Full wwPDB EM Validation Report (i)

Sep 12, 2026 – 01:13 PM EDT

PDB ID	:	12DL / pdb_000012dl
EMDB ID	:	EMD-76334
Title	:	Native structure of the cytoplasmic lattice (CPL) asymmetric unit from mouse MII eggs
Authors	:	Li, Y.; Zheng, W.; Leem, J.; Wu, C.; Tang, S.; Mogessie, B.; Xiong, Y.
Deposited on	:	2026-03-29
Resolution	:	3.50 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.

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

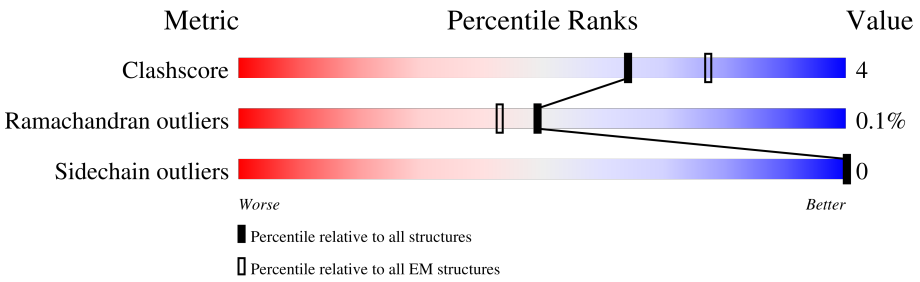
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

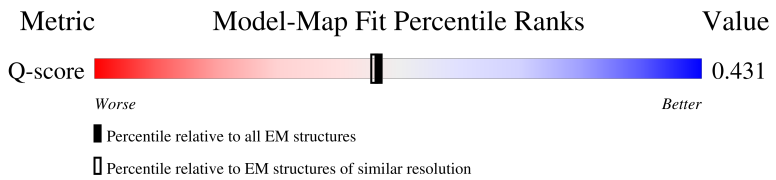
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	FA	445	86% 11% •
2	GA	1163	72% 10% 19%
2	GB	1163	70% 11% 18%
3	IA	164	70% 9% 22%

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Mol	Chain	Length	Quality of chain
3	JA	164	59% 13% 28%
4	HA	581	53% 9% 38%
4	HB	581	55% 8% 38%
5	KA	227	24% 75%
6	LA	440	26% 70%
7	MA	937	88% 12%
8	AA	682	85% 11%
8	AB	682	85% 11%
8	AC	682	84% 12%
8	AD	682	86% 10%
8	AE	682	85% 11%
8	AF	682	87% 10%
8	AG	682	87% 9%
8	AH	682	85% 11%
8	AI	682	85% 11%
8	AJ	682	85% 11%
9	EA	449	92% 6%
10	DA	993	84% 13%
10	DB	993	87% 10%
11	BA	782	73% 8% 20%
11	BB	782	7% 72% 9% 20%
12	CA	147	89% 10%
12	CB	147	80% 20%
13	OA	466	87% 11%
14	QA	163	6% 85% 11%

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Mol	Chain	Length	Quality of chain
14	QB	163	5% 84% 10% 6%
14	QC	163	• 86% 10% •
15	NA	469	85% 13% •
16	PA	468	85% 13% •

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 133296 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 Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	FA	429	3365	2114	577	649	25	0	0

- Molecule 2 is a protein called NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	GB	949	7479	4758	1266	1390	65	0	0
2	GA	946	7453	4744	1260	1384	65	0	0

- Molecule 3 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	IA	128	1026	660	177	184	5	0	0
3	JA	118	953	609	165	174	5	0	0

- Molecule 4 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	HB	363	2868	1820	502	526	20	0	0
4	HA	363	2868	1820	502	526	20	0	0

- Molecule 5 is a protein called Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	KA	57	460	293	85	76	6	0	0

- Molecule 6 is a protein called KH domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LA	133	1100	709	199	184	8	0	0

- Molecule 7 is a protein called NLR family, pyrin domain containing 4F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	MA	935	7536	4813	1256	1397	70	0	0

- Molecule 8 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AC	656	5185	3316	856	975	38	0	0
8	AD	656	5185	3316	856	975	38	0	0
8	AE	656	5185	3316	856	975	38	0	0
8	AF	656	5185	3316	856	975	38	0	0
8	AG	656	5185	3316	856	975	38	0	0
8	AH	656	5185	3316	856	975	38	0	0
8	AA	656	5185	3316	856	975	38	0	0
8	AB	656	5185	3316	856	975	38	0	0
8	AI	656	5185	3316	856	975	38	0	0
8	AJ	656	5185	3316	856	975	38	0	0

- Molecule 9 is a protein called Tubulin alpha-1C chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	EA	444	3464	2188	588	666	22	0	0

- Molecule 10 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	DA	958	7662	4875	1313	1412	62	0	0
10	DB	958	7663	4875	1313	1413	62	0	0

- Molecule 11 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BA	629	5082	3184	925	939	34	0	0
11	BB	629	5082	3184	925	939	34	0	0

- Molecule 12 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	CA	146	1166	746	199	214	7	0	0
12	CB	146	1166	746	199	214	7	0	0

- Molecule 13 is a protein called F-box and WD-40 domain protein 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	OA	456	3683	2371	628	655	29	0	0

- Molecule 14 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	QB	154	1236	778	200	252	6	0	0
14	QA	157	1260	793	205	256	6	0	0
14	QC	157	1260	794	204	255	7	0	0

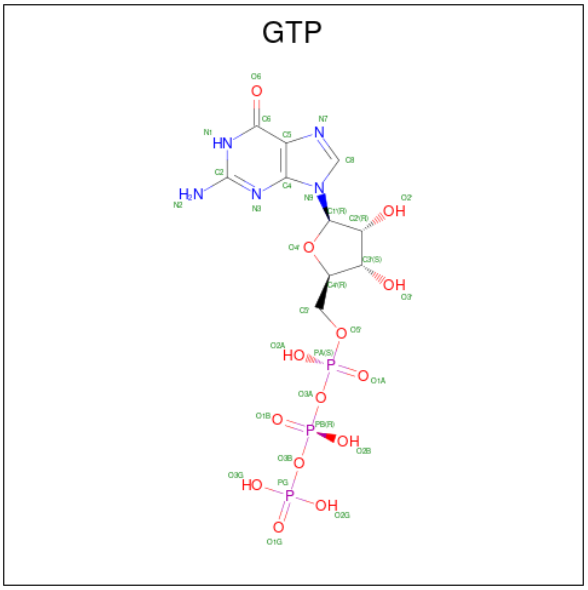
- Molecule 15 is a protein called Expressed sequence C85627.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	NA	463	3755	2421	625	680	29	0	0

- Molecule 16 is a protein called F-box and WD-40 domain protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	PA	461	3781	2451	632	674	24	0	0

- Molecule 17 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	FA	1	32	10	5	14	3	0
			Total	C	N	O	P	
17	EA	1	32	10	5	14	3	0

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
18	FA	1	1	1	0
			Total	Mg	
18	EA	1	1	1	0

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
19	KA	1	1	1	0
			Total	Zn	
19	BA	5	5	5	0
			Total	Zn	
19	BB	5	5	5	0

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

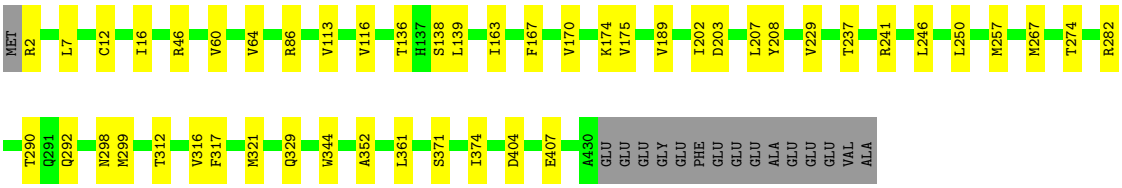
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
20	EA	1	1	1	0

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.

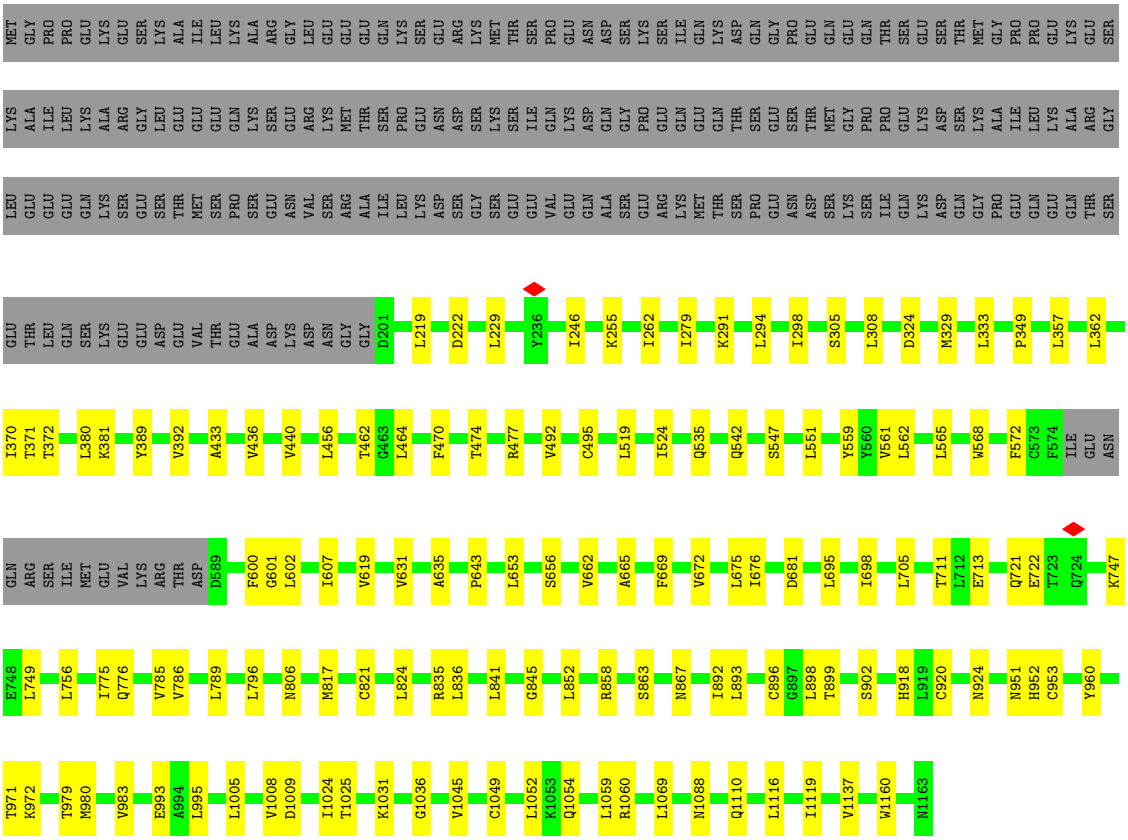
- Molecule 1: Tubulin beta-4B chain

Chain FA:



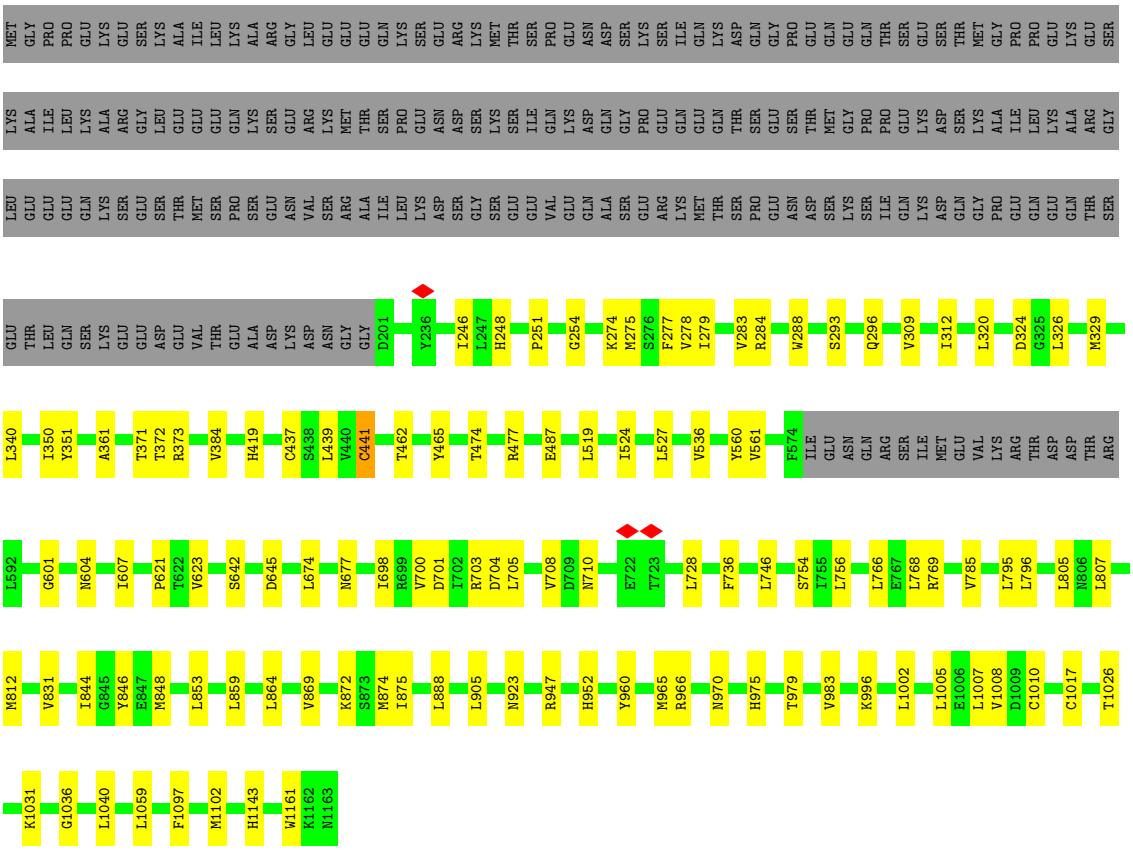
- Molecule 2: NACHT, LRR and PYD domains-containing protein 5

Chain GB:



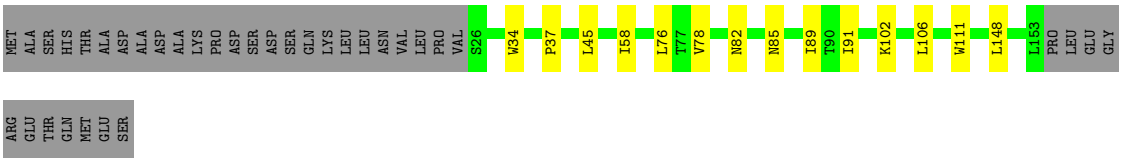
• Molecule 2: NACHT, LRR and PYD domains-containing protein 5

Chain GA: 72% 10% 19%



• Molecule 3: Oocyte-expressed protein homolog

Chain IA: 70% 9% 22%



• Molecule 3: Oocyte-expressed protein homolog

Chain JA: 59% 13% 28%

• Molecule 4: Transducin-like enhancer protein 6

Chain HB: 55% 8% 38%

MET THR SER HIS ARG GLN SER SER ASP THR PHE GLY GLY ILE LEU PRO SER THR LEU SER SER ARG TYR LEU SER ILE VAL ASN GLN LEU PRO GLU GLU PHE SER SER VAL VAL SER GLU MET MET VAL HIS LEU GLU ASN ILE PHE SER LEU ALA GLU ASN PHE PHE GLN ALA ILE GLU

ARG PHE SER ARG THR PRO ASP LEU LEU GLU ARG ASN LYS MET SER ILE GLY VAL GLY ALA GLU GLY ASP SER TRP PRO CYS HIS VAL SER HIS GLU ALA PRO MET GLY SER ALA GLN THR THR GLU ASN SER ALA LYS GLU GLU ASP LYS GLN VAL PRO GLU SER ALA ALA LEU GLN HIS

PRO LYS PHE LYS SER THR PRO GLY PRO GLN LEU PRO THR ARG ARG ARG PHE LEU SER GLU SER ASP GLU LEU GLN ASP P147 W151 Q175 LYS ASN GLN GLN GLU HIS GLY GLY GLU ASP SER SER GLN GLU SER LYS ASP SER GLY LEU CYS ASP PHE LYS PRO GLU PRO GLN PRO

ARG HIS ARG ASN SER LEU SER ASP SER ALA ASP PRO PHE LEU ILE LYS SER PRO SER ALA LEU LEU ASP TYR TYR GLN GLU ASP VAL SER ARG PRO GLN PRO GLU THR GLN GLU SER SER GLY ARG ALA D248 W256 W273 Q274 R277 V289 L297 V298 V299 S302 S303

T310 C311 V322 E332 V339 Q340 V344 L351 V422 R423 D439 D440 L456 R457 L484 K509 I513 L516 A526 S527 V528 G529 M530 I534 T535 V536 L545 F546 Q547 P553 V554 R555 C556 F557 T560 I566 I567 T568 C573

V576 V577 Y581

- Molecule 4: Transducin-like enhancer protein 6

Chain HA: 53% 9% 38%

MET THR SER HIS ARG GLN SER SER ASP THR PHE GLY GLY ILE LEU PRO SER THR LEU SER SER ARG TYR LEU SER ILE VAL ASN GLN LEU PRO GLU GLU PHE SER SER VAL VAL SER GLU MET MET VAL HIS LEU GLU ASN ILE PHE SER LEU ALA GLU ASN PHE PHE GLN ALA ILE GLU

ARG PHE SER ARG THR PRO ASP LEU LEU GLU ARG ASN LYS MET SER ILE GLY VAL GLY ALA GLU GLY ASP SER TRP PRO CYS HIS VAL SER HIS GLU ALA PRO MET GLY SER ALA GLN THR THR GLU ASN SER ALA LYS GLU GLU ASP LYS GLN VAL PRO GLU SER ALA ALA LEU GLN HIS

PRO LYS PHE LYS SER THR PRO GLY PRO GLN LEU PRO THR ARG ARG ARG PHE LEU SER GLU SER ASP GLU LEU GLN ASP P147 W151 Q175 LYS ASN GLN GLN GLU HIS GLY GLY GLU ASP SER SER GLN GLU SER LYS ASP SER GLY LEU CYS ASP PHE LYS PRO GLU PRO GLN PRO

ARG HIS ARG ASN SER LEU SER ASP SER ALA ASP PRO PHE LEU ILE LYS SER PRO SER ALA LEU LEU ASP TYR TYR GLN GLU ASP VAL SER ARG PRO GLN PRO GLU THR GLN GLU SER SER GLY ARG ALA D248 V260 R277 V289 L296 V301 S302 K317 V322

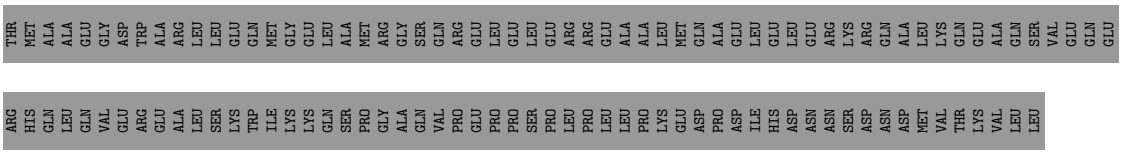
P331 L335 K336 C337 V344 Y345 L346 L351 N364 L365 L378 L403 R412 R417 T418 I421 V437 I442 L451 W454 D455 L456 L463 E464 H465 L466 F467 Q468 S469 Q470 I471 L484 L485 G486 L487 L516 S519 V528 T535 V536

T541 G542 A543 K544 L545 F546 Q547 V551 V554 M559 T560 L565 I566 G569 S570 R571 Y577 H578 Y581

- Molecule 5: Zinc finger BED domain-containing protein 3

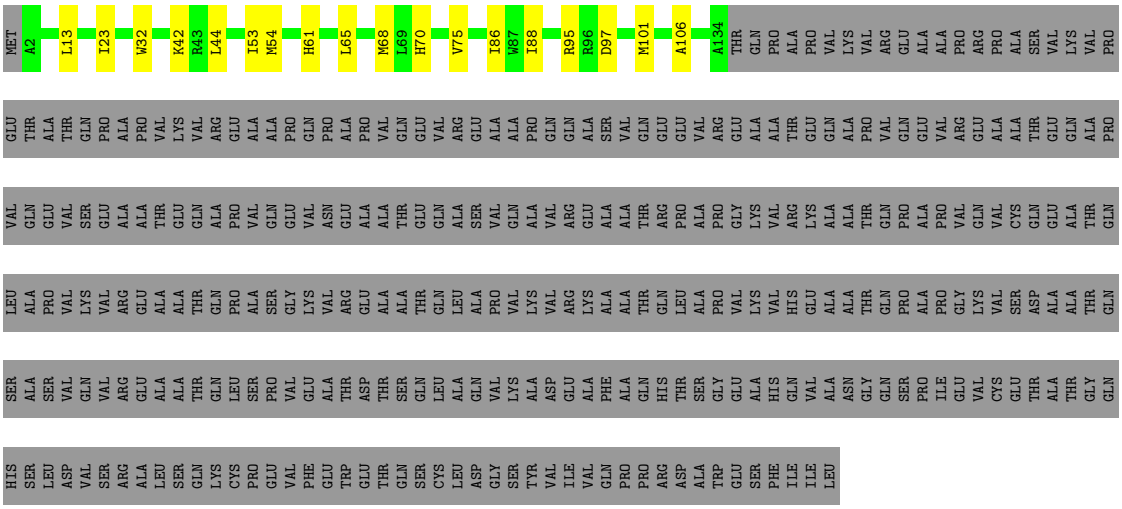
Chain KA: 24% 75%

LYS SER LYS LYS PRO LEU LYS ILE THR MET GLU ASP SER ARG ARG LEU ASN ASP PRO ALA GLU GLN GLY GLY LEU CYS PRO ALA PRO VAL GLY PRO S34 Y35 F73 P90 GLU LEU LYS LYS SER ALA ALA PRO SER SER PRO THR THR MET PRO CYS PRO PRO PRO PRO SER PRO



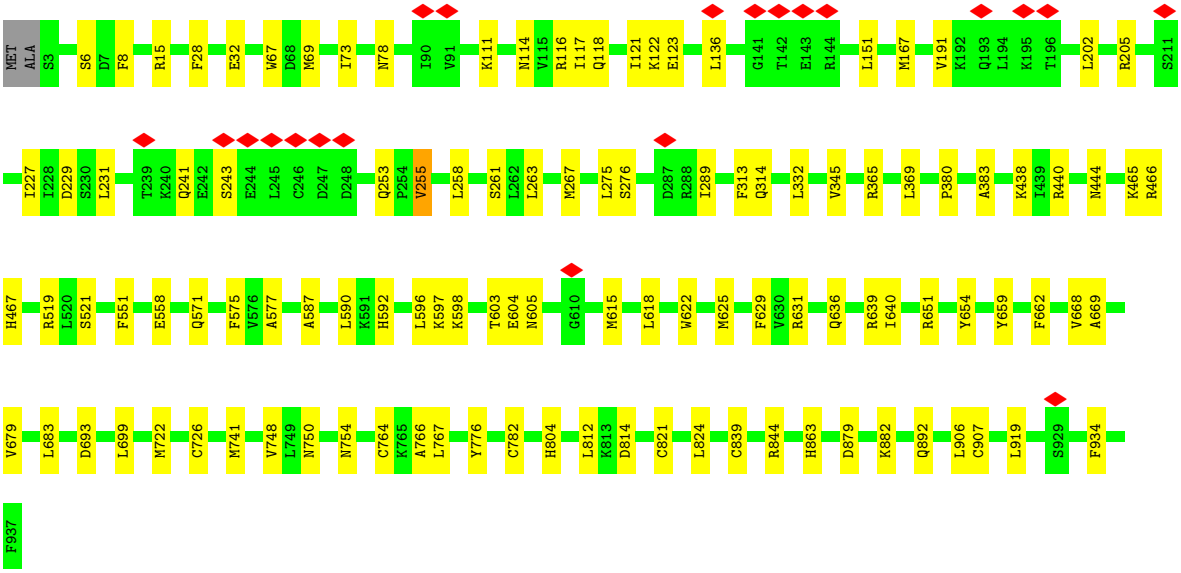
• Molecule 6: KH domain-containing protein 3

Chain LA:



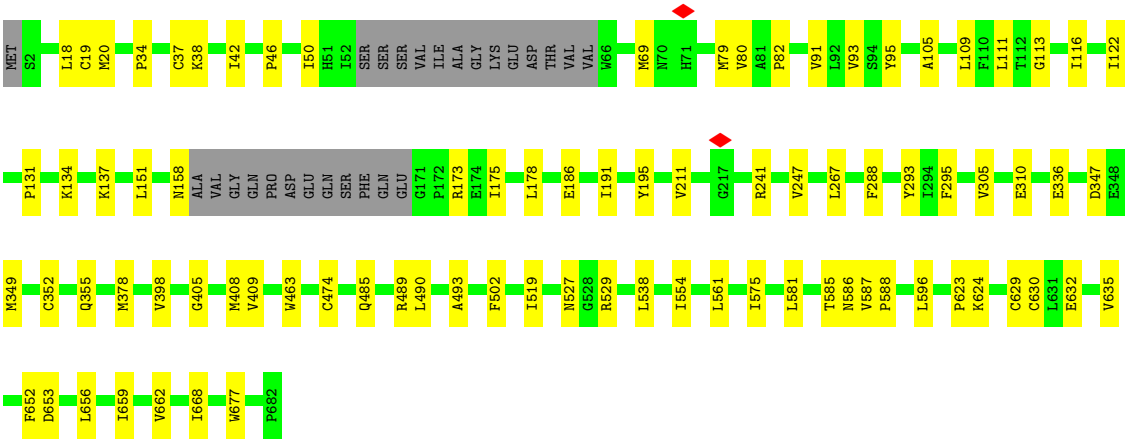
• Molecule 7: NLR family, pyrin domain containing 4F

Chain MA:



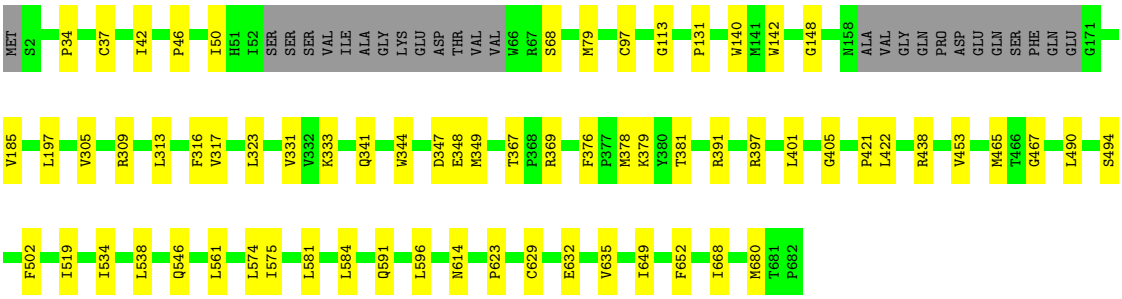
• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AC:



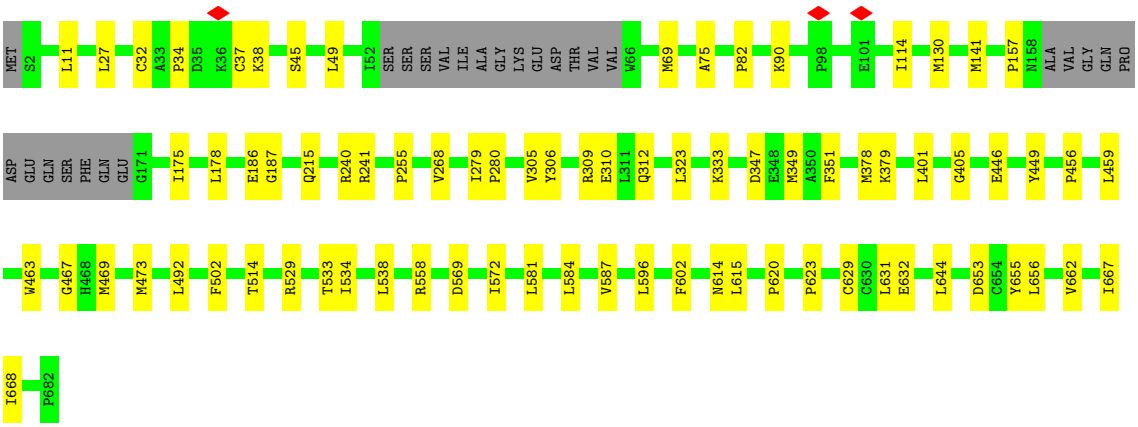
• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AD:



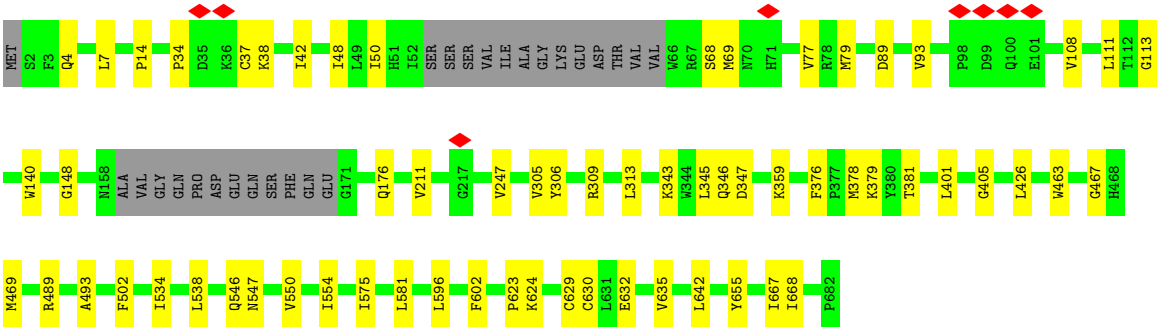
• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AE:



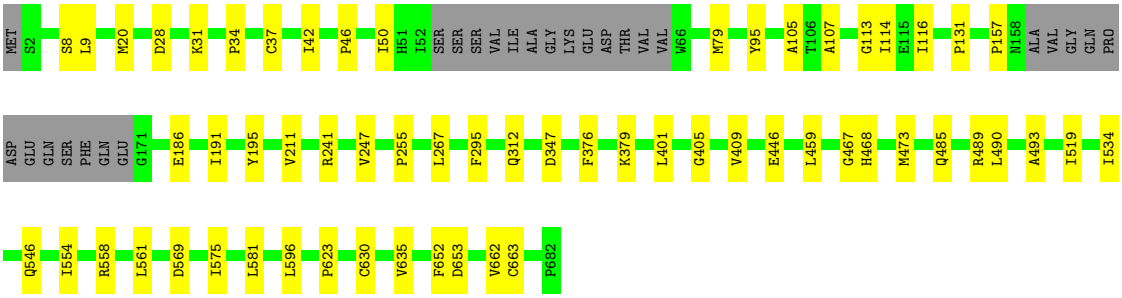
• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AF:



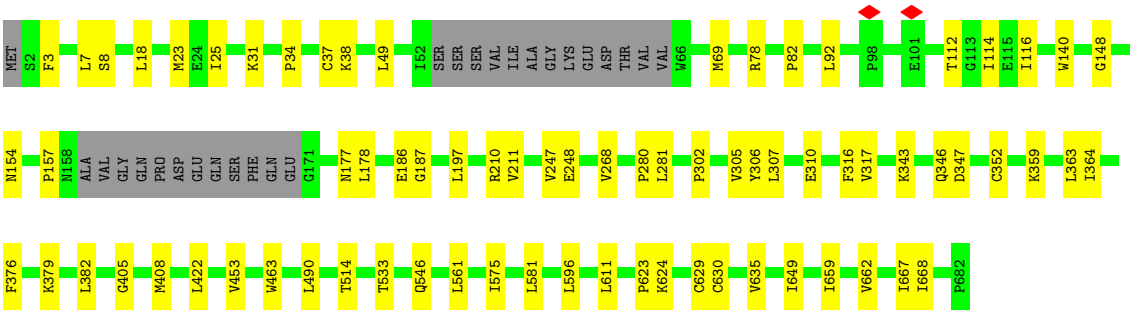
• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AG: 87% 9% •



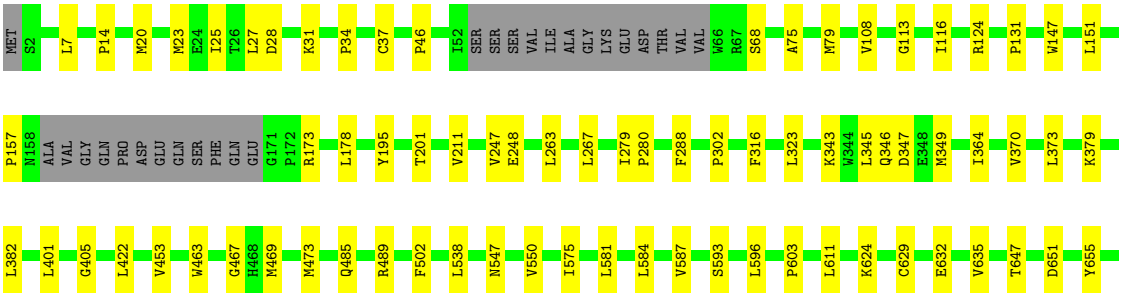
• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AH: 85% 11% •



• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AA: 85% 11% •



P682

• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AB: 85% 11% •

MET S2 L7 M20 I25 D28 K31 P34 C37 P46 I50 H51 I52 SER SER SER VAL ILE ALA GLY LYS GLU ASP THR VAL VAL W66 V77 R78 M79 G113 I116 P131 N158 ALA VAL GLY GLN PRO ASP GLU GLN SER PHE GLN GLU

G171 I175 L178 Q196 E205 K208 V211 V247 F257 I261 V268 I294 F295 V305 C308 Q341 S342 K343 W344 L345 Q346 D347 A350 F351 L365 R369 F376 K379 L401 G405 V409 L422 L426 Y449

V453 P456 V457 G467 M473 S494 T514 L515 N527 T533 I534 Q546 N547 V550 E564 L574 I575 L581 L584 V587 S593 L596 P623 K624 G627 T628 C629 E632 V635 F652 I667 I668 P682

• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AI: 85% 11% •

MET S2 N5 S6 L7 L11 I25 D35 K36 I42 R43 G44 I50 H51 I52 SER SER SER VAL ILE ALA GLY LYS GLU ASP THR VAL VAL W66 H71 P82 S83 V91 Y95 Q100 E101 A105 G113 I114 E115 N158 ALA VAL GLY GLN PRO

ASP GLU GLN SER PHE GLN GLU G171 L178 M181 E186 Y195 Q196 L197 T209 Y246 P255 I261 S262 L263 S264 L265 S266 L267 I279 P280 I294 F295 L303 E304 V305 C308 R309 E310 L345 Q346 D347 E348 M349 L373 E374 D375 F376 P377 M378 K379

R397 L401 G405 M408 V409 R438 E446 V453 L459 G467 M473 C474 Q485 R489 L490 N527 G528 R529 I534 Q546 L561 I575 L581 L584 V587 L596 P623 K624 C629 C630 V635 L656 I659

V662 C663 A664 I668 P682

• Molecule 8: Inactive protein-arginine deiminase type-6

Chain AJ: 85% 11% •

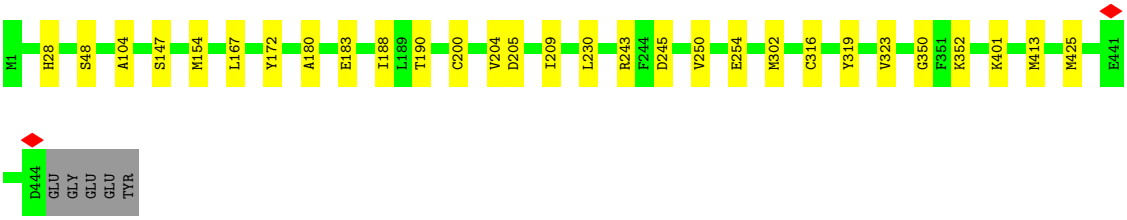
MET S2 F3 L7 L18 C19 M20 V21 I25 D28 K31 P34 C37 I42 P46 I52 SER SER SER VAL ILE ALA GLY LYS GLU ASP THR VAL VAL W66 V80 A81 P82 V93 T112 I116 P131 W140 M141 W142 G148 N158

ALA VAL GLY GLN PRO ASP GLU GLN SER PHE GLN GLU G171 Q176 L197 V305 Y306 R309 F316 V317 D318 S319 L345 Q346 D347 C352 K359 L363 E394 R397 S400 L401 G405 E436 M440 N441 W463 G467 Q485 R489

Q504 K507 E508 G509 Y510 T514 I519 T533 L538 R544 E545 Q546 N547 V550 T559 L581 K595 L596 P623 K624 C629 C630 L642 I649 F652 C663 A664 I667 I668 P682

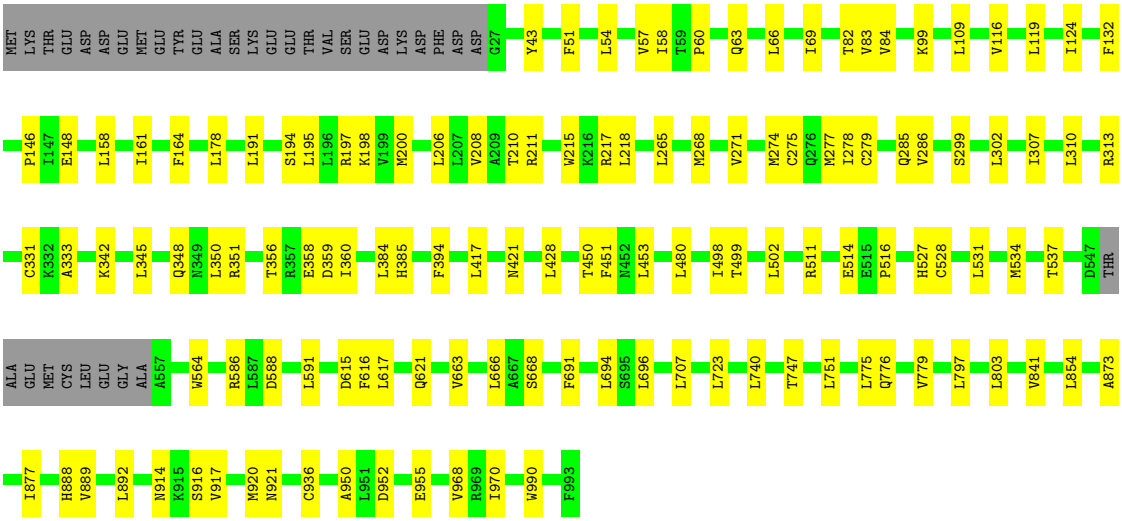
• Molecule 9: Tubulin alpha-1C chain

Chain EA: 92% 6% •



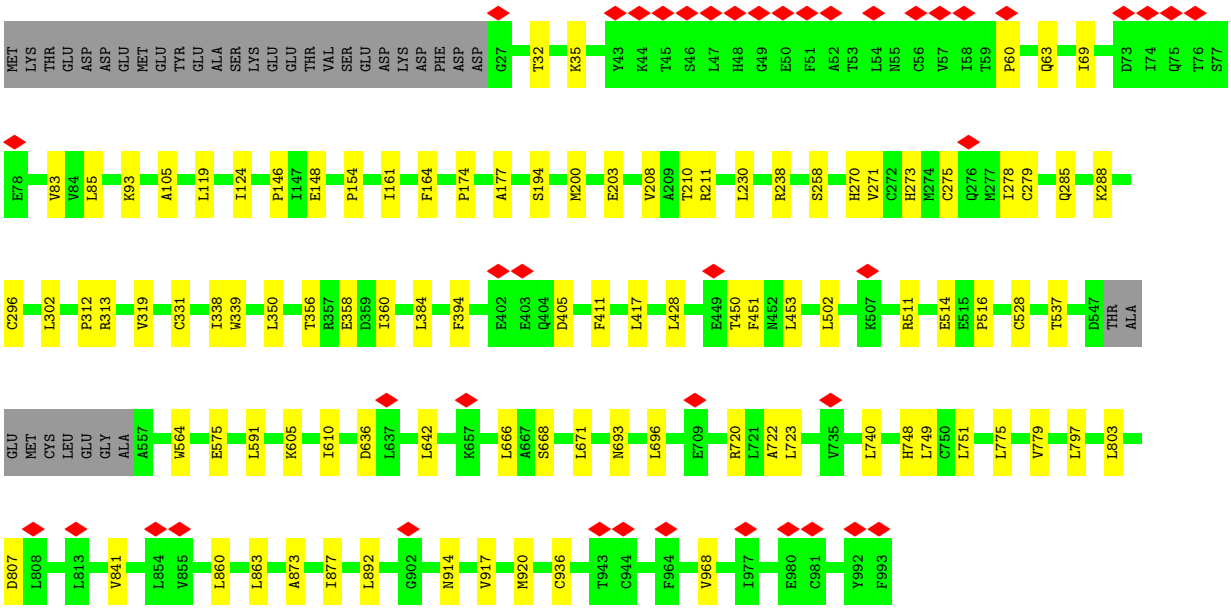
• Molecule 10: NACHT, LRR and PYD domains-containing protein 14

Chain DA:



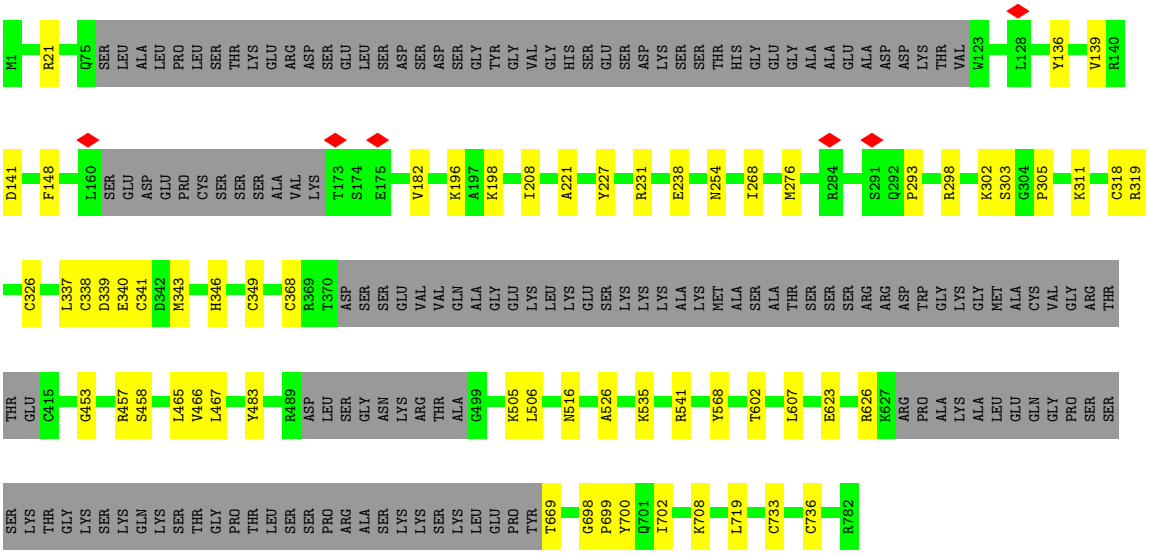
• Molecule 10: NACHT, LRR and PYD domains-containing protein 14

Chain DB:



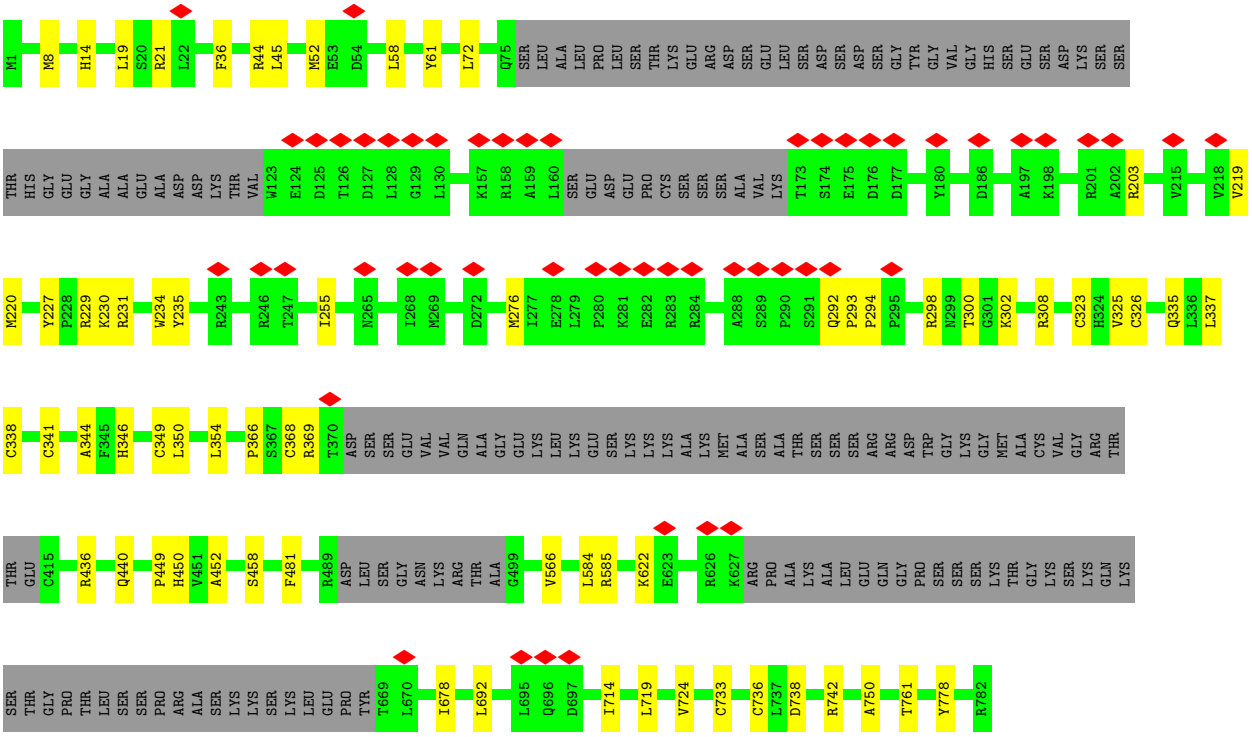
• Molecule 11: E3 ubiquitin-protein ligase UHRF1

Chain BA:



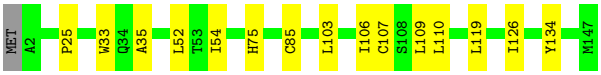
- Molecule 11: E3 ubiquitin-protein ligase UHRF1

Chain BB:



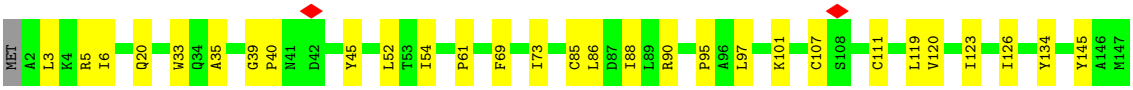
- Molecule 12: Ubiquitin-conjugating enzyme E2 D3

Chain CA:



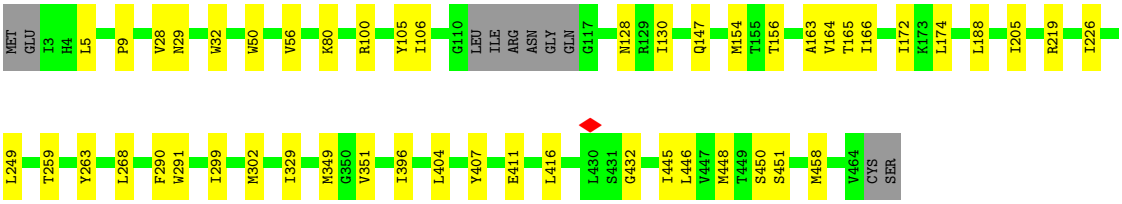
• Molecule 12: Ubiquitin-conjugating enzyme E2 D3

Chain CB:



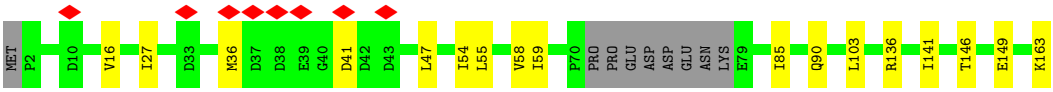
• Molecule 13: F-box and WD-40 domain protein 19

Chain OA:



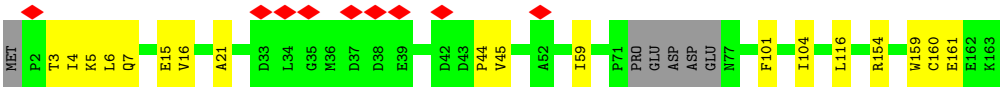
• Molecule 14: S-phase kinase-associated protein 1

Chain QB:



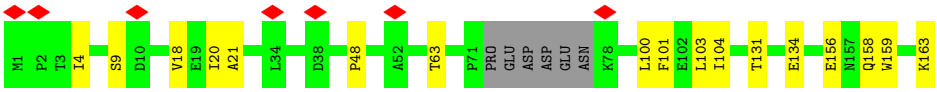
• Molecule 14: S-phase kinase-associated protein 1

Chain QA:



• Molecule 14: S-phase kinase-associated protein 1

Chain QC:

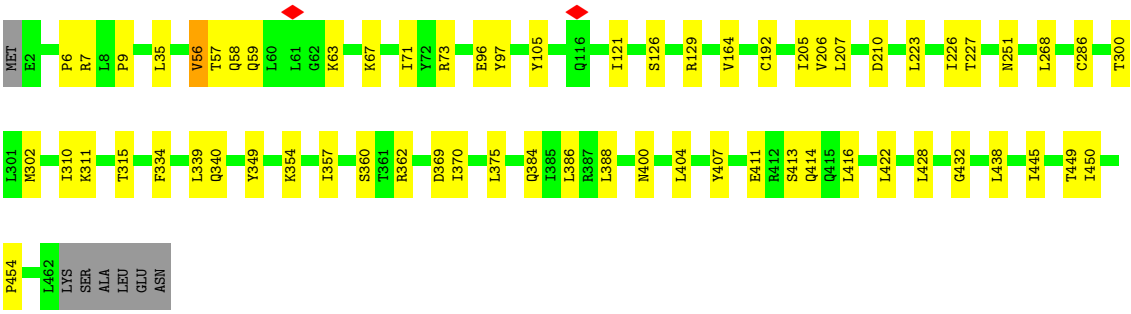


• Molecule 15: Expressed sequence C85627

Chain NA:

• Molecule 16: F-box and WD-40 domain protein 21

Chain PA:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249541	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.702	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, GTP, ZN

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	FA	0.21	0/3440	0.36	0/4663
2	GA	0.19	0/7585	0.36	1/10258 (0.0%)
2	GB	0.18	0/7611	0.34	0/10293
3	IA	0.18	0/1046	0.30	0/1415
3	JA	0.20	0/971	0.36	0/1315
4	HA	0.20	0/2934	0.36	0/3982
4	HB	0.21	0/2934	0.36	0/3982
5	KA	0.17	0/477	0.28	0/649
6	LA	0.17	0/1131	0.32	0/1527
7	MA	0.12	0/7678	0.34	0/10339
8	AA	0.13	0/5302	0.32	0/7189
8	AB	0.13	0/5302	0.31	0/7189
8	AC	0.16	0/5302	0.32	0/7189
8	AD	0.14	0/5302	0.32	0/7189
8	AE	0.15	0/5302	0.32	0/7189
8	AF	0.14	0/5302	0.31	0/7189
8	AG	0.15	0/5302	0.33	0/7189
8	AH	0.15	0/5302	0.32	0/7189
8	AI	0.16	0/5302	0.31	0/7189
8	AJ	0.16	0/5302	0.33	0/7189
9	EA	0.21	0/3542	0.30	0/4809
10	DA	0.19	0/7806	0.36	0/10553
10	DB	0.10	0/7807	0.29	0/10553
11	BA	0.18	0/5198	0.30	0/7027
11	BB	0.10	0/5198	0.27	0/7027
12	CA	0.21	0/1201	0.33	0/1637
12	CB	0.14	0/1201	0.36	0/1637
13	OA	0.18	0/3774	0.33	0/5124
14	QA	0.13	0/1281	0.33	0/1731
14	QB	0.13	0/1256	0.30	0/1697
14	QC	0.10	0/1281	0.29	0/1731
15	NA	0.20	0/3848	0.33	0/5228

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	PA	0.18	0/3883	0.32	0/5270
All	All	0.16	0/136103	0.33	1/184337 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	NA	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	GA	441	CYS	CA-CB-SG	5.70	127.51	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	NA	8	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FA	3365	0	3244	29	0
2	GA	7453	0	7533	67	0
2	GB	7479	0	7557	82	0
3	IA	1026	0	1060	10	0
3	JA	953	0	974	22	0
4	HA	2868	0	2848	33	0
4	HB	2868	0	2848	25	0
5	KA	460	0	431	1	0
6	LA	1100	0	1112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	MA	7536	0	7597	67	0
8	AA	5185	0	5185	43	0
8	AB	5185	0	5185	43	0
8	AC	5185	0	5185	52	0
8	AD	5185	0	5185	37	0
8	AE	5185	0	5185	44	0
8	AF	5185	0	5185	35	0
8	AG	5185	0	5185	36	0
8	AH	5185	0	5185	44	0
8	AI	5185	0	5185	45	0
8	AJ	5185	0	5185	43	0
9	EA	3464	0	3361	19	0
10	DA	7662	0	7769	73	0
10	DB	7663	0	7769	52	0
11	BA	5082	0	4956	37	0
11	BB	5082	0	4956	41	0
12	CA	1166	0	1147	8	0
12	CB	1166	0	1147	19	0
13	OA	3683	0	3733	29	0
14	QA	1260	0	1244	11	0
14	QB	1236	0	1218	11	0
14	QC	1260	0	1249	10	0
15	NA	3755	0	3766	34	0
16	PA	3781	0	3787	37	0
17	EA	32	0	12	0	0
17	FA	32	0	12	0	0
18	EA	1	0	0	0	0
18	FA	1	0	0	0	0
19	BA	5	0	0	0	0
19	BB	5	0	0	0	0
19	KA	1	0	0	0	0
20	EA	1	0	0	0	0
All	All	133296	0	133180	1098	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 4.

All (1098) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GA:437:CYS:HA	2:GA:441:CYS:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GA:462:THR:HG21	2:GA:601:GLY:HA3	1.61	0.82
11:BA:338:CYS:SG	11:BA:341:CYS:HB2	2.25	0.75
3:IA:37:PRO:HB3	4:HB:322:VAL:HG21	1.69	0.73
14:QA:4:ILE:HD13	14:QA:21:ALA:HB2	1.72	0.71
8:AG:581:LEU:HD12	8:AG:596:LEU:HB3	1.71	0.71
8:AA:581:LEU:HD12	8:AA:596:LEU:HB3	1.71	0.71
14:QC:20:ILE:HD13	14:QC:63:THR:HG22	1.74	0.70
4:HA:296:LEU:HD11	4:HA:569:GLY:HA3	1.73	0.70
2:GB:462:THR:HG21	2:GB:601:GLY:HA3	1.73	0.70
8:AC:46:PRO:HD3	8:AJ:131:PRO:HD3	1.74	0.70
11:BA:516:ASN:HD22	11:BA:535:LYS:HB2	1.56	0.70
4:HB:566:ILE:HG23	4:HB:577:TYR:HB2	1.75	0.69
8:AH:343:LYS:HE3	8:AH:346:GLN:H	1.57	0.69
8:AG:131:PRO:HD3	8:AB:46:PRO:HD3	1.74	0.69
1:FA:60:VAL:HG21	1:FA:86:ARG:HG2	1.75	0.69
11:BB:326:CYS:HB3	11:BB:349:CYS:SG	2.34	0.68
8:AC:581:LEU:HD12	8:AC:596:LEU:HB3	1.75	0.68
8:AH:310:GLU:H	8:AH:662:VAL:HG23	1.59	0.68
8:AJ:581:LEU:HD12	8:AJ:596:LEU:HB3	1.74	0.68
8:AE:347:ASP:HA	8:AE:405:GLY:HA3	1.76	0.68
3:JA:121:VAL:HA	3:JA:124:LYS:HE3	1.77	0.67
8:AB:534:ILE:HD11	8:AB:623:PRO:HG3	1.76	0.67
8:AC:131:PRO:HD3	8:AJ:46:PRO:HD3	1.77	0.67
10:DA:914:ASN:HD21	10:DA:917:VAL:HB	1.60	0.67
13:OA:263:TYR:HB2	13:OA:329:ILE:HD11	1.77	0.67
1:FA:237:THR:HG23	1:FA:241:ARG:HE	1.59	0.67
4:HA:484:LEU:HD23	4:HA:516:LEU:HD13	1.75	0.67
8:AI:181:MET:HE1	8:AI:263:LEU:HD22	1.75	0.66
8:AC:42:ILE:HG12	8:AC:50:ILE:HD13	1.76	0.66
2:GB:893:LEU:HD23	2:GB:898:LEU:HD21	1.77	0.66
2:GA:923:ASN:HA	2:GA:952:HIS:HB3	1.78	0.66
4:HB:422:VAL:HG12	4:HB:423:ARG:HD2	1.78	0.66
8:AB:581:LEU:HD12	8:AB:596:LEU:HB3	1.78	0.66
14:QB:36:MET:HE2	14:QB:41:ASP:HB3	1.76	0.65
10:DA:119:LEU:HD12	10:DA:124:ILE:HD11	1.78	0.65
10:DB:275:CYS:HB2	10:DB:279:CYS:H	1.61	0.65
1:FA:12:CYS:HB3	1:FA:138:SER:HB2	1.77	0.65
4:HB:484:LEU:HD23	4:HB:516:LEU:HD13	1.79	0.65
9:EA:352:LYS:HB3	10:DA:51:PHE:CZ	2.31	0.65
8:AH:581:LEU:HD12	8:AH:596:LEU:HB3	1.79	0.65
8:AB:401:LEU:HD11	8:AB:467:GLY:HA3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AJ:20:MET:HE1	8:AJ:116:ILE:H	1.61	0.65
11:BA:669:THR:HG21	11:BA:698:GLY:HA2	1.78	0.64
8:AI:195:TYR:HB3	8:AI:267:LEU:HD11	1.77	0.64
4:HA:535:THR:HG22	4:HA:547:GLN:HG2	1.78	0.64
8:AB:20:MET:HE1	8:AB:116:ILE:H	1.61	0.64
1:FA:7:LEU:HD23	1:FA:64:VAL:HB	1.79	0.64
8:AH:157:PRO:HB3	8:AH:379:LYS:HD2	1.80	0.64
4:HA:471:ILE:HD12	4:HA:485:LEU:HD23	1.79	0.64
12:CA:35:ALA:HB3	12:CA:52:LEU:HB2	1.80	0.64
7:MA:15:ARG:HG3	3:JA:100:ARG:HH11	1.62	0.63
6:LA:97:ASP:HB2	3:JA:122:LYS:HE2	1.79	0.63
10:DB:119:LEU:HD12	10:DB:124:ILE:HD11	1.79	0.63
8:AC:38:LYS:HB3	8:AC:69:MET:HE2	1.80	0.63
8:AJ:140:TRP:HD1	8:AJ:148:GLY:HA3	1.63	0.63
13:OA:166:ILE:HG12	13:OA:172:ILE:HG12	1.79	0.63
8:AG:459:LEU:HD13	8:AG:473:MET:HE1	1.80	0.63
8:AE:534:ILE:HD11	8:AE:623:PRO:HG3	1.81	0.63
2:GB:631:VAL:HG21	2:GB:653:LEU:HD11	1.82	0.62
8:AE:514:THR:HA	8:AE:533:THR:HA	1.81	0.62
8:AJ:347:ASP:HA	8:AJ:405:GLY:HA3	1.82	0.62
8:AA:581:LEU:HB3	8:AA:596:LEU:HD12	1.81	0.62
4:HA:412:ARG:HD3	4:HA:421:ILE:HD12	1.82	0.62
4:HA:344:VAL:HG12	4:HA:364:ASN:HB3	1.82	0.62
1:FA:292:GLN:HG2	1:FA:298:ASN:HD22	1.64	0.61
8:AD:519:ILE:HD12	8:AD:652:PHE:HZ	1.65	0.61
8:AF:426:LEU:HB3	8:AF:469:MET:HE1	1.82	0.61
8:AC:585:THR:HG22	8:AC:586:ASN:H	1.65	0.61
8:AE:279:ILE:HD12	8:AE:280:PRO:HD2	1.83	0.61
2:GA:278:VAL:HG22	2:GA:320:LEU:HB3	1.83	0.61
8:AE:186:GLU:HG2	8:AE:241:ARG:HD3	1.82	0.61
8:AI:376:PHE:HB2	8:AI:379:LYS:HE2	1.83	0.61
11:BB:231:ARG:HD3	11:BB:298:ARG:HG3	1.81	0.61
2:GB:1024:ILE:HD12	2:GB:1059:LEU:HD11	1.81	0.61
8:AD:131:PRO:HD3	8:AA:46:PRO:HD3	1.83	0.61
8:AH:347:ASP:HA	8:AH:405:GLY:HA3	1.81	0.61
15:NA:208:ILE:HD13	15:NA:271:LEU:HD21	1.81	0.61
4:HA:469:SER:HB3	4:HA:487:LEU:HB3	1.82	0.61
7:MA:577:ALA:HB3	7:MA:603:THR:HG22	1.83	0.61
16:PA:121:ILE:HD11	16:PA:445:ILE:HG13	1.82	0.61
16:PA:226:ILE:HG22	16:PA:227:THR:HG23	1.83	0.61
16:PA:300:THR:HG23	16:PA:315:THR:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:HA:417:ARG:HG3	4:HA:418:THR:HG23	1.83	0.61
8:AH:514:THR:HA	8:AH:533:THR:HA	1.83	0.61
8:AE:653:ASP:HA	8:AE:656:LEU:HD23	1.83	0.61
16:PA:67:LYS:HE2	16:PA:71:ILE:HD11	1.81	0.61
1:FA:317:PHE:HB3	1:FA:321:MET:HE1	1.83	0.60
7:MA:814:ASP:HB3	7:MA:844:ARG:HE	1.66	0.60
8:AG:20:MET:HE1	8:AG:116:ILE:H	1.65	0.60
8:AH:140:TRP:HD1	8:AH:148:GLY:HA3	1.65	0.60
2:GA:288:TRP:HB2	2:GA:351:TYR:HB3	1.82	0.60
8:AC:588:PRO:HG3	11:BA:505:LYS:HD2	1.83	0.60
8:AE:34:PRO:HB2	8:AE:37:CYS:HB2	1.84	0.60
8:AF:534:ILE:HD11	8:AF:623:PRO:HG3	1.82	0.60
8:AA:485:GLN:HB3	8:AA:489:ARG:HH22	1.64	0.60
1:FA:267:MET:HG2	1:FA:374:ILE:HD13	1.82	0.60
10:DA:194:SER:HB3	10:DA:200:MET:HB2	1.84	0.60
8:AI:581:LEU:HD12	8:AI:596:LEU:HB3	1.82	0.60
7:MA:615:MET:HG2	7:MA:618:LEU:HD12	1.81	0.60
8:AA:211:VAL:HG22	8:AA:247:VAL:HG12	1.84	0.60
8:AB:624:LYS:HZ3	8:AB:627:GLY:H	1.50	0.60
8:AJ:3:PHE:HD2	8:AJ:20:MET:HB2	1.66	0.60
8:AJ:21:VAL:HG21	8:AJ:82:PRO:HG3	1.84	0.60
16:PA:126:SER:HB3	16:PA:129:ARG:HB2	1.83	0.60
2:GA:324:ASP:HA	2:GA:371:THR:HB	1.82	0.60
8:AG:347:ASP:HA	8:AG:405:GLY:HA3	1.83	0.60
10:DB:85:LEU:HD11	10:DB:230:LEU:HB2	1.84	0.60
7:MA:231:LEU:HD11	7:MA:275:LEU:HD22	1.83	0.59
14:QA:7:GLN:HB2	14:QA:44:PRO:HB2	1.84	0.59
8:AE:27:LEU:HB2	8:AE:75:ALA:HB3	1.83	0.59
2:GB:971:THR:HG23	2:GB:972:LYS:HG3	1.85	0.59
7:MA:191:VAL:HG12	7:MA:255:VAL:HG22	1.84	0.59
8:AE:114:ILE:HG22	8:AE:187:GLY:HA3	1.85	0.59
16:PA:164:VAL:HG11	16:PA:206:VAL:HG21	1.84	0.59
1:FA:316:VAL:HA	1:FA:352:ALA:HB3	1.84	0.59
8:AE:38:LYS:HD3	8:AE:69:MET:HE2	1.85	0.59
8:AE:349:MET:HE1	8:AE:378:MET:HG3	1.85	0.59
8:AJ:34:PRO:HB2	8:AJ:37:CYS:HB2	1.85	0.59
10:DA:164:PHE:HB3	10:DA:210:THR:HG22	1.85	0.59
7:MA:114:ASN:HB3	7:MA:116:ARG:HG2	1.85	0.59
13:OA:411:GLU:HB2	14:QB:163:LYS:HB3	1.85	0.59
16:PA:205:ILE:HD13	16:PA:268:LEU:HD11	1.85	0.59
4:HB:535:THR:HG22	4:HB:547:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AB:584:LEU:HD21	8:AB:593:SER:H	1.68	0.59
8:AE:620:PRO:HG3	8:AE:631:LEU:HD11	1.85	0.59
10:DA:265:LEU:HD23	10:DA:299:SER:HA	1.85	0.59
1:FA:170:VAL:HG22	1:FA:203:ASP:HA	1.85	0.58
10:DA:313:ARG:HH12	10:DA:450:THR:HA	1.68	0.58
8:AI:575:ILE:HD12	8:AI:635:VAL:HG23	1.86	0.58
2:GA:326:LEU:HD23	2:GA:329:MET:HG3	1.84	0.58
8:AB:494:SER:HB2	8:AB:574:LEU:HD12	1.86	0.58
14:QB:27:ILE:HD11	14:QB:47:LEU:HD21	1.85	0.58
1:FA:136:THR:HG22	1:FA:167:PHE:HB2	1.85	0.58
16:PA:360:SER:HB3	16:PA:388:LEU:HD22	1.85	0.58
8:AD:494:SER:HB2	8:AD:574:LEU:HD12	1.84	0.58
8:AH:34:PRO:HB2	8:AH:37:CYS:HB2	1.85	0.58
3:IA:45:LEU:HD21	3:IA:102:LYS:HD3	1.86	0.58
8:AG:46:PRO:HD3	8:AB:131:PRO:HD3	1.85	0.58
8:AA:279:ILE:HD12	8:AA:280:PRO:HD2	1.85	0.58
8:AI:295:PHE:HB2	8:AI:409:VAL:HG21	1.86	0.58
11:BA:208:ILE:HD11	11:BA:276:MET:HB2	1.85	0.58
16:PA:56:VAL:HG13	16:PA:59:GLN:HE21	1.69	0.58
10:DB:914:ASN:HD21	10:DB:917:VAL:HB	1.69	0.58
11:BB:724:VAL:HG11	11:BB:761:THR:HB	1.84	0.58
1:FA:267:MET:HE3	1:FA:299:MET:HE2	1.86	0.57
9:EA:167:LEU:HD22	9:EA:200:CYS:HB3	1.86	0.57
2:GA:874:MET:HG3	2:GA:905:LEU:HD11	1.87	0.57
8:AC:42:ILE:HG13	8:AC:93:VAL:HG22	1.85	0.57
1:FA:16:ILE:HD12	1:FA:229:VAL:HG11	1.84	0.57
2:GB:841:LEU:HD13	2:GB:867:ASN:HD21	1.69	0.57
10:DB:779:VAL:HA	10:DB:807:ASP:HB3	1.86	0.57
16:PA:302:MET:HE3	16:PA:311:LYS:HD3	1.86	0.57
2:GB:892:ILE:HA	2:GB:920:CYS:HB3	1.84	0.57
2:GA:979:THR:HG23	2:GA:1008:VAL:HB	1.86	0.57
8:AF:376:PHE:HB2	8:AF:379:LYS:HE2	1.86	0.57
10:DA:502:LEU:HD13	10:DA:528:CYS:HA	1.86	0.57
13:OA:164:VAL:HG22	13:OA:174:LEU:HD12	1.86	0.57
14:QA:154:ARG:HG2	15:NA:30:GLN:HE22	1.70	0.57
10:DA:210:THR:HG21	10:DA:218:LEU:HD22	1.86	0.57
15:NA:318:THR:HG22	15:NA:337:ILE:HD12	1.87	0.57
7:MA:571:GLN:HB3	7:MA:597:LYS:HB2	1.86	0.57
8:AC:653:ASP:HA	8:AC:656:LEU:HD13	1.87	0.57
2:GA:869:VAL:HG11	2:GA:874:MET:HE2	1.87	0.57
8:AI:255:PRO:HG3	8:AI:446:GLU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:68:MET:HE1	3:JA:124:LYS:HD2	1.85	0.57
8:AD:534:ILE:HD11	8:AD:623:PRO:HG3	1.86	0.57
10:DA:588:ASP:HB3	10:DA:617:LEU:HD12	1.85	0.57
11:BB:227:TYR:HB3	11:BB:230:LYS:HB2	1.87	0.57
10:DA:161:ILE:HB	10:DA:208:VAL:HG12	1.86	0.56
8:AH:114:ILE:HD12	8:AH:187:GLY:HA3	1.87	0.56
10:DA:271:VAL:HB	10:DA:274:MET:HG2	1.85	0.56
2:GA:474:THR:HA	2:GA:477:ARG:HG3	1.87	0.56
9:EA:316:CYS:HA	9:EA:352:LYS:HB2	1.86	0.56
7:MA:764:CYS:HA	7:MA:767:LEU:HB3	1.86	0.56
8:AD:401:LEU:HD11	8:AD:467:GLY:HA3	1.87	0.56
8:AD:490:LEU:HD21	8:AD:561:LEU:HD13	1.87	0.56
8:AI:534:ILE:HD11	8:AI:623:PRO:HG3	1.88	0.56
10:DA:451:PHE:HB2	10:DA:453:LEU:HD22	1.87	0.56
10:DA:514:GLU:HB3	10:DA:516:PRO:HD2	1.87	0.56
15:NA:126:MET:HE2	15:NA:460:LEU:HD12	1.86	0.56
8:AD:140:TRP:CD1	8:AD:148:GLY:HA3	2.40	0.56
8:AA:584:LEU:HD21	8:AA:593:SER:H	1.71	0.56
10:DA:331:CYS:HB3	10:DA:394:PHE:HB2	1.87	0.56
4:HA:403:LEU:HD21	4:HA:437:VAL:HG21	1.88	0.56
7:MA:651:ARG:HH12	7:MA:679:VAL:HG11	1.69	0.56
10:DA:69:ILE:HG23	10:DA:83:VAL:HG11	1.88	0.56
11:BA:467:LEU:HD13	11:BA:541:ARG:HG2	1.88	0.56
2:GA:807:LEU:HD13	2:GA:812:MET:HE1	1.87	0.56
8:AC:485:GLN:HB3	8:AC:489:ARG:HH12	1.69	0.56
8:AB:347:ASP:HA	8:AB:405:GLY:HA3	1.88	0.56
8:AJ:401:LEU:HD11	8:AJ:467:GLY:HA3	1.87	0.56
2:GB:246:ILE:HG22	2:GB:370:ILE:HB	1.88	0.56
12:CB:107:CYS:HA	12:CB:111:CYS:H	1.70	0.56
2:GB:676:ILE:HG23	2:GB:681:ASP:HB3	1.87	0.55
7:MA:202:LEU:HA	7:MA:205:ARG:HD3	1.88	0.55
10:DA:356:THR:HG23	10:DA:358:GLU:H	1.72	0.55
10:DB:356:THR:HG23	10:DB:358:GLU:H	1.71	0.55
13:OA:219:ARG:HB2	13:OA:226:ILE:HD11	1.88	0.55
2:GB:495:CYS:HB3	2:GB:559:TYR:HB2	1.88	0.55
2:GB:979:THR:HG22	2:GB:980:MET:HG3	1.89	0.55
8:AC:502:PHE:HB3	8:AC:538:LEU:HD11	1.88	0.55
8:AC:656:LEU:HD11	11:BA:457:ARG:HH12	1.72	0.55
8:AA:584:LEU:HD12	8:AA:587:VAL:HG11	1.89	0.55
8:AB:79:MET:HE2	8:AB:113:GLY:HA3	1.88	0.55
8:AI:279:ILE:HD12	8:AI:280:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AD:46:PRO:HD3	8:AA:131:PRO:HD3	1.86	0.55
10:DB:860:LEU:HD21	10:DB:863:LEU:HD12	1.88	0.55
4:HA:322:VAL:HG21	3:JA:37:PRO:HB3	1.89	0.55
6:LA:53:ILE:HG22	3:JA:133:ARG:HG3	1.88	0.55
7:MA:699:LEU:HD13	7:MA:726:CYS:HB3	1.88	0.55
8:AG:312:GLN:HE21	8:AG:662:VAL:HG11	1.71	0.55
8:AG:376:PHE:HB2	8:AG:379:LYS:HE2	1.89	0.55
12:CB:3:LEU:HA	12:CB:6:ILE:HD12	1.89	0.55
14:QC:4:ILE:HG23	14:QC:18:VAL:HG22	1.88	0.55
8:AI:83:SER:H	8:AI:113:GLY:HA3	1.71	0.55
11:BB:235:TYR:HB2	11:BB:255:ILE:HD11	1.89	0.55
1:FA:163:ILE:HG21	1:FA:250:LEU:HB3	1.89	0.55
8:AH:307:LEU:HD21	8:AH:317:VAL:HG13	1.88	0.55
15:NA:368:LEU:HB3	15:NA:381:PHE:HB2	1.89	0.55
8:AF:309:ARG:HD2	8:AF:313:LEU:HD22	1.88	0.55
10:DA:211:ARG:HH11	10:DA:384:LEU:HD12	1.71	0.55
15:NA:10:SER:HB3	15:NA:12:PRO:HD2	1.89	0.55
2:GB:1008:VAL:HG13	2:GB:1036:GLY:HA3	1.89	0.54
2:GA:519:LEU:HD22	2:GA:524:ILE:HD11	1.88	0.54
2:GA:674:LEU:HB2	2:GA:700:VAL:HG12	1.88	0.54
8:AE:312:GLN:HB2	8:AE:662:VAL:HG21	1.89	0.54
8:AA:79:MET:HE2	8:AA:113:GLY:HA3	1.88	0.54
2:GB:756:LEU:HB2	2:GB:785:VAL:HG12	1.90	0.54
2:GA:996:LYS:HG3	2:GA:1026:THR:HG21	1.88	0.54
8:AH:18:LEU:HD13	8:AH:112:THR:HG23	1.90	0.54
2:GB:711:THR:HB	2:GB:713:GLU:HG2	1.90	0.54
8:AH:82:PRO:HG2	8:AH:186:GLU:HB2	1.90	0.54
8:AA:343:LYS:HE3	8:AA:346:GLN:H	1.72	0.54
8:AI:347:ASP:HA	8:AI:405:GLY:HA3	1.88	0.54
7:MA:551:PHE:HE2	7:MA:575:PHE:HB2	1.72	0.54
8:AB:211:VAL:HG22	8:AB:247:VAL:HG12	1.89	0.54
13:OA:5:LEU:HD12	13:OA:9:PRO:HG2	1.89	0.54
2:GA:700:VAL:HG11	2:GA:736:PHE:HZ	1.73	0.54
7:MA:592:HIS:HA	7:MA:631:ARG:HH12	1.73	0.54
8:AF:581:LEU:HD12	8:AF:596:LEU:HB3	1.90	0.54
8:AJ:116:ILE:HD12	8:AJ:197:LEU:HD21	1.90	0.54
8:AF:401:LEU:HD11	8:AF:467:GLY:HA3	1.90	0.54
9:EA:352:LYS:HB3	10:DA:51:PHE:CE2	2.43	0.54
2:GB:219:LEU:HB3	2:GB:222:ASP:HB2	1.89	0.53
4:HA:301:VAL:HG13	4:HA:302:SER:H	1.73	0.53
8:AF:34:PRO:HB2	8:AF:37:CYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:MA:590:LEU:HB2	7:MA:625:MET:HB2	1.90	0.53
8:AD:42:ILE:HG12	8:AD:50:ILE:HD13	1.91	0.53
8:AE:11:LEU:HD23	8:AE:32:CYS:HB2	1.91	0.53
8:AH:352:CYS:HB2	8:AH:363:LEU:HB3	1.89	0.53
2:GA:309:VAL:HA	2:GA:312:ILE:HG22	1.91	0.53
7:MA:8:PHE:HZ	3:JA:101:MET:HG3	1.73	0.53
7:MA:111:LYS:HG3	7:MA:440:ARG:HG3	1.91	0.53
8:AC:79:MET:HE2	8:AC:113:GLY:HA3	1.90	0.53
8:AC:408:MET:HE1	8:AC:474:CYS:HA	1.89	0.53
8:AG:79:MET:HE2	8:AG:113:GLY:HA3	1.91	0.53
8:AA:7:LEU:HD12	8:AA:25:ILE:HG21	1.90	0.53
8:AI:42:ILE:HG12	8:AI:50:ILE:HD13	1.90	0.53
1:FA:274:THR:HG21	1:FA:361:LEU:HD21	1.90	0.53
16:PA:6:PRO:HD2	16:PA:9:PRO:HG2	1.89	0.53
4:HB:536:VAL:HG23	4:HB:545:LEU:HB2	1.89	0.53
7:MA:640:ILE:HB	7:MA:669:ALA:HA	1.90	0.53
2:GB:995:LEU:HD11	2:GB:1005:LEU:HD22	1.91	0.53
8:AI:401:LEU:HD11	8:AI:467:GLY:HA3	1.90	0.53
8:AJ:309:ARG:HE	8:AJ:317:VAL:HG11	1.74	0.53
10:DB:211:ARG:HH11	10:DB:384:LEU:HD12	1.72	0.53
11:BA:196:LYS:HG3	11:BA:198:LYS:H	1.73	0.53
11:BA:708:LYS:HD2	11:BA:719:LEU:HD13	1.91	0.53
7:MA:241:GLN:HG3	7:MA:243:SER:H	1.74	0.53
8:AC:295:PHE:HB2	8:AC:409:VAL:HG21	1.90	0.53
10:DB:161:ILE:HB	10:DB:208:VAL:HG12	1.91	0.53
13:OA:154:MET:HE3	13:OA:165:THR:HG22	1.90	0.53
4:HB:440:ASP:HB3	4:HB:457:ARG:HH11	1.74	0.53
8:AC:158:ASN:HB2	8:AC:173:ARG:HE	1.74	0.53
8:AC:581:LEU:HB3	8:AC:596:LEU:HD12	1.89	0.53
8:AJ:305:VAL:HG22	8:AJ:668:ILE:HD12	1.90	0.53
10:DB:275:CYS:HA	10:DB:278:ILE:HB	1.91	0.53
2:GB:858:ARG:HH21	15:NA:455:ARG:HG3	1.74	0.53
7:MA:722:MET:HA	7:MA:750:ASN:HB3	1.91	0.53
8:AH:546:GLN:HB3	8:AH:581:LEU:HD23	1.90	0.53
11:BB:323:CYS:HB2	11:BB:346:HIS:ND1	2.24	0.53
8:AE:401:LEU:HD11	8:AE:467:GLY:HA3	1.90	0.52
8:AI:408:MET:HE1	8:AI:474:CYS:HA	1.91	0.52
3:JA:121:VAL:O	3:JA:124:LYS:HG2	2.09	0.52
2:GB:796:LEU:HD13	2:GB:824:LEU:HD21	1.91	0.52
4:HB:339:VAL:HA	4:HB:344:VAL:HG21	1.89	0.52
8:AF:4:GLN:HE21	8:AF:7:LEU:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AF:547:ASN:HA	8:AF:550:VAL:HG12	1.90	0.52
8:AI:459:LEU:HD13	8:AI:473:MET:HE1	1.91	0.52
8:AA:547:ASN:HA	8:AA:550:VAL:HG12	1.91	0.52
2:GA:604:ASN:HB3	2:GA:607:ILE:HG12	1.90	0.52
10:DB:69:ILE:HG23	10:DB:83:VAL:HG11	1.91	0.52
8:AJ:18:LEU:HD23	8:AJ:112:THR:HB	1.92	0.52
11:BA:318:CYS:O	11:BA:319:ARG:HG2	2.09	0.52
10:DA:275:CYS:HB2	10:DA:279:CYS:H	1.75	0.52
10:DA:307:ILE:HD12	10:DA:310:LEU:HD12	1.92	0.52
4:HA:551:VAL:HG11	4:HA:571:ARG:HH11	1.74	0.52
8:AB:584:LEU:HD12	8:AB:587:VAL:HG11	1.92	0.52
10:DB:154:PRO:HG2	10:DB:203:GLU:HB2	1.92	0.52
11:BB:326:CYS:SG	11:BB:346:HIS:CE1	3.02	0.52
1:FA:113:VAL:HA	1:FA:116:VAL:HG12	1.91	0.52
7:MA:136:LEU:HD11	7:MA:151:LEU:HD21	1.90	0.52
8:AF:305:VAL:HG22	8:AF:668:ILE:HD12	1.93	0.51
10:DB:313:ARG:HH12	10:DB:450:THR:HA	1.76	0.51
7:MA:659:TYR:HA	7:MA:662:PHE:HB3	1.92	0.51
2:GB:806:ASN:HA	2:GB:835:ARG:HB2	1.91	0.51
8:AE:215:GLN:HE21	8:AE:240:ARG:HH22	1.57	0.51
8:AJ:140:TRP:CD1	8:AJ:148:GLY:HA3	2.44	0.51
8:AC:134:LYS:HA	8:AC:137:LYS:HE2	1.92	0.51
8:AE:310:GLU:H	8:AE:662:VAL:HG23	1.76	0.51
10:DB:194:SER:HB3	10:DB:200:MET:HB2	1.92	0.51
2:GB:924:ASN:H	2:GB:953:CYS:HB3	1.73	0.51
4:HB:303:SER:HB3	4:HB:560:THR:HB	1.93	0.51
4:HB:534:ILE:HD12	4:HB:568:THR:HG21	1.93	0.51
8:AD:581:LEU:HD12	8:AD:596:LEU:HB3	1.92	0.51
8:AG:347:ASP:HB3	8:AG:468:HIS:HE2	1.75	0.51
2:GA:677:ASN:HB3	2:GA:703:ARG:HH21	1.75	0.51
7:MA:466:ARG:HH21	7:MA:519:ARG:HB3	1.74	0.51
7:MA:587:ALA:HA	7:MA:625:MET:HB3	1.93	0.51
13:OA:156:THR:HG22	13:OA:163:ALA:HA	1.92	0.51
16:PA:354:LYS:HE3	16:PA:413:SER:O	2.11	0.51
8:AH:116:ILE:HD12	8:AH:197:LEU:HD21	1.92	0.51
10:DA:417:LEU:HD13	10:DA:428:LEU:HD12	1.93	0.51
16:PA:407:TYR:HB3	16:PA:416:LEU:HD22	1.91	0.51
15:NA:199:LYS:HB2	15:NA:242:LEU:HD22	1.93	0.51
6:LA:32:TRP:CD1	6:LA:70:HIS:HD1	2.29	0.51
8:AC:211:VAL:HG22	8:AC:247:VAL:HG12	1.93	0.51
8:AF:211:VAL:HG22	8:AF:247:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:NA:143:MET:HE3	15:NA:146:VAL:HB	1.92	0.51
2:GA:853:LEU:HD22	2:GA:888:LEU:HD12	1.92	0.51
2:GA:1008:VAL:HA	2:GA:1036:GLY:H	1.76	0.51
4:HA:337:CYS:HB3	4:HA:346:LEU:HD11	1.92	0.51
8:AE:502:PHE:HB3	8:AE:538:LEU:HD11	1.92	0.51
8:AE:581:LEU:HD12	8:AE:596:LEU:HB3	1.93	0.51
8:AA:629:CYS:HB3	8:AA:632:GLU:HB2	1.93	0.51
15:NA:31:VAL:HG12	15:NA:32:ASN:HD22	1.76	0.51
14:QB:55:LEU:HA	14:QB:58:VAL:HG12	1.93	0.50
8:AC:575:ILE:HD12	8:AC:635:VAL:HG23	1.93	0.50
8:AF:343:LYS:HZ1	8:AF:346:GLN:H	1.58	0.50
8:AH:140:TRP:CD1	8:AH:148:GLY:HA3	2.45	0.50
10:DA:275:CYS:HA	10:DA:278:ILE:HB	1.93	0.50
10:DA:531:LEU:HD21	10:DA:534:MET:HB2	1.92	0.50
11:BB:622:LYS:HD3	12:CB:20:GLN:HA	1.93	0.50
16:PA:7:ARG:HD3	16:PA:35:LEU:HD21	1.92	0.50
8:AC:310:GLU:H	8:AC:662:VAL:HG23	1.75	0.50
8:AI:303:LEU:HD23	8:AI:304:GLU:HG3	1.92	0.50
8:AJ:28:ASP:HB3	8:AJ:31:LYS:HE3	1.93	0.50
2:GB:747:LYS:HG3	2:GB:776:GLN:HG3	1.93	0.50
2:GB:863:SER:HB2	2:GB:892:ILE:HD13	1.93	0.50
4:HA:317:LYS:HD3	4:HA:331:PRO:HG3	1.92	0.50
1:FA:246:LEU:HD22	1:FA:352:ALA:HA	1.92	0.50
6:LA:88:ILE:HG22	6:LA:95:ARG:HH21	1.76	0.50
8:AE:49:LEU:HD13	8:AH:49:LEU:HD13	1.93	0.50
8:AH:268:VAL:HG12	8:AH:280:PRO:HA	1.92	0.50
15:NA:305:MET:HE2	15:NA:351:CYS:H	1.77	0.50
8:AA:323:LEU:HD21	8:AA:647:THR:HG21	1.94	0.50
8:AB:175:ILE:HG23	8:AB:178:LEU:HD12	1.94	0.50
8:AJ:514:THR:HG22	8:AJ:533:THR:HG22	1.94	0.50
11:BB:738:ASP:HB3	11:BB:742:ARG:HH12	1.77	0.50
12:CB:86:LEU:HD22	12:CB:88:ILE:HG12	1.93	0.50
15:NA:310:PRO:HA	15:NA:348:ARG:HH22	1.76	0.50
2:GB:1025:THR:HG22	2:GB:1054:GLN:HG3	1.94	0.50
8:AG:546:GLN:HB3	8:AG:581:LEU:HD23	1.93	0.50
8:AB:527:ASN:HD22	8:AB:652:PHE:HE2	1.60	0.50
8:AJ:42:ILE:HG13	8:AJ:93:VAL:HG22	1.93	0.50
8:AJ:547:ASN:HA	8:AJ:550:VAL:HG12	1.94	0.50
11:BB:19:LEU:HD23	11:BB:58:LEU:HD11	1.93	0.50
16:PA:205:ILE:HD12	16:PA:207:LEU:HD21	1.94	0.50
2:GB:372:THR:HG21	2:GB:380:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:440:VAL:HG13	2:GB:464:LEU:HD13	1.94	0.50
7:MA:6:SER:HB2	7:MA:67:TRP:HE1	1.77	0.50
8:AG:95:TYR:HB2	8:AG:105:ALA:HB3	1.94	0.50
8:AA:178:LEU:HD22	8:AA:248:GLU:HB3	1.93	0.50
2:GB:291:LYS:HA	2:GB:349:PRO:HA	1.93	0.50
9:EA:172:TYR:HB3	9:EA:205:ASP:HA	1.94	0.50
10:DB:331:CYS:HB3	10:DB:394:PHE:HB2	1.94	0.50
8:AF:306:TYR:HB2	8:AF:667:ILE:HG13	1.94	0.49
10:DB:797:LEU:HD11	10:DB:803:LEU:HD23	1.94	0.49
13:OA:50:TRP:HB3	13:OA:56:VAL:HG21	1.93	0.49
2:GB:357:LEU:HG	2:GB:362:LEU:HD21	1.93	0.49
2:GA:701:ASP:HA	2:GA:754:SER:HB3	1.95	0.49
2:GA:1008:VAL:HG13	2:GA:1036:GLY:HA3	1.93	0.49
8:AH:316:PHE:HD1	8:AH:649:ILE:HG21	1.77	0.49
2:GA:340:LEU:HD12	2:GA:361:ALA:HB3	1.95	0.49
7:MA:28:PHE:HB3	7:MA:73:ILE:HD12	1.95	0.49
7:MA:118:GLN:HA	7:MA:121:ILE:HB	1.94	0.49
8:AI:310:GLU:H	8:AI:662:VAL:HG21	1.77	0.49
11:BB:678:ILE:HD13	11:BB:692:LEU:HD11	1.93	0.49
2:GB:980:MET:HA	2:GB:1009:ASP:HB3	1.94	0.49
8:AJ:504:GLN:HG2	8:AJ:507:LYS:HE2	1.94	0.49
13:OA:432:GLY:HA3	13:OA:450:SER:HA	1.95	0.49
14:QA:5:LYS:HG2	14:QA:15:GLU:HG3	1.93	0.49
9:EA:250:VAL:HG13	9:EA:254:GLU:HB2	1.94	0.49
10:DA:797:LEU:HD11	10:DA:803:LEU:HD23	1.94	0.49
10:DB:238:ARG:HH21	10:DB:270:HIS:HB3	1.77	0.49
10:DB:723:LEU:HD11	10:DB:751:LEU:HG	1.93	0.49
2:GB:246:ILE:HG12	2:GB:389:TYR:HB3	1.94	0.49
8:AG:401:LEU:HD11	8:AG:467:GLY:HA3	1.95	0.49
10:DB:93:LYS:HE3	10:DB:211:ARG:HG3	1.95	0.49
13:OA:28:VAL:HA	14:QB:136:ARG:HH11	1.76	0.49
13:OA:407:TYR:HB3	13:OA:416:LEU:HD22	1.94	0.49
2:GB:456:LEU:HD22	2:GB:607:ILE:HG12	1.94	0.49
2:GA:708:VAL:HG12	2:GA:710:ASN:H	1.76	0.49
8:AC:398:VAL:HG21	8:AC:587:VAL:HG12	1.95	0.49
8:AA:20:MET:HE1	8:AA:116:ILE:H	1.78	0.49
12:CA:33:TRP:HB2	12:CA:54:ILE:HB	1.94	0.49
12:CB:40:PRO:HD2	12:CB:45:TYR:HB2	1.94	0.49
12:CB:85:CYS:HA	12:CB:90:ARG:HH22	1.77	0.49
2:GB:492:VAL:HG12	2:GB:562:LEU:HD13	1.95	0.49
2:GB:749:LEU:HB2	2:GB:775:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AD:316:PHE:HD1	8:AD:649:ILE:HG21	1.76	0.49
8:AH:8:SER:HA	8:AH:31:LYS:HZ3	1.78	0.49
11:BB:203:ARG:HH11	11:BB:294:PRO:HB2	1.77	0.49
11:BB:338:CYS:SG	11:BB:341:CYS:HB2	2.53	0.49
13:OA:249:LEU:HD11	13:OA:259:THR:HB	1.95	0.49
16:PA:58:GLN:HA	16:PA:63:LYS:HD3	1.94	0.49
2:GB:329:MET:HE2	2:GB:333:LEU:HD21	1.94	0.49
2:GA:293:SER:HB3	2:GA:296:GLN:HG2	1.94	0.49
8:AH:659:ILE:HD12	11:BB:458:SER:H	1.77	0.49
8:AI:115:GLU:HB3	8:AI:186:GLU:H	1.78	0.49
2:GA:756:LEU:HB2	2:GA:785:VAL:HG12	1.95	0.49
8:AD:376:PHE:HB2	8:AD:379:LYS:HE2	1.95	0.49
10:DA:936:CYS:HB2	10:DA:968:VAL:HG21	1.94	0.49
10:DB:285:GLN:HA	10:DB:288:LYS:HG2	1.95	0.49
10:DB:564:TRP:CD2	10:DB:591:LEU:HD11	2.48	0.49
11:BA:623:GLU:HA	11:BA:626:ARG:HD2	1.95	0.49
12:CA:103:LEU:HD23	12:CA:106:ILE:HD12	1.93	0.49
15:NA:389:LEU:HD22	15:NA:449:ARG:HH22	1.78	0.49
6:LA:13:LEU:HD23	6:LA:23:ILE:HA	1.95	0.48
8:AI:473:MET:HE2	8:AI:561:LEU:HD11	1.95	0.48
8:AI:490:LEU:HD21	8:AI:561:LEU:HD13	1.95	0.48
14:QA:6:LEU:HD23	14:QA:45:VAL:HB	1.95	0.48
2:GB:675:LEU:HD11	4:HB:256:TRP:HH2	1.79	0.48
8:AJ:489:ARG:HE	8:AJ:642:LEU:HD11	1.77	0.48
10:DA:586:ARG:HD2	10:DA:615:ASP:HB2	1.94	0.48
11:BB:227:TYR:HE1	11:BB:308:ARG:HG3	1.77	0.48
3:JA:50:GLU:HB2	3:JA:53:VAL:HG22	1.94	0.48
8:AC:91:VAL:HB	8:AC:109:LEU:HB3	1.96	0.48
9:EA:147:SER:HB2	9:EA:190:THR:HB	1.95	0.48
2:GB:389:TYR:OH	3:IA:34:TRP:HA	2.13	0.48
2:GB:960:TYR:CZ	2:GB:983:VAL:HB	2.49	0.48
2:GA:561:VAL:HA	2:GA:621:PRO:HB3	1.96	0.48
4:HB:289:VAL:HG13	4:HB:573:CYS:HB3	1.95	0.48
11:BA:340:GLU:HB3	11:BA:368:CYS:SG	2.53	0.48
16:PA:404:LEU:HD22	16:PA:422:LEU:HD12	1.95	0.48
4:HA:302:SER:HB2	4:HA:351:LEU:HD21	1.95	0.48
8:AE:268:VAL:HA	8:AE:280:PRO:HA	1.95	0.48
8:AF:347:ASP:HA	8:AF:405:GLY:HA3	1.95	0.48
8:AI:373:LEU:O	8:AI:374:GLU:HG3	2.13	0.48
8:AJ:538:LEU:HG	8:AJ:544:ARG:HH21	1.78	0.48
10:DB:164:PHE:HB3	10:DB:210:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:DB:417:LEU:HD13	10:DB:428:LEU:HD12	1.94	0.48
15:NA:448:ILE:HG22	15:NA:462:THR:HG22	1.94	0.48
4:HB:513:ILE:HG21	4:HB:516:LEU:HD23	1.95	0.48
10:DA:747:THR:HB	10:DA:776:GLN:HG2	1.95	0.48
13:OA:291:TRP:CE2	13:OA:299:ILE:HD12	2.49	0.48
16:PA:105:TYR:HE2	16:PA:438:LEU:HB3	1.79	0.48
2:GA:246:ILE:HD11	2:GA:384:VAL:HG21	1.95	0.48
8:AD:465:MET:HE1	8:AD:584:LEU:HA	1.95	0.48
8:AD:502:PHE:HB3	8:AD:538:LEU:HD11	1.96	0.48
8:AF:546:GLN:HB3	8:AF:581:LEU:HD23	1.94	0.48
8:AG:195:TYR:HB3	8:AG:267:LEU:HD11	1.94	0.48
8:AJ:306:TYR:HB2	8:AJ:667:ILE:HG13	1.95	0.48
12:CA:85:CYS:HB2	12:CA:119:LEU:HG	1.95	0.48
2:GB:824:LEU:HD12	2:GB:852:LEU:HD11	1.94	0.48
8:AD:347:ASP:HA	8:AD:405:GLY:HA3	1.95	0.48
8:AE:584:LEU:HD12	8:AE:587:VAL:HG11	1.95	0.48
8:AF:343:LYS:HZ2	8:AF:345:LEU:H	1.61	0.48
8:AH:302:PRO:HG3	8:AH:611:LEU:HA	1.94	0.48
10:DB:740:LEU:HD12	10:DB:775:LEU:HD11	1.95	0.48
2:GA:1031:LYS:HA	2:GA:1059:LEU:HA	1.96	0.48
8:AA:603:PRO:HD3	8:AA:655:TYR:CZ	2.48	0.48
8:AJ:624:LYS:HA	8:AJ:629:CYS:HA	1.95	0.48
10:DB:451:PHE:HB2	10:DB:453:LEU:HD22	1.95	0.48
2:GA:698:ILE:HG22	2:GA:746:LEU:HD11	1.96	0.48
2:GB:433:ALA:HB3	2:GB:436:VAL:HG23	1.96	0.47
2:GB:535:GLN:HE21	2:GB:542:GLN:HA	1.78	0.47
7:MA:263:LEU:HB3	7:MA:289:ILE:HD12	1.95	0.47
8:AG:157:PRO:HB3	8:AG:379:LYS:HD2	1.95	0.47
8:AJ:140:TRP:HZ3	8:AJ:142:TRP:CE2	2.32	0.47
10:DA:740:LEU:HD12	10:DA:775:LEU:HD11	1.96	0.47
11:BA:699:PRO:HB3	11:BA:702:ILE:HD12	1.94	0.47
15:NA:82:THR:HG21	15:NA:112:ARG:HH22	1.78	0.47
8:AG:42:ILE:HG12	8:AG:50:ILE:HD13	1.96	0.47
7:MA:263:LEU:HD21	7:MA:275:LEU:HD11	1.96	0.47
8:AD:305:VAL:HG22	8:AD:668:ILE:HD12	1.96	0.47
10:DA:60:PRO:HA	10:DA:63:GLN:HG2	1.96	0.47
11:BA:139:VAL:HG21	11:BA:182:VAL:HG21	1.96	0.47
2:GA:703:ARG:NH1	2:GA:704:ASP:HB2	2.29	0.47
8:AA:27:LEU:HB2	8:AA:75:ALA:HB3	1.96	0.47
11:BA:602:THR:HG23	11:BA:607:LEU:HB2	1.95	0.47
4:HB:567:ILE:HG13	4:HB:576:VAL:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:MA:776:TYR:HA	7:MA:804:HIS:HB3	1.95	0.47
8:AD:79:MET:HE2	8:AD:113:GLY:HA3	1.96	0.47
8:AI:623:PRO:HG2	8:AI:630:CYS:SG	2.55	0.47
10:DB:693:ASN:HA	10:DB:722:ALA:HB3	1.97	0.47
11:BB:300:THR:HG22	11:BB:302:LYS:HG2	1.95	0.47
14:QC:100:LEU:HA	14:QC:103:LEU:HD12	1.95	0.47
2:GB:979:THR:HG23	2:GB:1008:VAL:HB	1.96	0.47
2:GA:1097:PHE:HB3	2:GA:1102:MET:HG2	1.96	0.47
4:HB:302:SER:HB2	4:HB:351:LEU:HD21	1.97	0.47
8:AF:575:ILE:HD12	8:AF:635:VAL:HG23	1.97	0.47
8:AG:558:ARG:HH22	8:AG:569:ASP:HB2	1.78	0.47
8:AH:379:LYS:HA	8:AH:382:LEU:HG	1.96	0.47
8:AA:195:TYR:HB3	8:AA:267:LEU:HD11	1.96	0.47
8:AB:34:PRO:HB2	8:AB:37:CYS:HB2	1.97	0.47
10:DA:499:THR:HG22	10:DA:527:HIS:HB3	1.97	0.47
11:BB:14:HIS:HB2	11:BB:36:PHE:HE1	1.79	0.47
15:NA:157:LEU:HD13	15:NA:168:THR:HG22	1.96	0.47
3:IA:78:VAL:HG22	3:IA:89:ILE:HG12	1.97	0.47
4:HB:151:TRP:HZ2	4:HB:289:VAL:HG11	1.78	0.47
7:MA:821:CYS:HA	7:MA:824:LEU:HD12	1.97	0.47
8:AF:14:PRO:HB3	8:AF:108:VAL:HB	1.96	0.47
8:AF:50:ILE:HG12	8:AF:77:VAL:HG12	1.97	0.47
8:AH:49:LEU:HD12	8:AH:78:ARG:HE	1.80	0.47
8:AB:50:ILE:HG12	8:AB:77:VAL:HG12	1.97	0.47
8:AI:44:GLY:HA2	8:AI:91:VAL:HA	1.97	0.47
9:EA:104:ALA:HB2	9:EA:413:MET:HE3	1.97	0.47
11:BB:323:CYS:HB3	11:BB:326:CYS:SG	2.54	0.47
2:GB:653:LEU:HD21	2:GB:665:ALA:HB3	1.96	0.47
8:AC:347:ASP:HA	8:AC:405:GLY:HA3	1.96	0.47
8:AA:401:LEU:HD11	8:AA:467:GLY:HA3	1.96	0.47
8:AB:28:ASP:HB3	8:AB:31:LYS:HZ1	1.78	0.47
10:DB:174:PRO:HG2	10:DB:177:ALA:HB3	1.97	0.47
14:QA:101:PHE:HA	14:QA:104:ILE:HD12	1.97	0.47
4:HA:451:LEU:HD13	4:HA:485:LEU:HD21	1.96	0.47
6:LA:54:MET:HA	3:JA:133:ARG:HD2	1.97	0.47
8:AG:9:LEU:HD22	8:AG:107:ALA:HB1	1.96	0.47
8:AA:302:PRO:HG3	8:AA:611:LEU:HA	1.96	0.47
8:AA:469:MET:HB3	8:AA:473:MET:HE2	1.97	0.47
8:AB:514:THR:HA	8:AB:533:THR:HA	1.96	0.47
8:AE:323:LEU:HD11	8:AE:614:ASN:HB3	1.95	0.47
8:AG:34:PRO:HB2	8:AG:37:CYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AI:584:LEU:HD12	8:AI:587:VAL:HG11	1.97	0.47
10:DB:32:THR:HA	10:DB:35:LYS:HG2	1.97	0.47
16:PA:310:ILE:HG23	16:PA:340:GLN:HG2	1.97	0.47
2:GA:251:PRO:HG3	2:GA:373:ARG:HE	1.80	0.46
2:GA:768:LEU:HB2	2:GA:795:LEU:HD11	1.97	0.46
8:AD:367:THR:HG22	8:AD:391:ARG:HB3	1.97	0.46
8:AG:490:LEU:HD21	8:AG:561:LEU:HD13	1.97	0.46
8:AB:351:PHE:CE1	8:AB:667:ILE:HD12	2.50	0.46
10:DA:132:PHE:HB2	10:DA:191:LEU:HD12	1.96	0.46
10:DB:35:LYS:HE2	10:DB:105:ALA:HB1	1.97	0.46
11:BA:453:GLY:HA2	11:BA:466:VAL:HG12	1.97	0.46
14:QB:16:VAL:HG22	14:QB:59:ILE:HD12	1.97	0.46
8:AA:347:ASP:HA	8:AA:405:GLY:HA3	1.95	0.46
11:BA:298:ARG:HD2	11:BA:298:ARG:HA	1.80	0.46
15:NA:312:LYS:HZ1	15:NA:345:TYR:HB2	1.80	0.46
2:GA:796:LEU:HD21	2:GA:805:LEU:HD22	1.97	0.46
4:HB:298:VAL:HB	4:HB:311:CYS:HB3	1.97	0.46
8:AC:519:ILE:HD12	8:AC:652:PHE:HE2	1.81	0.46
8:AG:114:ILE:HD11	8:AG:191:ILE:HD11	1.97	0.46
8:AH:490:LEU:HD21	8:AH:561:LEU:HD13	1.97	0.46
8:AA:157:PRO:HB3	8:AA:379:LYS:HB3	1.97	0.46
8:AB:547:ASN:HA	8:AB:550:VAL:HG12	1.97	0.46
8:AI:95:TYR:HB2	8:AI:105:ALA:HB3	1.95	0.46
13:OA:105:TYR:HE1	13:OA:445:ILE:HD12	1.81	0.46
2:GB:294:LEU:HD22	2:GB:362:LEU:HD11	1.97	0.46
7:MA:365:ARG:HD3	7:MA:558:GLU:HG3	1.98	0.46
12:CB:120:VAL:HG11	12:CB:123:ILE:HD12	1.98	0.46
2:GB:1008:VAL:HA	2:GB:1036:GLY:H	1.80	0.46
7:MA:598:LYS:HD3	7:MA:636:GLN:HB3	1.97	0.46
8:AC:122:ILE:HD13	8:AC:137:LYS:HG2	1.97	0.46
8:AC:186:GLU:HG2	8:AC:241:ARG:HD3	1.98	0.46
8:AF:79:MET:HG2	8:AF:113:GLY:HA3	1.97	0.46
8:AH:154:ASN:HD21	8:AH:210:ARG:HH21	1.63	0.46
8:AB:205:GLU:HB3	8:AB:261:ILE:HG23	1.97	0.46
8:AI:305:VAL:HG22	8:AI:668:ILE:HG23	1.97	0.46
11:BA:208:ILE:HD11	11:BA:276:MET:HE2	1.96	0.46
13:OA:29:ASN:HD21	13:OA:32:TRP:CD1	2.34	0.46
13:OA:302:MET:HE3	13:OA:349:MET:HB3	1.98	0.46
15:NA:391:LEU:HD22	15:NA:400:VAL:HG22	1.96	0.46
2:GA:274:LYS:HE3	2:GA:275:MET:HE2	1.98	0.46
2:GA:766:LEU:HD22	2:GA:769:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IA:111:TRP:CE2	3:IA:148:LEU:HD21	2.51	0.46
8:AF:463:TRP:H	8:AF:463:TRP:CD1	2.32	0.46
9:EA:48:SER:HB3	9:EA:245:ASP:CG	2.40	0.46
15:NA:276:PHE:HE2	15:NA:330:ILE:HG13	1.80	0.46
16:PA:334:PHE:HE2	16:PA:370:ILE:HG12	1.80	0.46
2:GB:672:VAL:HG22	2:GB:695:LEU:HD11	1.98	0.46
2:GA:705:LEU:HA	3:JA:99:THR:HG21	1.97	0.46
7:MA:639:ARG:HG2	7:MA:668:VAL:HG21	1.98	0.46
8:AC:116:ILE:HG13	8:AC:267:LEU:HD22	1.96	0.46
8:AE:305:VAL:HG22	8:AE:668:ILE:HD12	1.98	0.46
8:AJ:345:LEU:HD12	8:AJ:664:ALA:HB1	1.98	0.46
12:CA:126:ILE:HG22	12:CA:134:TYR:HB2	1.97	0.46
15:NA:210:LEU:HD23	15:NA:220:ILE:HG12	1.97	0.46
2:GB:821:CYS:HA	2:GB:852:LEU:HD12	1.98	0.46
2:GB:836:LEU:HD21	2:GB:841:LEU:HD11	1.97	0.46
8:AD:421:PRO:HD2	8:AD:680:MET:HE3	1.98	0.46
8:AH:178:LEU:HD22	8:AH:248:GLU:HB3	1.98	0.46
11:BB:52:MET:HA	11:BB:61:TYR:CZ	2.51	0.46
4:HB:557:PHE:HE1	4:HB:566:ILE:HD11	1.81	0.46
8:AB:546:GLN:HB3	8:AB:581:LEU:HD23	1.97	0.46
8:AI:546:GLN:HB3	8:AI:581:LEU:HD23	1.97	0.46
10:DA:351:ARG:HH21	11:BA:339:ASP:HB3	1.80	0.46
10:DA:668:SER:H	10:DA:696:LEU:HB2	1.80	0.46
11:BB:220:MET:SD	11:BB:234:TRP:HB3	2.56	0.46
2:GA:288:TRP:HB3	2:GA:329:MET:HE1	1.97	0.46
4:HA:536:VAL:HG23	4:HA:545:LEU:HB2	1.98	0.46
2:GB:305:SER:HB3	2:GB:308:LEU:HD23	1.98	0.45
2:GB:635:ALA:HB1	2:GB:669:PHE:HA	1.98	0.45
2:GB:1088:ASN:HA	2:GB:1116:LEU:HA	1.98	0.45
3:IA:58:ILE:HD13	3:IA:78:VAL:HG21	1.97	0.45
8:AE:175:ILE:HG23	8:AE:178:LEU:HD12	1.97	0.45
8:AA:364:ILE:HG13	8:AA:382:LEU:HD21	1.99	0.45
8:AB:426:LEU:HD13	8:AB:473:MET:HE1	1.97	0.45
8:AJ:7:LEU:HD12	8:AJ:25:ILE:HG21	1.98	0.45
16:PA:251:ASN:HD21	16:PA:286:CYS:HB3	1.81	0.45
2:GB:711:THR:HG21	3:IA:106:LEU:HD13	1.99	0.45
4:HB:299:VAL:HG22	4:HB:310:THR:HG22	1.98	0.45
8:AF:489:ARG:HG3	8:AF:642:LEU:HD21	1.97	0.45
8:AG:255:PRO:HG3	8:AG:446:GLU:HB3	1.98	0.45
8:AB:295:PHE:HB2	8:AB:409:VAL:HG21	1.98	0.45
10:DA:666:LEU:HB2	10:DA:694:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BB:341:CYS:SG	11:BB:368:CYS:HB3	2.57	0.45
2:GA:1002:LEU:HD21	2:GA:1005:LEU:HB2	1.99	0.45
8:AE:45:SER:HB2	8:AE:90:LYS:H	1.82	0.45
8:AI:178:LEU:HB3	8:AI:246:TYR:HB3	1.97	0.45
9:EA:180:ALA:HB3	9:EA:183:GLU:HG3	1.99	0.45
10:DA:694:LEU:HD12	10:DA:707:LEU:HD11	1.98	0.45
16:PA:300:THR:HG21	16:PA:357:ILE:HD11	1.98	0.45
7:MA:863:HIS:ND1	7:MA:892:GLN:HG3	2.32	0.45
8:AC:18:LEU:HD11	8:AC:191:ILE:HD11	1.99	0.45
8:AC:310:GLU:HG2	8:AC:336:GLU:HG2	1.98	0.45
8:AC:355:GLN:HB3	8:AC:677:TRP:CD1	2.51	0.45
8:AC:623:PRO:HG2	8:AC:630:CYS:SG	2.56	0.45
8:AB:196:GLN:HB3	8:AB:268:VAL:HG23	1.98	0.45
2:GB:951:ASN:HB3	2:GB:952:HIS:H	1.52	0.45
2:GA:284:ARG:HH22	2:GA:536:VAL:HG11	1.81	0.45
8:AB:422:LEU:HD12	8:AB:453:VAL:HB	1.97	0.45
8:AJ:352:CYS:HB2	8:AJ:363:LEU:HB3	1.99	0.45
10:DA:116:VAL:HG12	10:DA:158:LEU:HB3	1.98	0.45
8:AC:493:ALA:HB3	8:AC:554:ILE:HD13	1.99	0.45
8:AE:459:LEU:HD13	8:AE:473:MET:HE1	1.99	0.45
8:AA:575:ILE:HD12	8:AA:635:VAL:HG23	1.98	0.45
11:BA:733:CYS:HB2	11:BA:736:CYS:SG	2.55	0.45
1:FA:175:VAL:HB	1:FA:208:TYR:CZ	2.51	0.45
8:AC:95:TYR:HB2	8:AC:105:ALA:HB3	1.99	0.45
8:AD:37:CYS:HB3	8:AD:97:CYS:HB3	1.86	0.45
8:AG:519:ILE:HG13	8:AG:652:PHE:HZ	1.82	0.45
8:AH:177:ASN:HA	8:AH:359:LYS:HD3	1.99	0.45
8:AA:14:PRO:HB3	8:AA:108:VAL:HB	1.99	0.45
14:QA:159:TRP:C	14:QA:161:GLU:H	2.25	0.45
15:NA:179:ASP:HB3	15:NA:186:LEU:HD11	1.99	0.45
2:GB:1049:CYS:HA	2:GB:1052:LEU:HB2	1.99	0.45
8:AD:575:ILE:HD12	8:AD:635:VAL:HG23	1.99	0.45
8:AE:463:TRP:H	8:AE:463:TRP:CD1	2.34	0.45
8:AI:308:CYS:HB3	8:AI:664:ALA:HB3	1.99	0.45
10:DB:740:LEU:HD11	10:DB:749:LEU:HD22	1.98	0.45
14:QC:101:PHE:HA	14:QC:104:ILE:HD12	1.98	0.45
1:FA:290:THR:HG21	1:FA:329:GLN:HB3	1.99	0.45
2:GA:848:MET:HE2	2:GA:848:MET:HB3	1.90	0.45
8:AD:323:LEU:HD11	8:AD:614:ASN:HB3	1.98	0.45
8:AF:502:PHE:HB3	8:AF:538:LEU:HD11	1.98	0.45
8:AH:624:LYS:HA	8:AH:629:CYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:DA:564:TRP:CD2	10:DA:591:LEU:HD11	2.52	0.45
10:DA:921:ASN:HA	10:DA:950:ALA:HB3	1.99	0.45
10:DB:511:ARG:HE	10:DB:537:THR:HG21	1.81	0.45
10:DB:642:LEU:HD22	10:DB:671:LEU:HD21	1.98	0.45
10:DB:720:ARG:HA	10:DB:748:HIS:HB2	1.99	0.45
2:GB:255:LYS:HG2	2:GB:392:VAL:HG21	1.99	0.45
7:MA:313:PHE:O	7:MA:314:GLN:HG3	2.17	0.45
8:AC:527:ASN:O	8:AC:529:ARG:HG2	2.17	0.45
8:AD:34:PRO:HB2	8:AD:37:CYS:HB2	1.98	0.45
8:AE:130:MET:HE3	8:AH:92:LEU:HD23	1.98	0.45
12:CB:5:ARG:NH1	12:CB:61:PRO:HG3	2.31	0.45
3:JA:100:ARG:O	3:JA:104:ILE:HG12	2.17	0.45
2:GB:492:VAL:HG23	2:GB:572:PHE:HZ	1.82	0.44
2:GB:786:VAL:HA	2:GB:789:LEU:HG	1.99	0.44
7:MA:167:MET:HE3	7:MA:227:ILE:HB	1.99	0.44
8:AD:378:MET:HA	8:AD:381:THR:HG22	1.99	0.44
8:AI:7:LEU:HD23	8:AI:25:ILE:HD13	1.98	0.44
8:AI:209:THR:HB	8:AI:261:ILE:HD13	1.97	0.44
8:AJ:319:SER:HB2	8:AJ:649:ILE:HG12	1.98	0.44
8:AJ:463:TRP:CD1	8:AJ:463:TRP:H	2.34	0.44
10:DA:43:TYR:CE1	10:DA:54:LEU:HD21	2.52	0.44
10:DA:211:ARG:NH1	10:DA:384:LEU:HD12	2.32	0.44
14:QA:16:VAL:HG11	14:QA:59:ILE:HD12	1.98	0.44
7:MA:332:LEU:HD22	7:MA:369:LEU:HD12	1.98	0.44
8:AB:575:ILE:HD12	8:AB:635:VAL:HG23	2.00	0.44
10:DA:663:VAL:HG13	10:DA:691:PHE:HB3	2.00	0.44
1:FA:174:LYS:HB3	1:FA:208:TYR:CD2	2.53	0.44
7:MA:741:MET:HG2	7:MA:766:ALA:HB1	2.00	0.44
7:MA:906:LEU:HD12	7:MA:919:LEU:HD21	1.99	0.44
8:AC:19:CYS:HB3	8:AC:111:LEU:HD21	1.99	0.44
10:DB:339:TRP:CZ3	10:DB:411:PHE:HA	2.53	0.44
14:QB:146:THR:H	14:QB:149:GLU:HB2	1.83	0.44
1:FA:267:MET:HE2	1:FA:371:SER:HB3	2.00	0.44
4:HB:528:VAL:HB	4:HB:554:VAL:HB	2.00	0.44
8:AC:151:LEU:HG	8:AC:288:PHE:HB3	1.98	0.44
8:AC:195:TYR:HB3	8:AC:267:LEU:HD11	1.98	0.44
8:AG:116:ILE:HG13	8:AG:267:LEU:HD22	1.99	0.44
8:AG:534:ILE:HD11	8:AG:623:PRO:HG3	1.98	0.44
10:DA:132:PHE:CE1	10:DA:195:LEU:HD21	2.52	0.44
2:GB:519:LEU:HG	2:GB:524:ILE:HD11	1.98	0.44
7:MA:111:LYS:HE2	7:MA:440:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:MA:345:VAL:HG22	7:MA:369:LEU:HD13	2.00	0.44
8:AC:82:PRO:HG2	8:AC:186:GLU:HB2	1.99	0.44
8:AI:485:GLN:HG3	8:AI:489:ARG:HH22	1.83	0.44
10:DB:610:ILE:HA	10:DB:636:ASP:HB2	2.00	0.44
11:BA:526:ALA:HB3	11:BA:568:TYR:CE1	2.52	0.44
13:OA:80:LYS:NZ	13:OA:396:ILE:HD11	2.33	0.44
13:OA:130:ILE:HD11	13:OA:165:THR:HG21	2.00	0.44
15:NA:60:ILE:HD11	15:NA:116:ARG:HG2	2.00	0.44
15:NA:202:PHE:HD1	15:NA:207:ALA:HB2	1.82	0.44
8:AD:313:LEU:HG	8:AD:317:VAL:HG11	1.98	0.44
8:AF:623:PRO:HG2	8:AF:630:CYS:SG	2.58	0.44
8:AI:82:PRO:HG2	8:AI:186:GLU:HB2	1.98	0.44
11:BB:350:LEU:HD11	11:BB:354:LEU:HD23	2.00	0.44
2:GB:492:VAL:HG21	2:GB:568:TRP:CD1	2.52	0.44
4:HA:565:LEU:HD23	4:HA:578:HIS:HA	1.99	0.44
6:LA:106:ALA:HA	3:JA:133:ARG:HH12	1.81	0.44
8:AD:349:MET:HE1	8:AD:378:MET:HE2	1.99	0.44
8:AD:422:LEU:HD12	8:AD:453:VAL:HB	1.99	0.44
10:DA:723:LEU:HD11	10:DA:751:LEU:HG	2.00	0.44
11:BA:231:ARG:HD3	11:BA:298:ARG:HG3	1.98	0.44
11:BA:302:LYS:HA	11:BA:303:SER:HA	1.60	0.44
2:GB:381:LYS:HD2	4:HB:332:GLU:HG3	1.99	0.44
2:GB:817:MET:HG2	2:GB:845:GLY:HA2	2.00	0.44
2:GA:560:TYR:HB3	2:GA:623:VAL:HG11	1.99	0.44
6:LA:75:VAL:HG22	6:LA:86:ILE:HG22	2.00	0.44
8:AA:201:THR:HB	8:AA:263:LEU:HD23	1.99	0.44
8:AI:5:ASN:HB2	8:AJ:559:THR:HG22	2.00	0.44
8:AI:656:LEU:HD21	8:AI:659:ILE:HG13	2.00	0.44
8:AJ:508:GLU:HG3	8:AJ:510:TYR:HD1	1.83	0.44
10:DB:502:LEU:HD13	10:DB:528:CYS:HA	1.99	0.44
11:BB:44:ARG:HB2	11:BB:72:LEU:HB3	2.00	0.44
11:BB:335:GLN:HB3	11:BB:344:ALA:HB1	1.99	0.44
11:BB:566:VAL:HG21	11:BB:585:ARG:HG3	1.99	0.44
8:AC:629:CYS:HB3	8:AC:632:GLU:HB2	2.00	0.44
9:EA:209:ILE:HG23	9:EA:230:LEU:HD23	2.00	0.44
10:DA:888:HIS:HA	10:DA:916:SER:HB2	1.99	0.44
11:BA:319:ARG:HB2	11:BA:343:MET:SD	2.57	0.44
11:BB:8:MET:HG3	11:BB:72:LEU:HD13	1.99	0.44
14:QA:3:THR:HG21	14:QA:15:GLU:HB3	1.99	0.44
16:PA:449:THR:HG22	16:PA:454:PRO:HA	1.99	0.44
2:GA:642:SER:HB3	2:GA:645:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:HB:297:LEU:O	4:HB:556:CYS:HB3	2.18	0.43
7:MA:229:ASP:HA	7:MA:276:SER:HB3	2.00	0.43
7:MA:668:VAL:O	7:MA:693:ASP:HB3	2.18	0.43
8:AE:492:LEU:HD13	8:AE:572:ILE:HG23	1.99	0.43
8:AF:176:GLN:HG3	8:AF:359:LYS:HD2	2.00	0.43
8:AF:493:ALA:HB3	8:AF:554:ILE:HD13	2.00	0.43
8:AI:485:GLN:HB2	8:AI:489:ARG:HH12	1.83	0.43
14:QC:163:LYS:HB3	16:PA:411:GLU:HB2	2.00	0.43
1:FA:292:GLN:HG2	1:FA:298:ASN:ND2	2.33	0.43
8:AC:34:PRO:HB2	8:AC:37:CYS:HB2	2.00	0.43
10:DB:405:ASP:HA	11:BB:229:ARG:HD2	2.00	0.43
11:BB:436:ARG:H	11:BB:440:GLN:NE2	2.16	0.43
12:CB:85:CYS:SG	12:CB:119:LEU:HG	2.58	0.43
15:NA:407:LEU:HD11	15:NA:425:LEU:HD12	2.00	0.43
16:PA:57:THR:O	16:PA:58:GLN:HG3	2.18	0.43
16:PA:432:GLY:HA2	16:PA:450:ILE:HA	1.99	0.43
3:JA:138:LEU:HA	3:JA:141:LEU:HD12	1.99	0.43
2:GA:277:PHE:CE2	2:GA:279:ILE:HD11	2.53	0.43
7:MA:604:GLU:HG2	7:MA:605:ASN:H	1.83	0.43
8:AC:463:TRP:CD1	8:AC:463:TRP:H	2.35	0.43
8:AE:602:PHE:HA	8:AE:655:TYR:OH	2.18	0.43
8:AH:422:LEU:HD12	8:AH:453:VAL:HB	2.00	0.43
11:BA:136:TYR:CZ	11:BA:293:PRO:HB3	2.53	0.43
12:CB:126:ILE:HG22	12:CB:134:TYR:HB2	2.00	0.43
13:OA:205:ILE:HD13	13:OA:268:LEU:HD21	2.00	0.43
2:GB:1045:VAL:HG21	2:GB:1069:LEU:HD11	1.99	0.43
2:GB:1110:GLN:HB3	2:GB:1137:VAL:HG12	2.00	0.43
11:BB:219:VAL:HG23	11:BB:276:MET:HA	1.99	0.43
2:GB:653:LEU:HB3	2:GB:662:VAL:HG22	2.00	0.43
4:HA:528:VAL:HB	4:HA:554:VAL:HG13	2.00	0.43
7:MA:253:GLN:HB3	7:MA:258:LEU:HB2	2.00	0.43
7:MA:748:VAL:HG13	7:MA:776:TYR:HB3	2.00	0.43
8:AE:351:PHE:HE1	8:AE:667:ILE:HD12	1.83	0.43
8:AH:3:PHE:HE2	8:AH:281:LEU:HD13	1.84	0.43
8:AH:211:VAL:HG22	8:AH:247:VAL:HG22	2.00	0.43
8:AH:305:VAL:HG22	8:AH:668:ILE:HD12	2.00	0.43
8:AB:308:CYS:HB2	8:AB:345:LEU:HD22	1.99	0.43
10:DA:348:GLN:HA	10:DA:351:ARG:HG2	2.00	0.43
10:DB:258:SER:HB3	10:DB:296:CYS:HB3	2.01	0.43
13:OA:188:LEU:HD23	13:OA:188:LEU:HA	1.84	0.43
4:HA:277:ARG:HH12	7:MA:78:ASN:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:HA:344:VAL:HB	4:HA:365:LEU:HD12	1.99	0.43
7:MA:465:LYS:N	7:MA:521:SER:HB2	2.34	0.43
8:AE:309:ARG:HD2	8:AE:333:LYS:HE2	2.00	0.43
8:AB:376:PHE:HB2	8:AB:379:LYS:HE2	2.00	0.43
8:AI:197:LEU:HD23	8:AI:265:LEU:HD11	2.00	0.43
10:DA:58:ILE:HA	10:DA:99:LYS:HZ1	1.82	0.43
10:DA:268:MET:HE3	10:DA:385:HIS:CG	2.53	0.43
10:DA:278:ILE:HG12	10:DA:302:LEU:HD21	2.01	0.43
4:HB:530:MET:HG3	4:HB:553:PRO:HB3	2.00	0.43
7:MA:596:LEU:H	7:MA:596:LEU:HD23	1.83	0.43
8:AC:20:MET:HE1	8:AC:116:ILE:H	1.83	0.43
8:AE:306:TYR:HB2	8:AE:667:ILE:HG13	2.01	0.43
8:AI:473:MET:HG3	8:AI:490:LEU:HD11	2.01	0.43
10:DA:198:LYS:HD3	10:DA:198:LYS:HA	1.85	0.43
6:LA:44:LEU:HB3	6:LA:86:ILE:HG13	2.01	0.43
7:MA:69:MET:O	7:MA:73:ILE:HG12	2.19	0.43
7:MA:380:PRO:HD2	7:MA:383:ALA:HB3	2.01	0.43
8:AD:546:GLN:HB3	8:AD:581:LEU:HD23	2.00	0.43
8:AG:653:ASP:OD2	8:AG:663:CYS:HB2	2.18	0.43
10:DA:511:ARG:HE	10:DA:537:THR:HG21	1.83	0.43
11:BA:326:CYS:HB3	11:BA:349:CYS:SG	2.59	0.43
13:OA:290:PHE:HB3	13:OA:351:VAL:HG23	2.01	0.43
2:GB:470:PHE:HE2	2:GB:607:ILE:HG23	1.84	0.43
2:GB:899:THR:HG23	2:GB:902:SER:H	1.84	0.43
4:HA:519:SER:HA	4:HA:559:MET:HE1	2.01	0.43
8:AC:519:ILE:HD12	8:AC:652:PHE:CE2	2.52	0.43
8:AE:157:PRO:HB3	8:AE:379:LYS:HD2	2.01	0.43
9:EA:319:TYR:HB3	9:EA:323:VAL:HG21	2.01	0.43
2:GB:561:VAL:HG21	2:GB:602:LEU:HB3	2.01	0.43
3:IA:76:LEU:HD12	3:IA:91:ILE:HG12	2.01	0.43
8:AC:490:LEU:HD21	8:AC:561:LEU:HD13	2.00	0.43
8:AD:140:TRP:HZ3	8:AD:142:TRP:CE2	2.37	0.43
8:AF:629:CYS:HB3	8:AF:632:GLU:HB2	2.00	0.43
8:AG:581:LEU:HB3	8:AG:596:LEU:HD12	2.00	0.43
8:AH:463:TRP:CD1	8:AH:463:TRP:H	2.37	0.43
10:DA:178:LEU:HD11	10:DA:197:ARG:HD2	2.01	0.43
10:DA:356:THR:HG22	10:DA:359:ASP:OD2	2.19	0.43
16:PA:354:LYS:HD2	16:PA:414:GLN:HG2	1.99	0.43
4:HA:463:LEU:HD21	4:HA:465:HIS:HB2	2.00	0.42
8:AF:140:TRP:CD1	8:AF:148:GLY:HA3	2.54	0.42
8:AJ:176:GLN:HG3	8:AJ:359:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:DB:146:PRO:HB2	10:DB:148:GLU:HG3	2.00	0.42
10:DB:271:VAL:HG12	10:DB:273:HIS:H	1.84	0.42
10:DB:350:LEU:HD11	10:DB:360:ILE:HG21	2.00	0.42
11:BB:366:PRO:HA	11:BB:369:ARG:HG2	2.00	0.42
11:BB:733:CYS:HB2	11:BB:736:CYS:SG	2.60	0.42
13:OA:29:ASN:HD22	14:QB:141:ILE:HG21	1.82	0.42
4:HA:151:TRP:HZ2	4:HA:289:VAL:HG11	1.84	0.42
6:LA:61:HIS:NE2	3:JA:132:ILE:HG21	2.35	0.42
8:AF:38:LYS:C	8:AF:69:MET:HG2	2.44	0.42
8:AA:34:PRO:HB2	8:AA:37:CYS:HB2	2.00	0.42
8:AJ:546:GLN:HB3	8:AJ:581:LEU:HD23	2.01	0.42
10:DA:421:ASN:ND2	10:DA:480:LEU:HD23	2.34	0.42
10:DB:514:GLU:HB3	10:DB:516:PRO:HD2	2.01	0.42
15:NA:107:CYS:HB2	15:NA:125:CYS:HB3	1.30	0.42
2:GB:896:CYS:HB2	2:GB:898:LEU:HD23	2.01	0.42
2:GB:918:HIS:HB3	2:GB:1160:TRP:CH2	2.54	0.42
4:HA:301:VAL:HG11	4:HA:560:THR:HA	2.01	0.42
8:AG:28:ASP:HB3	8:AG:31:LYS:HE3	2.01	0.42
8:AH:376:PHE:HB2	8:AH:379:LYS:HE2	2.00	0.42
9:EA:154:MET:HE3	9:EA:154:MET:HB3	1.97	0.42
11:BB:714:ILE:HD13	11:BB:750:ALA:HA	2.01	0.42
11:BB:719:LEU:HD12	11:BB:778:TYR:HB2	2.00	0.42
14:QB:54:ILE:HG23	14:QB:103:LEU:HD23	2.01	0.42
15:NA:96:ILE:HG21	15:NA:126:MET:HE1	2.00	0.42
2:GB:565:LEU:HD21	2:GB:619:VAL:HG22	2.01	0.42
2:GB:1116:LEU:HD22	2:GB:1119:ILE:HG12	2.01	0.42
3:IA:58:ILE:HA	5:KA:73:PHE:CD2	2.55	0.42
4:HA:566:ILE:HG23	4:HA:577:TYR:HB2	2.01	0.42
8:AC:659:ILE:HG21	11:BA:458:SER:H	1.84	0.42
8:AD:344:TRP:O	8:AD:348:GLU:HB2	2.19	0.42
8:AF:48:ILE:HD11	8:AF:111:LEU:HD11	2.00	0.42
8:AB:208:LYS:HD3	8:AB:257:PHE:CD1	2.54	0.42
8:AB:350:ALA:HB3	8:AB:365:LEU:HB3	2.02	0.42
8:AI:624:LYS:HA	8:AI:629:CYS:HA	2.01	0.42
10:DA:350:LEU:HD11	10:DA:360:ILE:HG21	2.01	0.42
12:CB:35:ALA:HB3	12:CB:52:LEU:HB2	2.00	0.42
12:CB:61:PRO:HG2	12:CB:95:PRO:HB3	2.00	0.42
13:OA:128:ASN:ND2	13:OA:147:GLN:HB2	2.34	0.42
2:GA:283:VAL:HG21	2:GA:326:LEU:H	1.84	0.42
6:LA:65:LEU:HD22	3:JA:129:PHE:HE2	1.84	0.42
8:AD:341:GLN:HE21	8:AD:369:ARG:HE	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AF:624:LYS:HA	8:AF:629:CYS:HA	2.01	0.42
8:AG:211:VAL:HG22	8:AG:247:VAL:HG13	2.01	0.42
8:AG:575:ILE:HD12	8:AG:635:VAL:HG23	2.00	0.42
8:AB:343:LYS:HE3	8:AB:346:GLN:H	1.83	0.42
8:AJ:397:ARG:HB2	8:AJ:400:SER:HB3	2.02	0.42
9:EA:188:ILE:HG23	9:EA:425:MET:HG3	2.00	0.42
9:EA:204:VAL:HG13	9:EA:302:MET:HE3	2.01	0.42
2:GB:229:LEU:HD13	2:GB:262:ILE:HD11	2.02	0.42
2:GB:600:PHE:O	2:GB:656:SER:HB3	2.20	0.42
2:GB:1031:LYS:HG3	2:GB:1060:ARG:HB2	2.02	0.42
3:IA:82:ASN:HB3	3:IA:85:ASN:HB3	2.01	0.42
8:AE:529:ARG:HG3	8:AE:655:TYR:CD2	2.55	0.42
11:BB:45:LEU:HD23	11:BB:45:LEU:H	1.85	0.42
16:PA:192:CYS:HA	16:PA:210:ASP:HA	2.00	0.42
3:JA:52:TRP:CD1	3:JA:53:VAL:HG13	2.55	0.42
4:HA:551:VAL:HG11	4:HA:571:ARG:NH1	2.35	0.42
7:MA:261:SER:HB3	7:MA:267:MET:HE3	2.01	0.42
8:AC:305:VAL:HG22	8:AC:668:ILE:HD12	2.01	0.42
8:AD:397:ARG:HH22	8:AD:438:ARG:HG2	1.84	0.42
8:AH:38:LYS:C	8:AH:69:MET:HG2	2.43	0.42
8:AH:364:ILE:HD13	8:AH:382:LEU:HD13	2.01	0.42
8:AA:173:ARG:HD3	8:AA:173:ARG:HA	1.88	0.42
11:BB:325:VAL:HB	11:BB:349:CYS:HB3	2.01	0.42
12:CA:75:HIS:CE1	12:CA:109:LEU:HG	2.55	0.42
13:OA:448:MET:HG2	13:OA:458:MET:HE1	2.01	0.42
16:PA:73:ARG:HA	16:PA:73:ARG:HD2	1.93	0.42
2:GA:844:ILE:HG22	2:GA:848:MET:HE3	2.02	0.42
2:GA:966:ARG:O	2:GA:970:ASN:HB2	2.20	0.42
4:HA:260:VAL:HG21	4:HA:578:HIS:CG	2.55	0.42
7:MA:253:GLN:HE21	7:MA:258:LEU:HA	1.84	0.42
8:AC:80:VAL:HG11	8:AJ:80:VAL:HG11	2.01	0.42
8:AC:293:TYR:HB2	8:AC:352:CYS:HB3	2.02	0.42
8:AG:623:PRO:HG2	8:AG:630:CYS:SG	2.60	0.42
8:AA:20:MET:HB2	8:AA:23:MET:HE2	2.01	0.42
8:AB:343:LYS:HE3	8:AB:346:GLN:HB2	2.02	0.42
8:AB:457:VAL:HG21	8:AB:564:GLU:HG3	2.01	0.42
10:DA:333:ALA:HB1	10:DA:345:LEU:HD11	2.02	0.42
12:CB:86:LEU:HD23	12:CB:88:ILE:H	1.85	0.42
16:PA:223:LEU:HD23	16:PA:223:LEU:HA	1.88	0.42
1:FA:202:ILE:HD13	1:FA:229:VAL:HG13	2.02	0.42
2:GB:547:SER:HB3	2:GB:551:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AA:345:LEU:HD12	8:AA:349:MET:HE2	2.02	0.42
8:AA:463:TRP:CD1	8:AA:463:TRP:H	2.37	0.42
8:AB:624:LYS:HA	8:AB:629:CYS:HA	2.01	0.42
10:DA:892:LEU:HD22	10:DA:920:MET:HE1	2.01	0.42
10:DB:60:PRO:HA	10:DB:63:GLN:HG2	2.01	0.42
10:DB:668:SER:H	10:DB:696:LEU:HB2	1.85	0.42
3:JA:126:VAL:O	3:JA:130:LEU:HG	2.20	0.42
2:GB:279:ILE:HG13	2:GB:298:ILE:HD12	2.02	0.42
2:GA:796:LEU:HD22	2:GA:831:VAL:HG21	2.02	0.42
4:HA:456:LEU:HD23	4:HA:456:LEU:HA	1.91	0.42
7:MA:907:CYS:HA	7:MA:934:PHE:HZ	1.83	0.42
8:AF:42:ILE:HG13	8:AF:93:VAL:HG22	2.02	0.42
8:AF:602:PHE:HA	8:AF:655:TYR:OH	2.20	0.42
8:AH:306:TYR:HB2	8:AH:667:ILE:HG13	2.01	0.42
8:AH:575:ILE:HD12	8:AH:635:VAL:HG23	2.01	0.42
10:DA:873:ALA:O	10:DA:877:ILE:HG12	2.19	0.42
14:QC:158:GLN:HG3	14:QC:159:TRP:HB2	2.01	0.42
16:PA:369:ASP:HB3	16:PA:375:LEU:HD21	2.02	0.42
2:GB:324:ASP:HA	2:GB:371:THR:HB	2.01	0.41
7:MA:438:LYS:HE3	7:MA:444:ASN:HA	2.01	0.41
8:AA:502:PHE:HB3	8:AA:538:LEU:HD11	2.01	0.41
8:AI:349:MET:HE1	8:AI:378:MET:HE2	2.02	0.41
8:AJ:623:PRO:HG2	8:AJ:630:CYS:SG	2.60	0.41
10:DA:66:LEU:HB3	10:DA:109:LEU:HD21	2.00	0.41
11:BB:449:PRO:HB3	11:BB:452:ALA:HB3	2.01	0.41
1:FA:139:LEU:HD21	1:FA:189:VAL:HG23	2.03	0.41
2:GB:474:THR:HA	2:GB:477:ARG:HG3	2.02	0.41
2:GA:419:HIS:CD2	2:GA:728:LEU:HD22	2.54	0.41
2:GA:1017:CYS:SG	2:GA:1040:LEU:HD22	2.60	0.41
8:AC:175:ILE:HG23	8:AC:178:LEU:HD12	2.02	0.41
8:AD:397:ARG:HA	8:AD:591:GLN:HE22	1.85	0.41
8:AE:141:MET:HE3	8:AE:141:MET:HB3	1.95	0.41
8:AE:469:MET:HE3	8:AE:469:MET:HB2	1.91	0.41
8:AE:558:ARG:HH22	8:AE:569:ASP:HB2	1.84	0.41
8:AA:624:LYS:HA	8:AA:629:CYS:HA	2.02	0.41
8:AI:294:ILE:HG12	8:AI:453:VAL:HG21	2.02	0.41
8:AI:527:ASN:O	8:AI:529:ARG:HG2	2.19	0.41
10:DB:338:ILE:HD13	10:DB:338:ILE:HA	1.97	0.41
1:FA:282:ARG:HD3	2:GA:1143:HIS:N	2.34	0.41
2:GB:993:GLU:HB3	2:GA:965:MET:HE1	2.01	0.41
2:GA:872:LYS:O	2:GA:875:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:MA:629:PHE:HB2	7:MA:662:PHE:CZ	2.55	0.41
8:AG:493:ALA:HB3	8:AG:554:ILE:HD13	2.03	0.41
8:AH:623:PRO:HG2	8:AH:630:CYS:SG	2.60	0.41
8:AA:316:PHE:HB2	8:AA:651:ASP:OD2	2.20	0.41
8:AB:341:GLN:HE21	8:AB:369:ARG:HE	1.68	0.41
10:DA:616:PHE:CG	10:DA:621:GLN:HG3	2.55	0.41
11:BB:21:ARG:HD2	11:BB:337:LEU:HD21	2.01	0.41
11:BB:450:HIS:HE1	12:CB:145:TYR:HA	1.86	0.41
12:CB:33:TRP:HB2	12:CB:54:ILE:HB	2.03	0.41
12:CB:107:CYS:HB3	12:CB:111:CYS:HB2	1.59	0.41
13:OA:106:ILE:HD12	13:OA:106:ILE:HA	1.93	0.41
15:NA:100:THR:HA	15:NA:457:PRO:HB3	2.01	0.41
15:NA:102:ILE:HG22	15:NA:130:MET:HG2	2.02	0.41
4:HA:541:THR:HG23	4:HA:543:ALA:H	1.85	0.41
6:LA:65:LEU:HD11	6:LA:101:MET:HE1	2.01	0.41
8:AD:629:CYS:HB3	8:AD:632:GLU:HB2	2.03	0.41
8:AF:48:ILE:HD11	8:AF:89:ASP:HB3	2.00	0.41
10:DA:498:ILE:HG22	10:DA:502:LEU:HD23	2.01	0.41
11:BA:227:TYR:CZ	11:BA:305:PRO:HD2	2.55	0.41
11:BA:305:PRO:HG2	11:BA:311:LYS:HG3	2.01	0.41
15:NA:138:ILE:HD12	15:NA:462:THR:HG21	2.03	0.41
4:HA:335:LEU:HD11	4:HA:378:LEU:HD21	2.03	0.41
7:MA:122:LYS:O	7:MA:123:GLU:HG3	2.21	0.41
8:AA:124:ARG:HH12	8:AA:147:TRP:HA	1.84	0.41
8:AB:305:VAL:HG22	8:AB:668:ILE:HD12	2.03	0.41
8:AJ:436:GLU:HG3	8:AJ:595:LYS:HD2	2.03	0.41
8:AJ:440:MET:HE3	8:AJ:440:MET:HB2	1.94	0.41
10:DB:278:ILE:HG23	10:DB:302:LEU:HD21	2.01	0.41
11:BA:141:ASP:HB2	11:BA:148:PHE:HE2	1.86	0.41
11:BB:292:GLN:HG3	11:BB:293:PRO:O	2.20	0.41
12:CB:39:GLY:HA2	12:CB:40:PRO:HD3	1.94	0.41
12:CB:97:LEU:HA	12:CB:101:LYS:HD2	2.01	0.41
2:GB:672:VAL:HG23	2:GB:698:ILE:HG13	2.02	0.41
2:GA:439:LEU:HD23	2:GA:465:TYR:CZ	2.56	0.41
8:AE:449:TYR:CZ	8:AE:456:PRO:HG2	2.56	0.41
8:AE:615:LEU:HD11	8:AE:644:LEU:HD22	2.02	0.41
8:AA:20:MET:HB2	8:AA:23:MET:HG3	2.03	0.41
10:DA:779:VAL:HG21	10:DA:990:TRP:CD1	2.56	0.41
15:NA:20:LEU:HB3	15:NA:24:SER:HB2	2.02	0.41
1:FA:344:TRP:CD2	9:EA:401:LYS:HG3	2.55	0.41
8:AE:255:PRO:HG3	8:AE:446:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AI:11:LEU:HD22	8:AI:105:ALA:HB1	2.02	0.41
10:DA:82:THR:HG22	10:DA:206:LEU:HB3	2.02	0.41
10:DA:970:ILE:HD13	11:BA:276:MET:HE3	2.03	0.41
11:BA:221:ALA:HB1	11:BA:268:ILE:HG21	2.03	0.41
13:OA:100:ARG:H	13:OA:100:ARG:HG2	1.71	0.41
16:PA:386:LEU:HD11	16:PA:400:ASN:HA	2.03	0.41
4:HB:526:ALA:HB2	4:HB:536:VAL:HG12	2.03	0.41
8:AF:378:MET:HA	8:AF:381:THR:HG22	2.03	0.41
8:AG:8:SER:HA	8:AG:31:LYS:NZ	2.36	0.41
8:AH:23:MET:HG3	8:AH:25:ILE:HG13	2.02	0.41
8:AB:7:LEU:HD12	8:AB:25:ILE:HG21	2.03	0.41
9:EA:28:HIS:CE1	9:EA:243:ARG:HB3	2.56	0.41
9:EA:350:GLY:HA2	10:DA:57:VAL:HG22	2.03	0.41
10:DA:217:ARG:NH2	10:DA:342:LYS:HE3	2.35	0.41
10:DB:642:LEU:HD11	10:DB:666:LEU:HD12	2.03	0.41
10:DB:936:CYS:HB2	10:DB:968:VAL:HG21	2.02	0.41
11:BA:346:HIS:HB2	11:BA:349:CYS:HB2	2.03	0.41
1:FA:2:ARG:NH2	1:FA:46:ARG:HH21	2.18	0.41
1:FA:203:ASP:O	1:FA:207:LEU:HG	2.21	0.41
2:GB:246:ILE:CG1	2:GB:389:TYR:HB3	2.50	0.41
2:GA:288:TRP:HA	2:GA:350:ILE:HB	2.02	0.41
2:GA:846:TYR:HE1	2:GA:864:LEU:HD13	1.86	0.41
2:GA:1007:LEU:HB3	2:GA:1010:CYS:SG	2.60	0.41
4:HB:456:LEU:HD23	4:HB:456:LEU:H	1.86	0.41
7:MA:622:TRP:HA	7:MA:625:MET:SD	2.61	0.41
7:MA:879:ASP:HA	7:MA:882:LYS:HE2	2.02	0.41
8:AD:185:VAL:HG11	8:AD:197:LEU:HD11	2.02	0.41
8:AD:305:VAL:HB	8:AD:331:VAL:HG22	2.03	0.41
8:AH:408:MET:HB3	8:AH:408:MET:HE2	1.85	0.41
8:AA:28:ASP:HB3	8:AA:31:LYS:HE3	2.02	0.41
8:AA:370:VAL:HB	8:AA:373:LEU:HD21	2.03	0.41
8:AA:422:LEU:HD12	8:AA:453:VAL:HB	2.03	0.41
8:AB:294:ILE:HG12	8:AB:453:VAL:HG21	2.03	0.41
8:AI:397:ARG:HH22	8:AI:438:ARG:HG2	1.85	0.41
8:AJ:394:GLU:HB2	8:AJ:441:ASN:ND2	2.35	0.41
8:AJ:485:GLN:HB3	8:AJ:489:ARG:HH12	1.85	0.41
8:AJ:519:ILE:HD12	8:AJ:652:PHE:CE1	2.56	0.41
10:DB:312:PRO:HD2	10:DB:319:VAL:HG21	2.02	0.41
11:BB:45:LEU:HG	11:BB:52:MET:HB2	2.03	0.41
12:CA:25:PRO:HA	12:CA:33:TRP:HA	2.02	0.41
13:OA:404:LEU:HD23	13:OA:446:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:QC:9:SER:HA	14:QC:48:PRO:HA	2.02	0.41
16:PA:349:TYR:HB2	16:PA:388:LEU:HD23	2.03	0.41
2:GA:703:ARG:CZ	3:JA:96:SER:HA	2.51	0.41
4:HA:467:PHE:CZ	4:HA:485:LEU:HD22	2.56	0.41
10:DA:285:GLN:NE2	10:DA:286:VAL:HG23	2.36	0.41
15:NA:351:CYS:HA	15:NA:362:CYS:HB3	2.02	0.41
14:QC:4:ILE:HD11	14:QC:21:ALA:HB3	2.02	0.41
14:QC:131:THR:HG23	14:QC:134:GLU:H	1.86	0.41
2:GB:643:PRO:HB2	2:GB:675:LEU:HD22	2.02	0.40
4:HA:442:ILE:HB	4:HA:454:TRP:HB2	2.02	0.40
8:AG:295:PHE:HB2	8:AG:409:VAL:HG21	2.03	0.40
8:AA:151:LEU:HG	8:AA:288:PHE:HB3	2.03	0.40
8:AB:449:TYR:CZ	8:AB:456:PRO:HG2	2.56	0.40
8:AJ:316:PHE:CD2	8:AJ:663:CYS:HA	2.57	0.40
10:DA:146:PRO:HB2	10:DA:148:GLU:HG3	2.03	0.40
10:DA:274:MET:HA	10:DA:277:MET:HE1	2.03	0.40
10:DA:854:LEU:HD11	10:DA:889:VAL:HG13	2.03	0.40
11:BA:21:ARG:HD2	11:BA:337:LEU:HD11	2.04	0.40
13:OA:80:LYS:HE2	13:OA:80:LYS:HB3	1.76	0.40
14:QA:116:LEU:HD12	14:QA:116:LEU:HA	1.95	0.40
15:NA:45:TRP:CD1	15:NA:70:LYS:HB2	2.56	0.40
16:PA:96:GLU:HG3	16:PA:97:TYR:CD2	2.56	0.40
2:GB:705:LEU:HD23	2:GB:705:LEU:HA	1.87	0.40
2:GA:487:GLU:HB3	2:GA:527:LEU:HD13	2.03	0.40
2:GA:1161:TRP:H	2:GA:1161:TRP:CD1	2.38	0.40
7:MA:32:GLU:HG3	7:MA:73:ILE:HD11	2.03	0.40
8:AD:309:ARG:HE	8:AD:333:LYS:HE2	1.87	0.40
8:AG:485:GLN:HE21	8:AG:489:ARG:NH2	2.19	0.40
9:EA:352:LYS:HB3	10:DA:51:PHE:HZ	1.80	0.40
11:BA:465:LEU:HD11	11:BA:483:TYR:CZ	2.57	0.40
15:NA:320:ASP:CG	15:NA:337:ILE:HD11	2.46	0.40
2:GA:859:LEU:HD12	2:GA:859:LEU:HA	1.90	0.40
6:LA:42:LYS:HZ1	6:LA:88:ILE:HD13	1.87	0.40
7:MA:654:TYR:HD1	7:MA:683:LEU:HD22	1.86	0.40
7:MA:812:LEU:HB3	7:MA:839:CYS:HB3	2.04	0.40
8:AE:82:PRO:HG2	8:AE:186:GLU:HB2	2.03	0.40
8:AH:7:LEU:HD12	8:AH:25:ILE:HG21	2.03	0.40
8:AB:515:LEU:HG	8:AB:623:PRO:HD3	2.03	0.40
8:AI:345:LEU:HD23	8:AI:664:ALA:HB1	2.03	0.40
10:DB:575:GLU:HB2	10:DB:605:LYS:HG3	2.03	0.40
11:BA:506:LEU:HD12	11:BA:506:LEU:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CA:107:CYS:HA	12:CA:110:LEU:HB2	2.04	0.40
12:CB:69:PHE:HD2	12:CB:73:ILE:HD13	1.87	0.40
14:QA:160:CYS:SG	15:NA:23:TYR:HA	2.61	0.40
1:FA:257:MET:HA	1:FA:312:THR:HG21	2.02	0.40
1:FA:404:ASP:OD1	1:FA:407:GLU:HG3	2.21	0.40
2:GB:721:GLN:CD	2:GB:722:GLU:H	2.29	0.40
2:GA:248:HIS:HA	2:GA:372:THR:O	2.22	0.40
2:GA:947:ARG:HG2	2:GA:975:HIS:HB2	2.03	0.40
2:GA:960:TYR:CZ	2:GA:983:VAL:HG22	2.57	0.40
7:MA:754:ASN:O	7:MA:782:CYS:HA	2.21	0.40
8:AG:186:GLU:HG2	8:AG:241:ARG:HD3	2.03	0.40
8:AB:629:CYS:HB3	8:AB:632:GLU:HB2	2.03	0.40
10:DA:952:ASP:HB2	10:DA:955:GLU:HG2	2.03	0.40
10:DB:892:LEU:HD22	10:DB:920:MET:HE1	2.03	0.40
11:BA:238:GLU:HG2	11:BA:254:ASN:HB2	2.02	0.40
14:QB:85:ILE:HG13	14:QB:90:GLN:NE2	2.37	0.40
14:QC:156:GLU:O	16:PA:71:ILE:HD13	2.22	0.40
16:PA:362:ARG:HH22	16:PA:384:GLN:NE2	2.20	0.40
3:JA:51:ALA:HA	3:JA:87:ALA:HB2	2.02	0.40
2:GA:254:GLY:O	3:JA:27:LEU:HD21	2.22	0.40
7:MA:15:ARG:HG3	3:JA:100:ARG:NH1	2.33	0.40
7:MA:114:ASN:O	7:MA:117:ILE:HG12	2.21	0.40
7:MA:639:ARG:HA	7:MA:668:VAL:HB	2.02	0.40
8:AC:349:MET:HE1	8:AC:378:MET:HE3	2.04	0.40
8:AC:624:LYS:HA	8:AC:629:CYS:HA	2.03	0.40
8:AE:629:CYS:HB3	8:AE:632:GLU:HG2	2.03	0.40
10:DA:84:VAL:HG11	10:DA:215:TRP:CZ3	2.57	0.40
10:DB:873:ALA:O	10:DB:877:ILE:HG12	2.21	0.40
11:BB:481:PHE:CZ	11:BB:584:LEU:HD12	2.56	0.40
14:QB:85:ILE:HG13	14:QB:90:GLN:HE21	1.86	0.40
16:PA:339:LEU:HD12	16:PA:339:LEU:HA	1.93	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	FA	427/445 (96%)	407 (95%)	20 (5%)	0	100	100
2	GA	942/1163 (81%)	874 (93%)	68 (7%)	0	100	100
2	GB	945/1163 (81%)	881 (93%)	64 (7%)	0	100	100
3	IA	126/164 (77%)	122 (97%)	4 (3%)	0	100	100
3	JA	116/164 (71%)	114 (98%)	2 (2%)	0	100	100
4	HA	359/581 (62%)	330 (92%)	29 (8%)	0	100	100
4	HB	359/581 (62%)	328 (91%)	29 (8%)	2 (1%)	21	54
5	KA	55/227 (24%)	50 (91%)	4 (7%)	1 (2%)	6	34
6	LA	131/440 (30%)	129 (98%)	2 (2%)	0	100	100
7	MA	933/937 (100%)	867 (93%)	64 (7%)	2 (0%)	43	74
8	AA	650/682 (95%)	623 (96%)	26 (4%)	1 (0%)	43	74
8	AB	650/682 (95%)	624 (96%)	26 (4%)	0	100	100
8	AC	650/682 (95%)	613 (94%)	37 (6%)	0	100	100
8	AD	650/682 (95%)	623 (96%)	26 (4%)	1 (0%)	43	74
8	AE	650/682 (95%)	623 (96%)	27 (4%)	0	100	100
8	AF	650/682 (95%)	615 (95%)	34 (5%)	1 (0%)	43	74
8	AG	650/682 (95%)	622 (96%)	28 (4%)	0	100	100
8	AH	650/682 (95%)	622 (96%)	28 (4%)	0	100	100
8	AI	650/682 (95%)	619 (95%)	31 (5%)	0	100	100
8	AJ	650/682 (95%)	622 (96%)	28 (4%)	0	100	100
9	EA	442/449 (98%)	431 (98%)	11 (2%)	0	100	100
10	DA	954/993 (96%)	914 (96%)	39 (4%)	1 (0%)	48	79
10	DB	954/993 (96%)	915 (96%)	38 (4%)	1 (0%)	48	79
11	BA	617/782 (79%)	592 (96%)	24 (4%)	1 (0%)	43	74
11	BB	617/782 (79%)	590 (96%)	27 (4%)	0	100	100
12	CA	144/147 (98%)	144 (100%)	0	0	100	100
12	CB	144/147 (98%)	140 (97%)	4 (3%)	0	100	100
13	OA	452/466 (97%)	430 (95%)	21 (5%)	1 (0%)	43	74
14	QA	153/163 (94%)	148 (97%)	5 (3%)	0	100	100
14	QB	150/163 (92%)	146 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	QC	153/163 (94%)	149 (97%)	4 (3%)	0	100	100
15	NA	461/469 (98%)	433 (94%)	27 (6%)	1 (0%)	43	74
16	PA	459/468 (98%)	429 (94%)	28 (6%)	2 (0%)	30	62
All	All	16593/18870 (88%)	15769 (95%)	809 (5%)	15 (0%)	49	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	OA	451	SER
7	MA	255	VAL
5	KA	35	TYR
7	MA	467	HIS
11	BA	700	TYR
16	PA	56	VAL
4	HB	439	ASP
8	AD	68	SER
8	AF	68	SER
8	AA	68	SER
4	HB	509	LYS
10	DA	841	VAL
10	DB	841	VAL
15	NA	9	PRO
16	PA	428	LEU

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	FA	367/380 (97%)	367 (100%)	0	100	100
2	GA	845/1054 (80%)	845 (100%)	0	100	100
2	GB	848/1054 (80%)	848 (100%)	0	100	100
3	IA	112/143 (78%)	112 (100%)	0	100	100
3	JA	105/143 (73%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	HA	320/516 (62%)	320 (100%)	0	100	100
4	HB	320/516 (62%)	320 (100%)	0	100	100
5	KA	48/196 (24%)	48 (100%)	0	100	100
6	LA	117/357 (33%)	117 (100%)	0	100	100
7	MA	861/862 (100%)	861 (100%)	0	100	100
8	AA	589/613 (96%)	589 (100%)	0	100	100
8	AB	589/613 (96%)	589 (100%)	0	100	100
8	AC	589/613 (96%)	589 (100%)	0	100	100
8	AD	589/613 (96%)	589 (100%)	0	100	100
8	AE	589/613 (96%)	589 (100%)	0	100	100
8	AF	589/613 (96%)	589 (100%)	0	100	100
8	AG	589/613 (96%)	589 (100%)	0	100	100
8	AH	589/613 (96%)	589 (100%)	0	100	100
8	AI	589/613 (96%)	589 (100%)	0	100	100
8	AJ	589/613 (96%)	589 (100%)	0	100	100
9	EA	372/376 (99%)	372 (100%)	0	100	100
10	DA	878/909 (97%)	878 (100%)	0	100	100
10	DB	878/909 (97%)	878 (100%)	0	100	100
11	BA	556/682 (82%)	556 (100%)	0	100	100
11	BB	556/682 (82%)	556 (100%)	0	100	100
12	CA	131/132 (99%)	131 (100%)	0	100	100
12	CB	131/132 (99%)	131 (100%)	0	100	100
13	OA	421/430 (98%)	421 (100%)	0	100	100
14	QA	144/150 (96%)	144 (100%)	0	100	100
14	QB	141/150 (94%)	141 (100%)	0	100	100
14	QC	144/150 (96%)	144 (100%)	0	100	100
15	NA	429/435 (99%)	429 (100%)	0	100	100
16	PA	425/431 (99%)	425 (100%)	0	100	100
All	All	15039/16919 (89%)	15039 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113)

such sidechains are listed below:

Mol	Chain	Res	Type
1	FA	15	GLN
1	FA	134	GLN
1	FA	335	ASN
2	GB	268	GLN
2	GB	426	GLN
2	GB	430	GLN
2	GB	542	GLN
2	GB	571	HIS
2	GB	693	GLN
2	GB	735	ASN
2	GB	914	GLN
2	GB	1110	GLN
2	GB	1133	GLN
2	GA	273	GLN
2	GA	471	HIS
2	GA	485	GLN
2	GA	801	ASN
2	GA	809	ASN
2	GA	1029	HIS
2	GA	1054	GLN
2	GA	1133	GLN
4	HB	164	GLN
4	HB	424	ASN
4	HB	441	ASN
4	HB	502	GLN
4	HB	578	HIS
4	HA	164	GLN
4	HA	419	GLN
4	HA	511	ASN
7	MA	107	HIS
7	MA	177	GLN
7	MA	391	GLN
7	MA	420	ASN
7	MA	509	GLN
7	MA	525	HIS
7	MA	665	ASN
8	AC	176	GLN
8	AC	272	HIS
8	AC	358	HIS
8	AC	451	GLN
8	AC	471	GLN
8	AC	591	GLN

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Mol	Chain	Res	Type
8	AD	272	HIS
8	AD	355	GLN
8	AD	358	HIS
8	AD	396	HIS
8	AD	451	GLN
8	AD	471	GLN
8	AE	5	ASN
8	AE	127	GLN
8	AE	215	GLN
8	AE	355	GLN
8	AE	392	GLN
8	AE	485	GLN
8	AF	4	GLN
8	AF	451	GLN
8	AF	607	GLN
8	AG	358	HIS
8	AG	441	ASN
8	AG	614	ASN
8	AH	406	ASN
8	AH	451	GLN
8	AA	272	HIS
8	AA	355	GLN
8	AA	392	GLN
8	AA	471	GLN
8	AB	355	GLN
8	AB	527	ASN
8	AI	154	ASN
8	AI	358	HIS
8	AI	506	GLN
8	AI	592	GLN
8	AJ	5	ASN
8	AJ	127	GLN
8	AJ	441	ASN
9	EA	393	HIS
10	DA	111	GLN
10	DA	126	GLN
10	DA	285	GLN
10	DA	430	GLN
10	DA	500	GLN
10	DA	506	GLN
10	DA	529	HIS
10	DA	607	GLN

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Mol	Chain	Res	Type
10	DA	776	GLN
10	DA	884	ASN
10	DA	913	ASN
10	DA	991	ASN
10	DB	111	GLN
10	DB	126	GLN
10	DB	343	HIS
10	DB	353	HIS
10	DB	500	GLN
10	DB	506	GLN
10	DB	772	GLN
10	DB	799	HIS
10	DB	823	HIS
10	DB	888	HIS
11	BA	134	ASN
11	BA	217	GLN
11	BA	477	ASN
11	BA	508	ASN
11	BA	773	GLN
11	BB	37	HIS
11	BB	222	ASN
11	BB	264	ASN
11	BB	450	HIS
11	BB	533	GLN
11	BB	773	GLN
12	CB	46	GLN
14	QA	158	GLN
16	PA	59	GLN
3	JA	85	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
17	GTP	FA	501	18	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
17	GTP	EA	502	18	33,34,34	0.90	0	50,54,54	1.55	9 (18%)

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
17	GTP	FA	501	18	-	6/22/38/38	0/3/3/3
17	GTP	EA	502	18	-	3/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	FA	501	GTP	C2-N3	2.02	1.38	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	FA	501	GTP	C5-C4-N3	-5.14	120.21	128.39
17	EA	502	GTP	C5-C4-N3	-5.03	120.38	128.39
17	FA	501	GTP	C2-N3-C4	4.69	120.37	112.30
17	EA	502	GTP	C2-N3-C4	4.46	119.98	112.30
17	EA	502	GTP	N9-C4-N3	3.29	132.54	125.95
17	FA	501	GTP	N9-C4-N3	3.27	132.49	125.95
17	FA	501	GTP	C2-N1-C6	-3.08	119.53	125.11
17	FA	501	GTP	N9-C8-N7	-2.82	108.16	113.40
17	EA	502	GTP	C2-N1-C6	-2.82	120.00	125.11
17	FA	501	GTP	C5-C6-N1	2.63	119.95	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	FA	501	GTP	C8-N7-C5	2.61	108.90	104.26
17	EA	502	GTP	N9-C8-N7	-2.57	108.63	113.40
17	EA	502	GTP	C5-C6-N1	2.48	119.56	113.25
17	FA	501	GTP	O6-C6-C5	-2.42	120.14	126.53
17	EA	502	GTP	C8-N7-C5	2.38	108.50	104.26
17	EA	502	GTP	O6-C6-C5	-2.29	120.48	126.53
17	EA	502	GTP	C3'-C2'-C1'	2.06	105.36	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

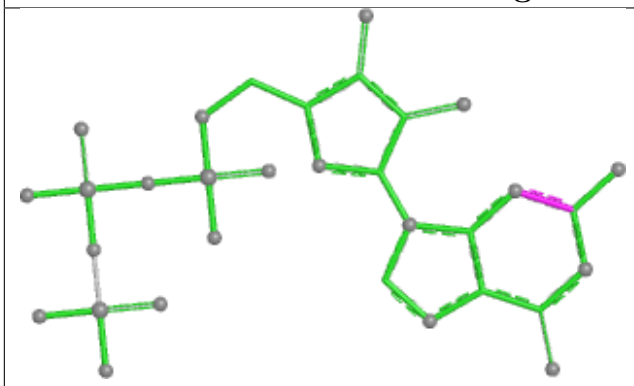
Mol	Chain	Res	Type	Atoms
17	FA	501	GTP	C5'-O5'-PA-O3A
17	FA	501	GTP	C5'-O5'-PA-O1A
17	FA	501	GTP	C5'-O5'-PA-O2A
17	EA	502	GTP	C5'-O5'-PA-O3A
17	EA	502	GTP	C5'-O5'-PA-O2A
17	EA	502	GTP	C4'-C5'-O5'-PA
17	FA	501	GTP	PB-O3B-PG-O2G
17	FA	501	GTP	C4'-C5'-O5'-PA
17	FA	501	GTP	PA-O3A-PB-O2B

There are no ring outliers.

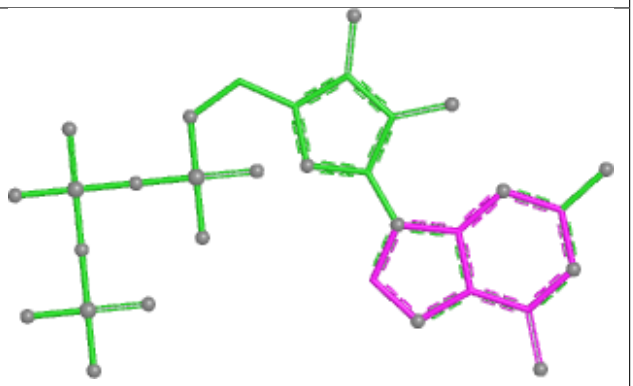
No monomer is involved in short contacts.

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.

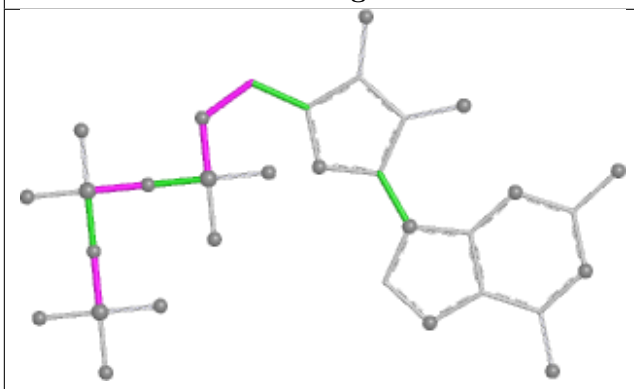
Ligand GTP FA 501



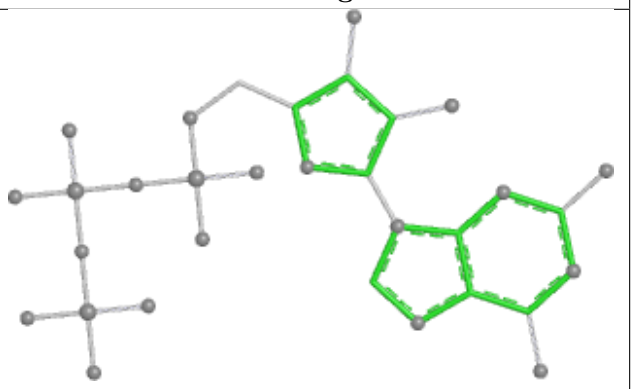
Bond lengths



Bond angles

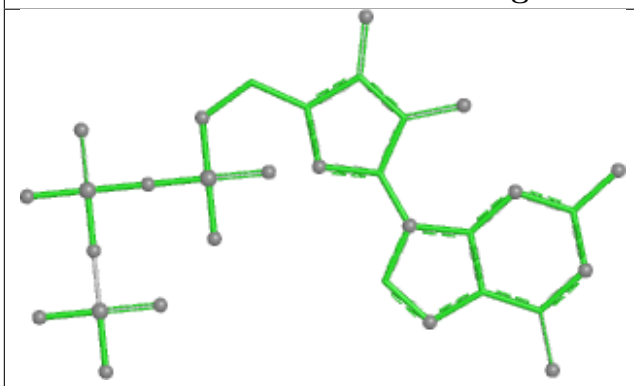


Torsions

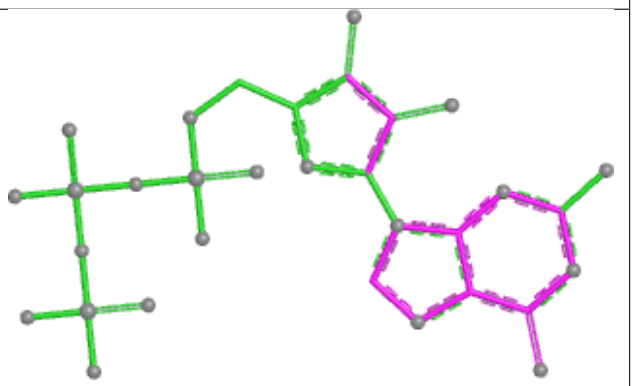


Rings

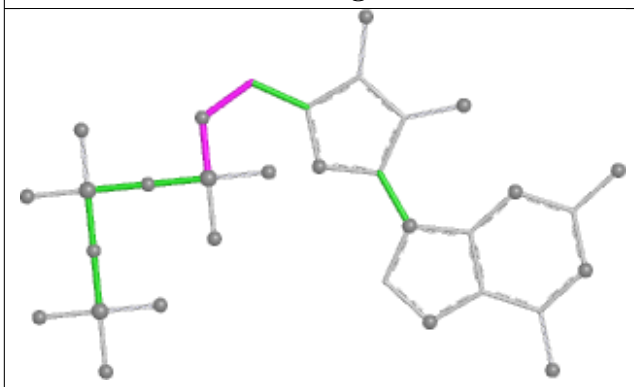
Ligand GTP EA 502



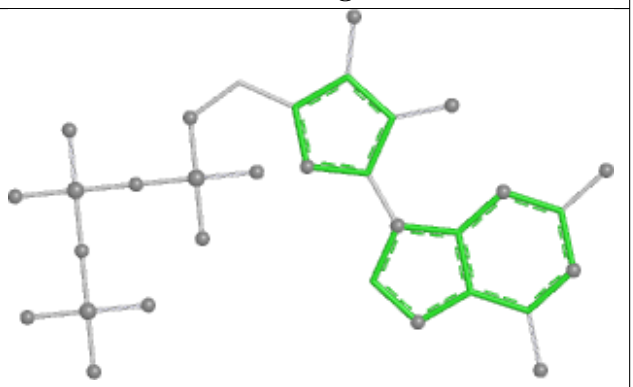
Bond lengths



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.

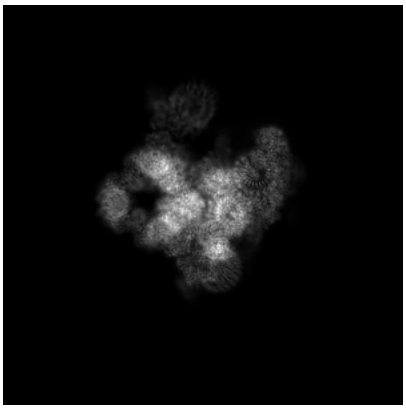
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-76334. These allow visual inspection of the internal detail of the map and identification of artifacts.

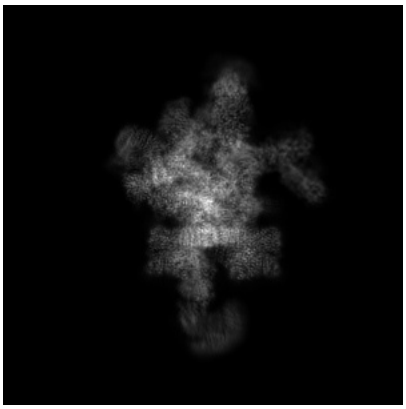
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

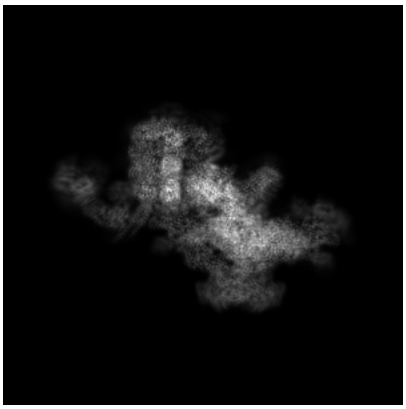
6.1.1 Primary map



X

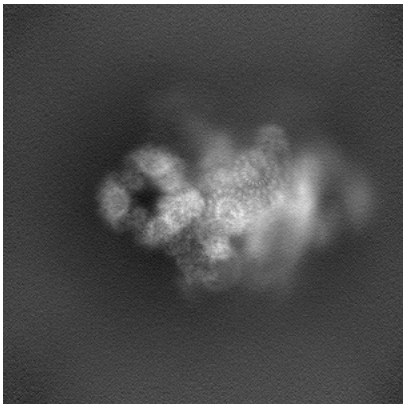


Y

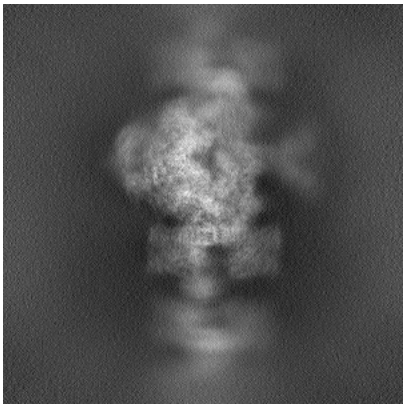


Z

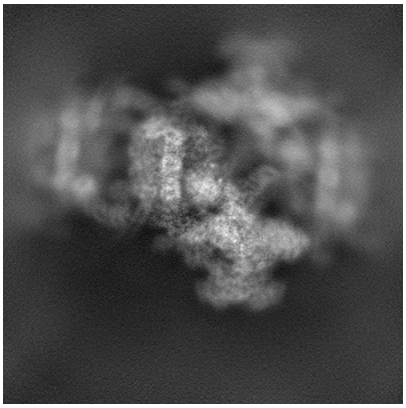
6.1.2 Raw map



X



Y

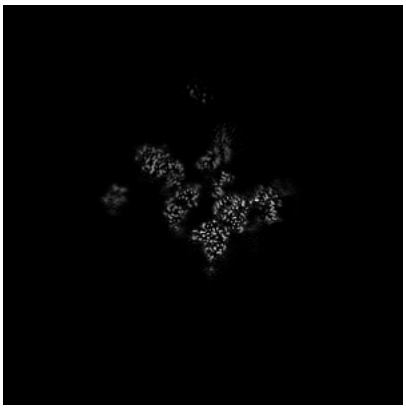


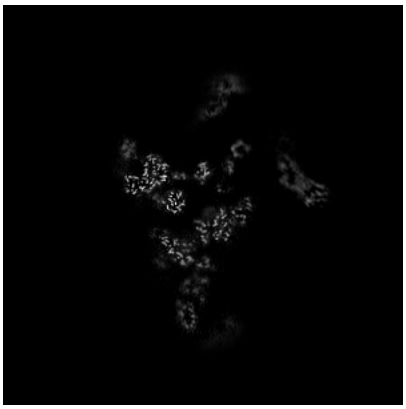
Z

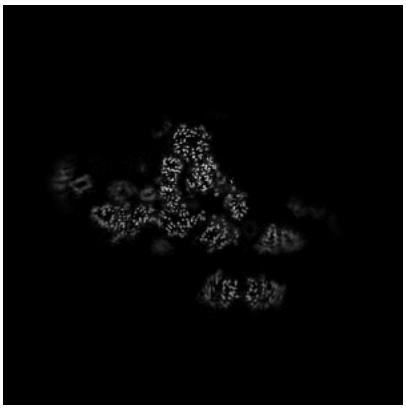
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

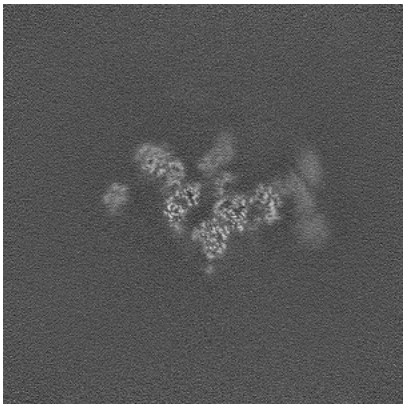
6.2.1 Primary map

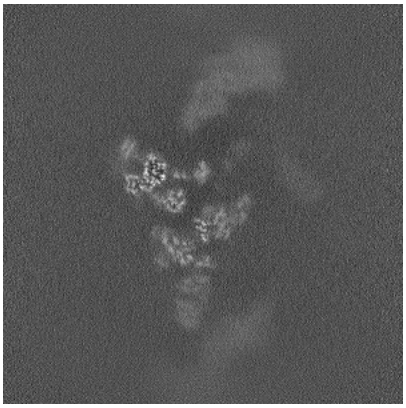

X Index: 256

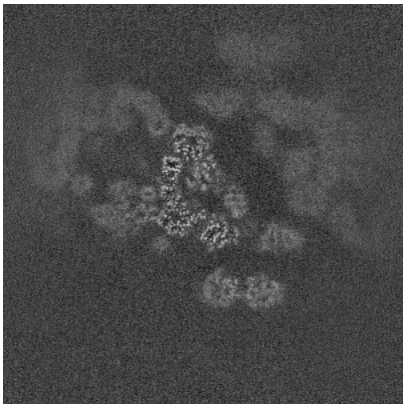

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256


Y Index: 256


Z Index: 256

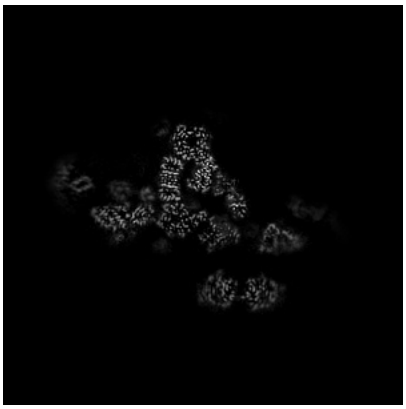
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

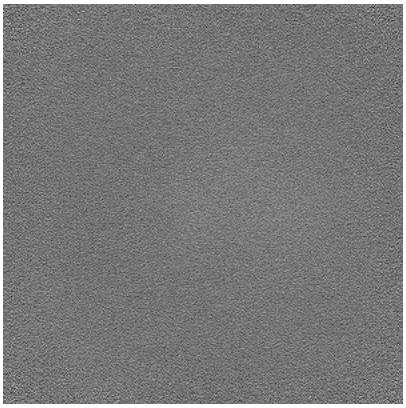
X Index: 291

Y Index: 275

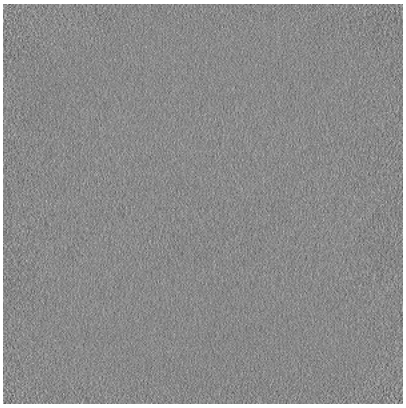


Z Index: 258

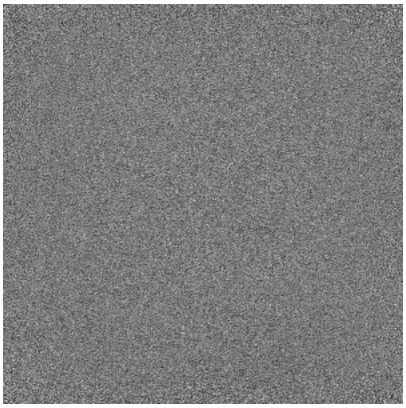
6.3.2 Raw map



X Index: 0



Y Index: 0

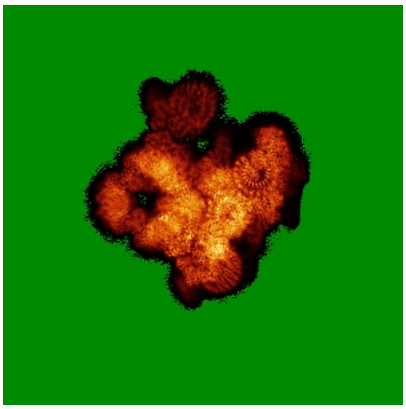


Z Index: 0

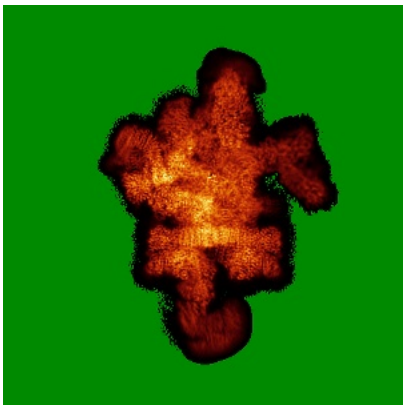
The images above show the largest variance slices of the map in three orthogonal directions.

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

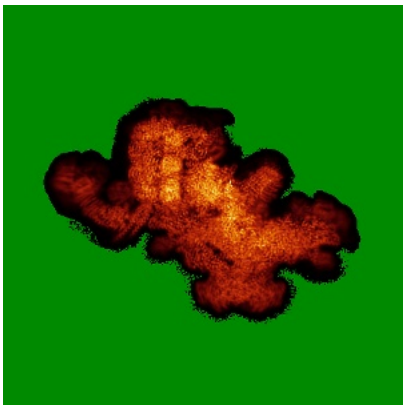
6.4.1 Primary map



X

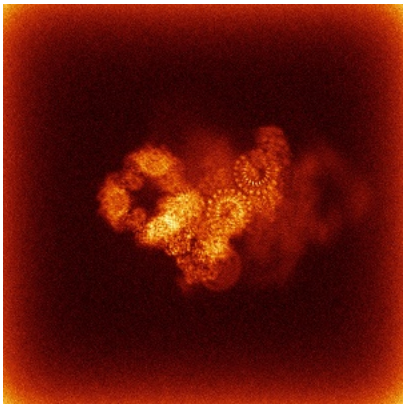


Y

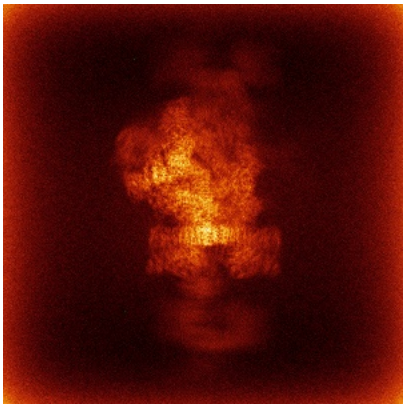


Z

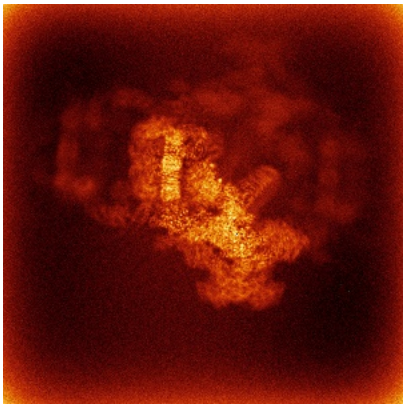
6.4.2 Raw map



X



Y



Z

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

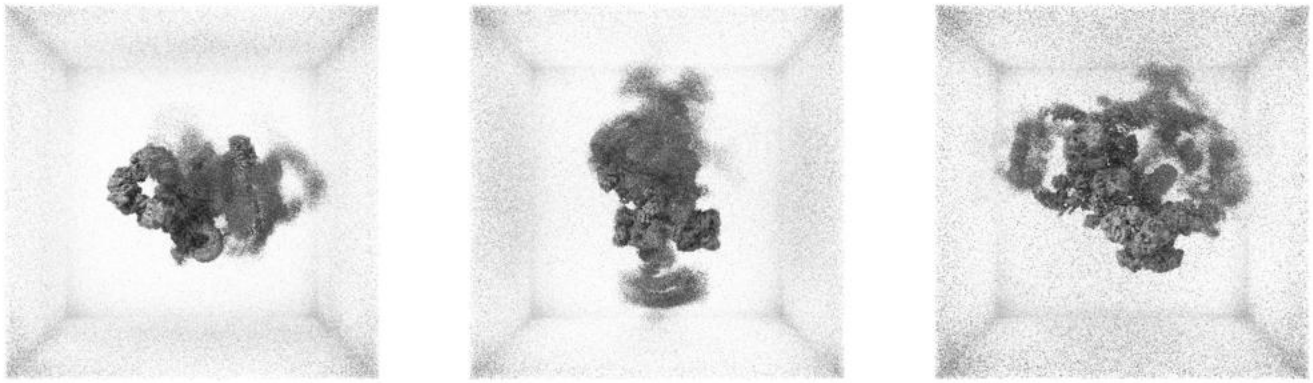
6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

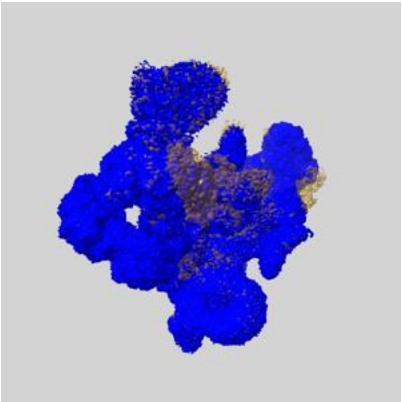
6.6 Mask visualisation (i)

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

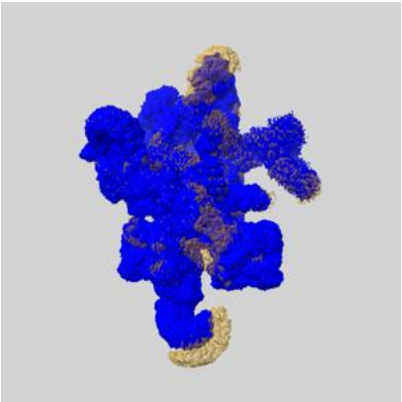
A mask typically either:

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

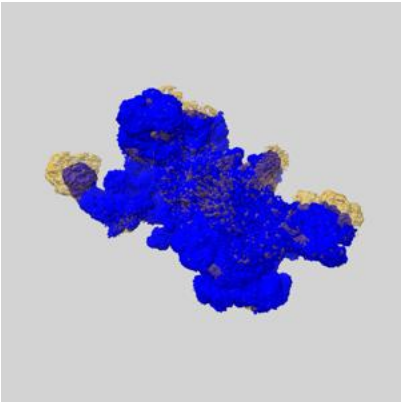
6.6.1 emd_76334_msk_1.map (i)



X



Y

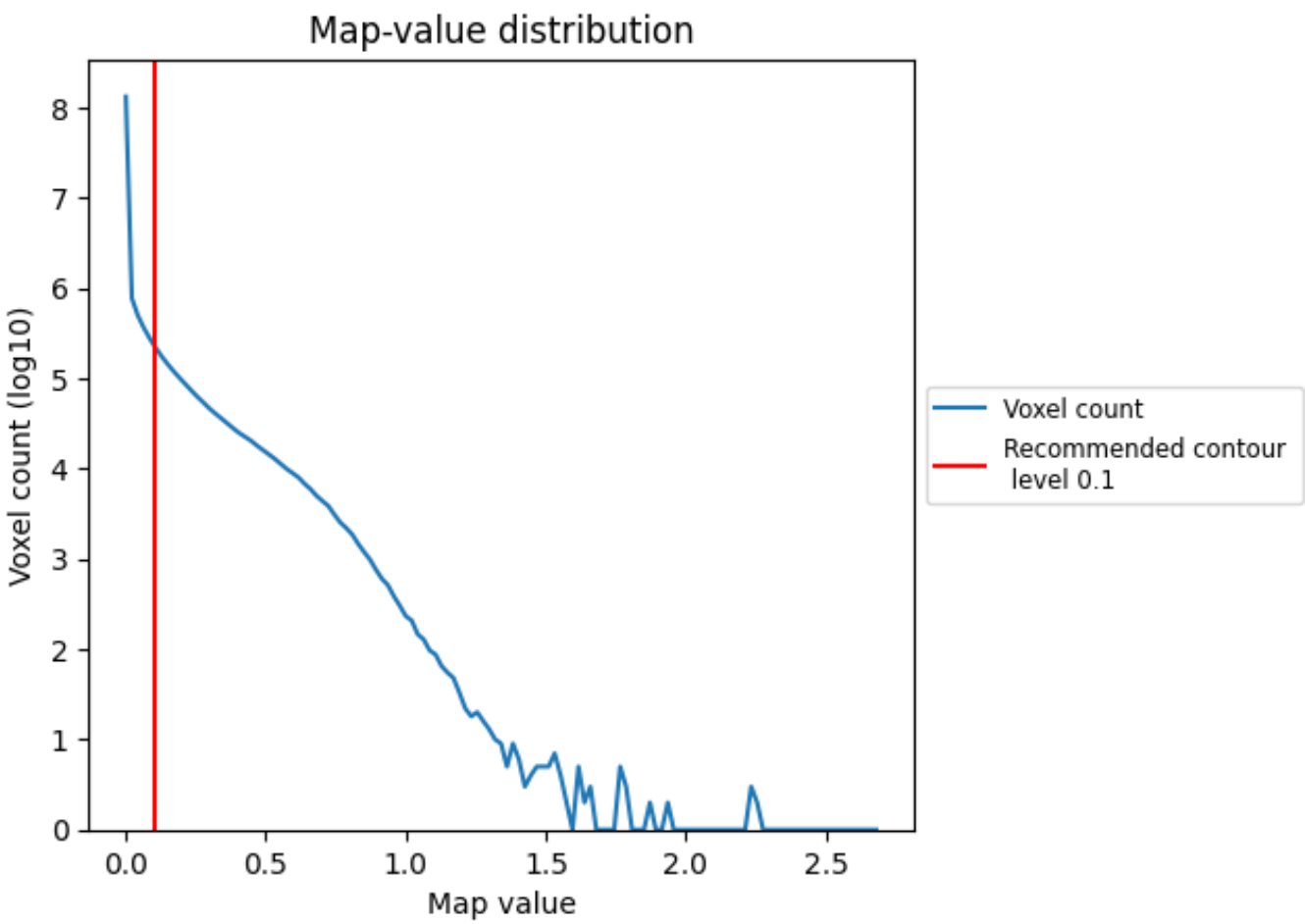


Z

7 Map analysis (i)

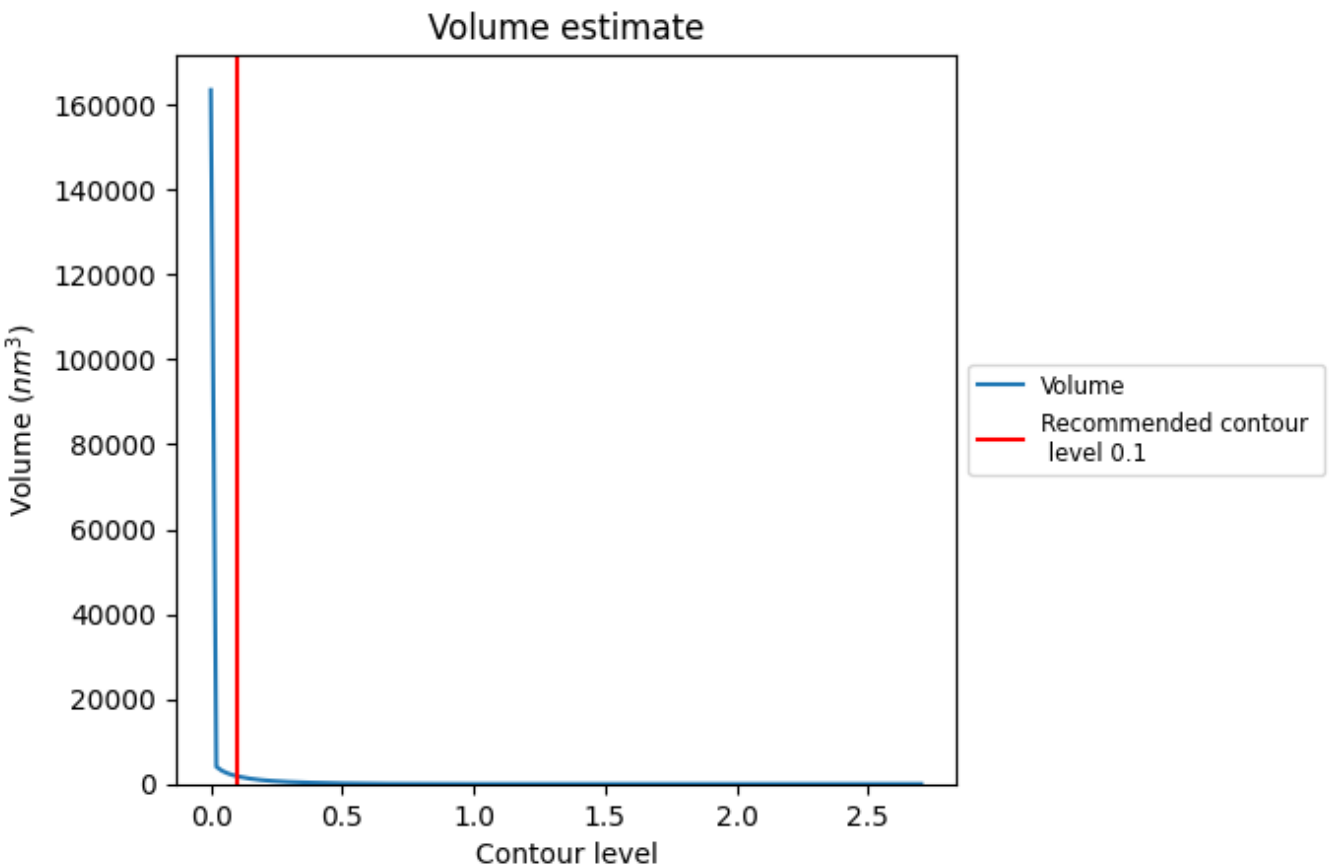
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

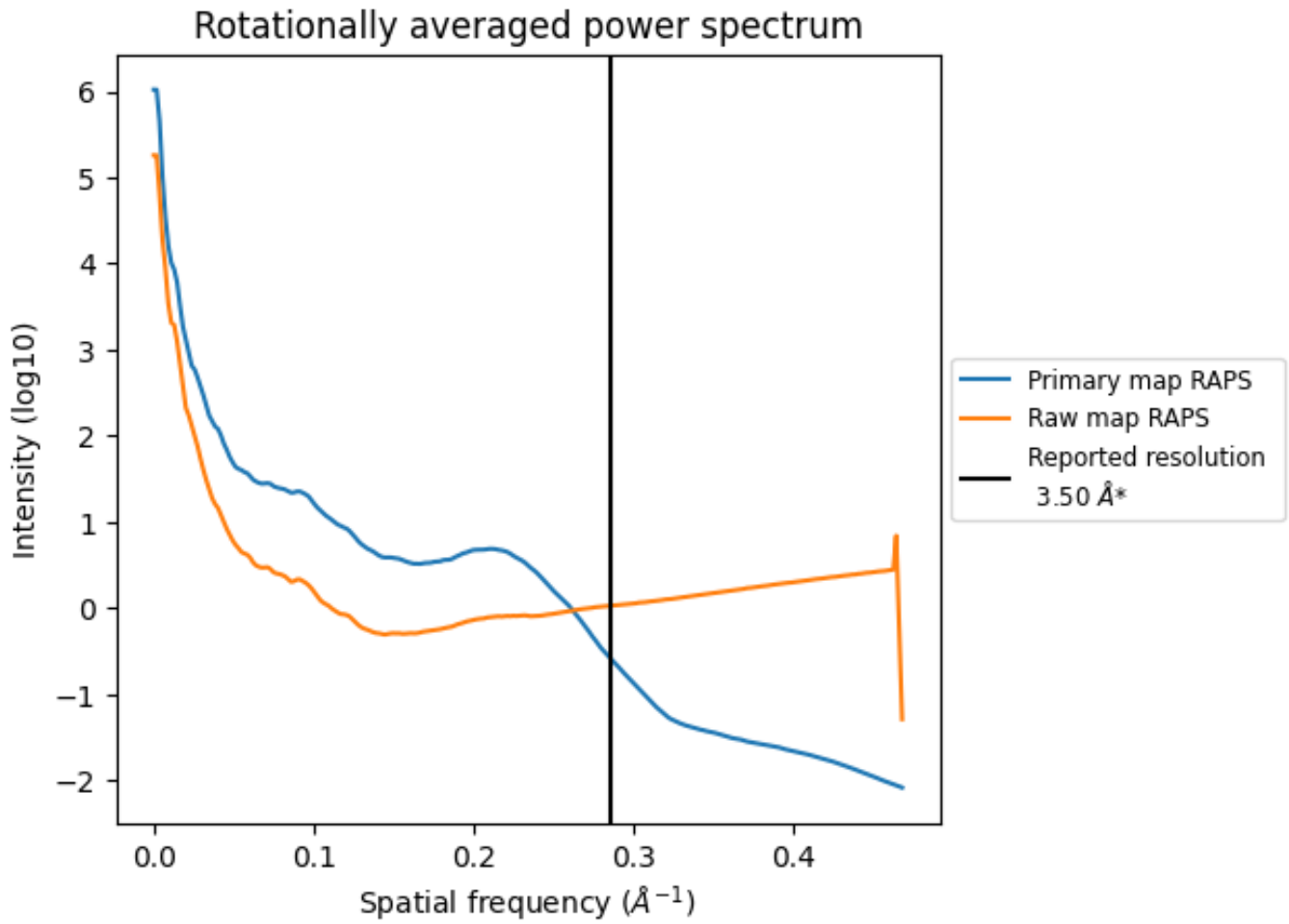
7.2 Volume estimate (i)



The volume at the recommended contour level is 1833 nm^3; this corresponds to an approximate mass of 1656 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)

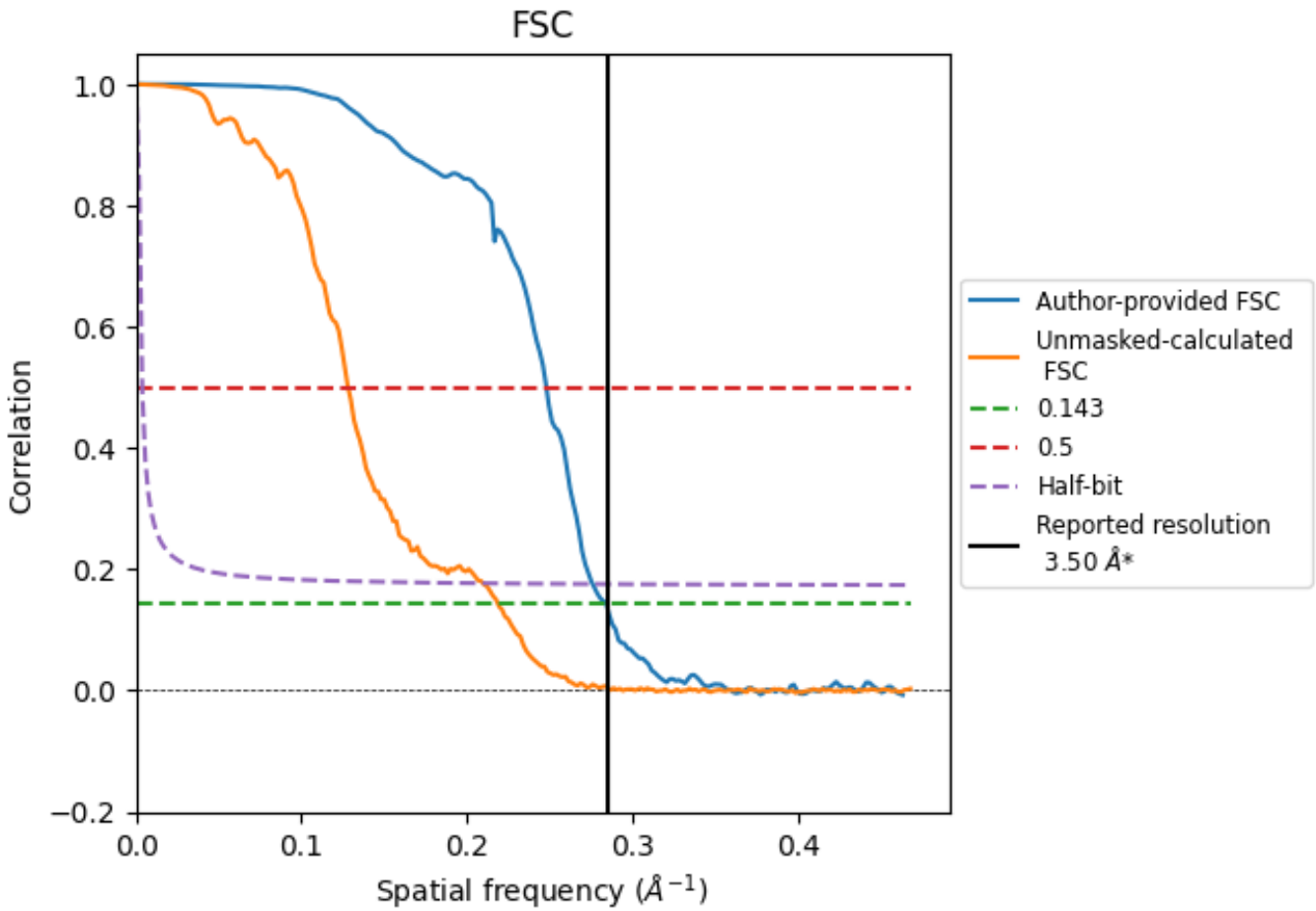


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

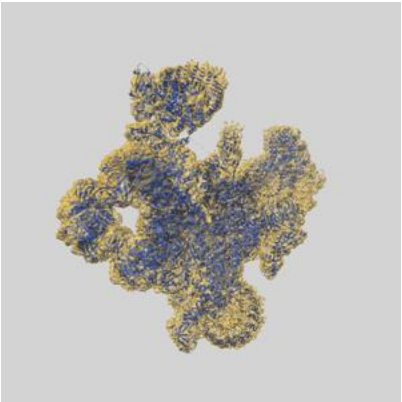
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.03	3.62
Unmasked-calculated*	4.57	7.81	4.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.5 by more than 10 %

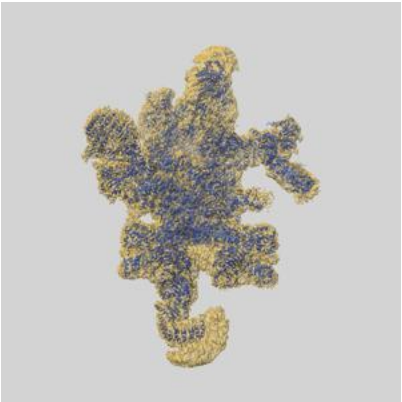
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-76334 and PDB model 12DL. Per-residue inclusion information can be found in section 3 on page 10.

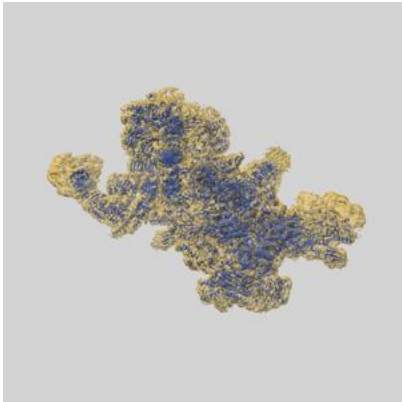
9.1 Map-model overlay (i)



X



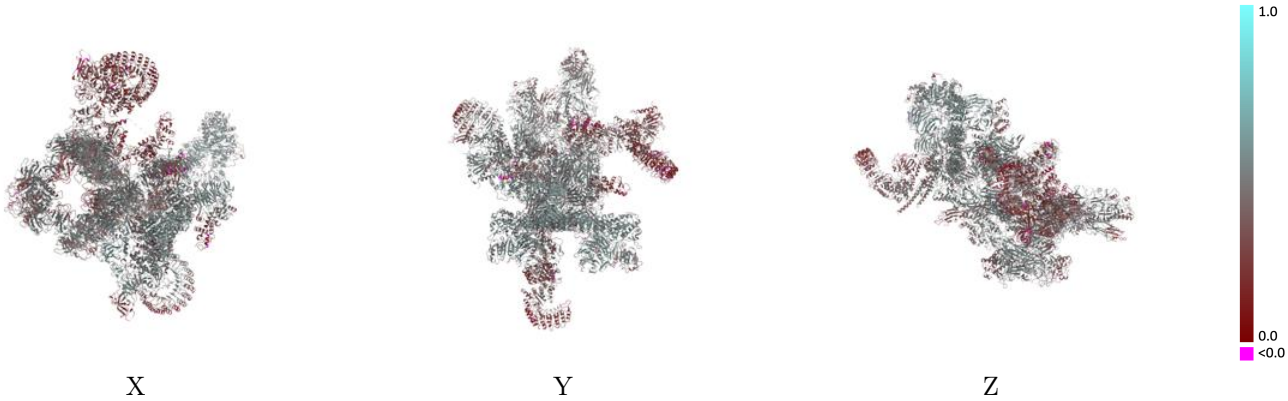
Y



Z

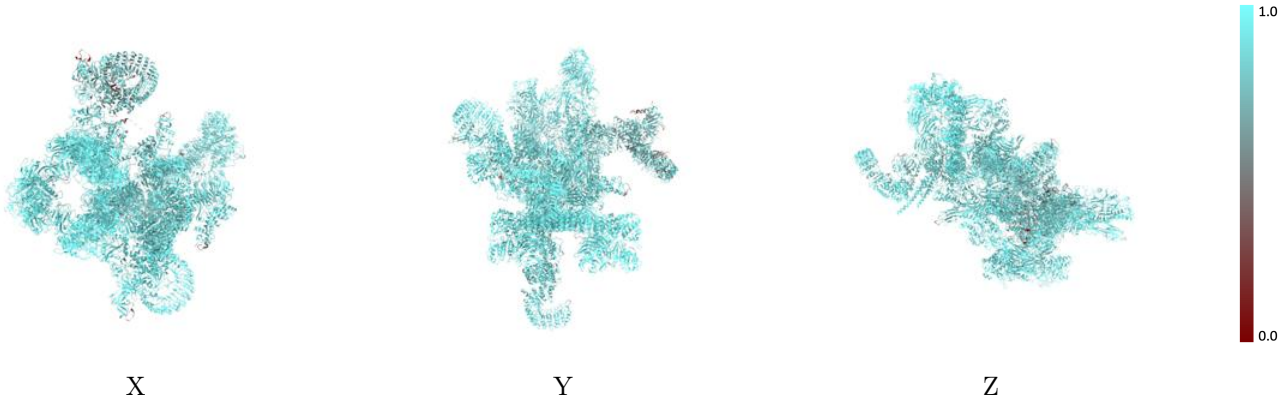
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



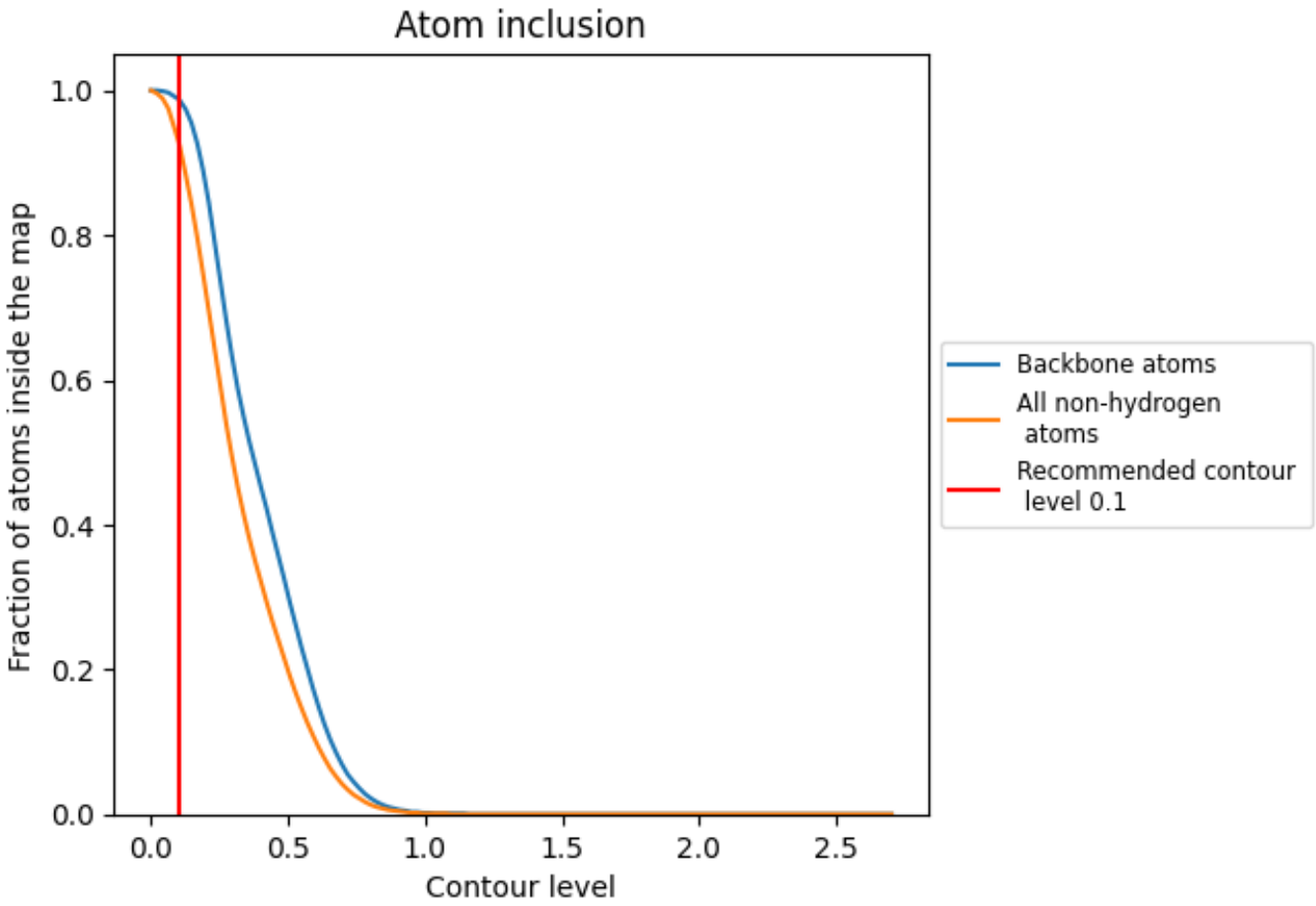
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9300	0.4310
AA	0.9590	0.4380
AB	0.9600	0.4330
AC	0.9710	0.4570
AD	0.9650	0.4560
AE	0.9540	0.4690
AF	0.9460	0.4380
AG	0.9590	0.4580
AH	0.9590	0.4430
AI	0.9570	0.4350
AJ	0.9520	0.4360
BA	0.9470	0.4550
BB	0.7530	0.2770
CA	0.9800	0.4890
CB	0.8570	0.2900
DA	0.9440	0.4420
DB	0.7330	0.2550
EA	0.9770	0.5300
FA	0.9780	0.4950
GA	0.9770	0.4960
GB	0.9620	0.5030
HA	0.9710	0.4960
HB	0.9570	0.5160
IA	0.9440	0.4930
JA	0.9630	0.4660
KA	0.9930	0.5360
LA	0.9380	0.4140
MA	0.8760	0.3050
NA	0.9710	0.5090
OA	0.9650	0.4760
PA	0.9610	0.4730
QA	0.8290	0.2650
QB	0.8270	0.2650
QC	0.8290	0.2470