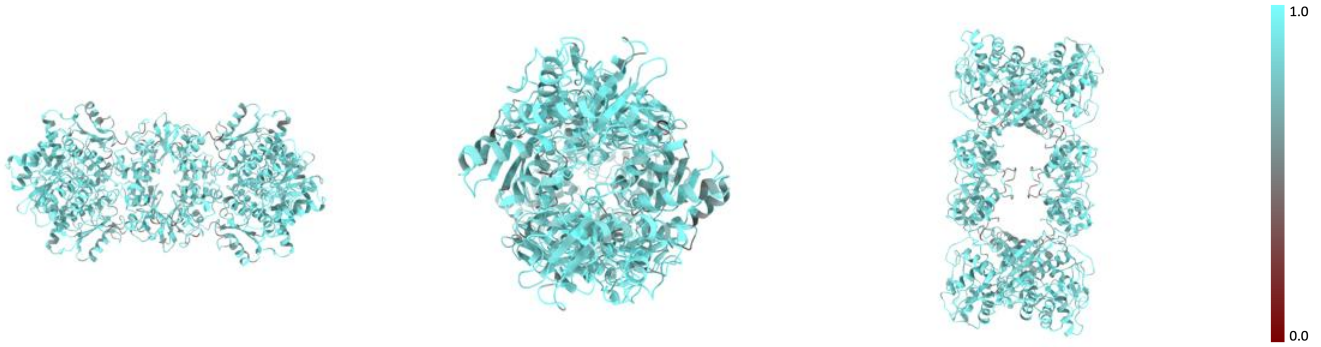
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

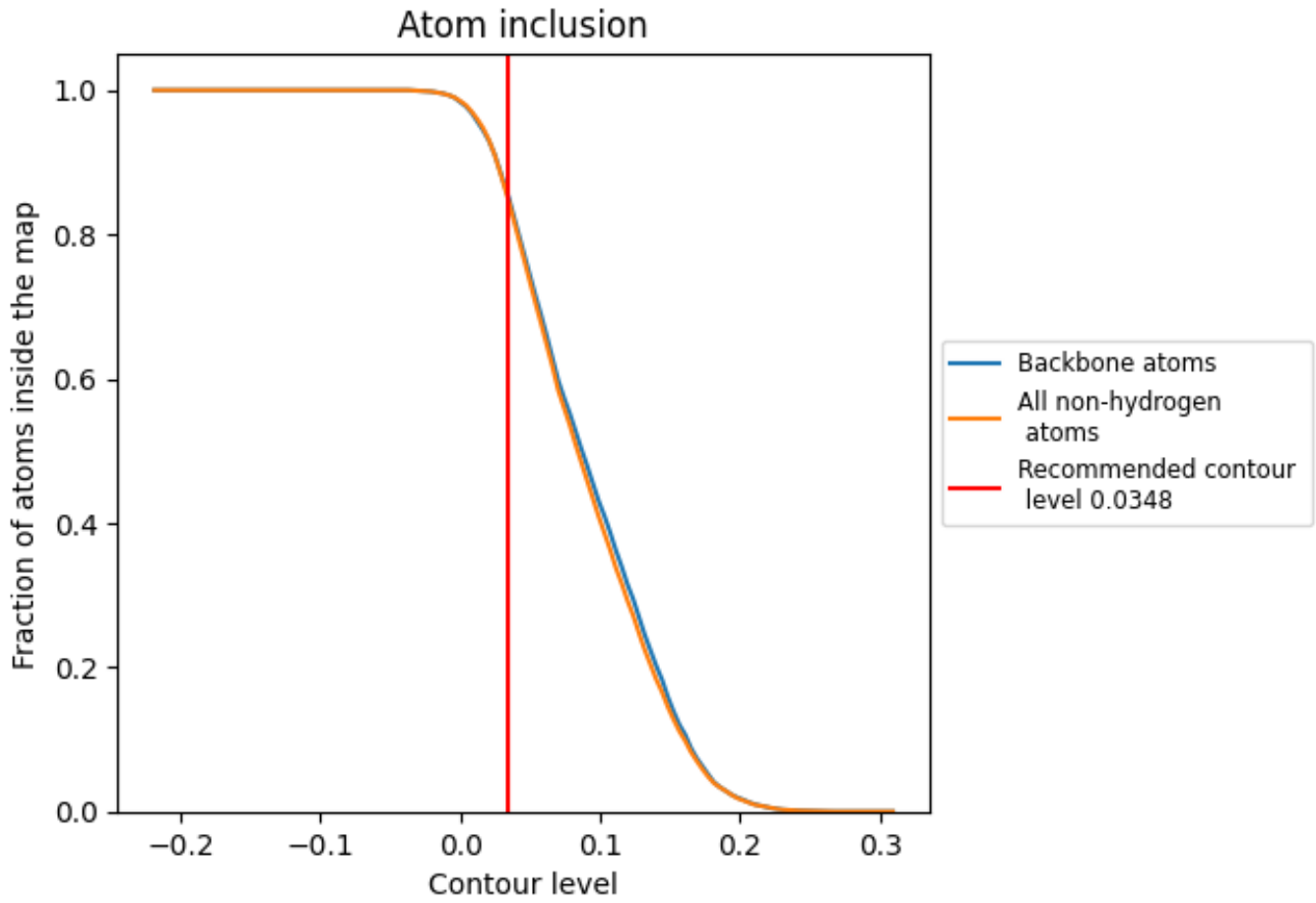
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0348).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.0348) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8457	0.5020
A	0.8416	0.5010
B	0.8558	0.5020
C	0.8574	0.5030
D	0.8447	0.5020