Full wwPDB EM Validation Report ⓘ

Oct 2, 2023 – 08:15 pm BST

PDB ID	:	8OXM
EMDB ID	:	EMD-17265
Title	:	ATM(Q2971A) activated by oxidative stress in complex with Mg AMP-PNP and p53 peptide
Authors	:	Howes, A.C.; Perisic, O.; Williams, R.L.
Deposited on	:	2023-05-02
Resolution	:	3.30 Å(reported)
Based on initial model	:	7SIC

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

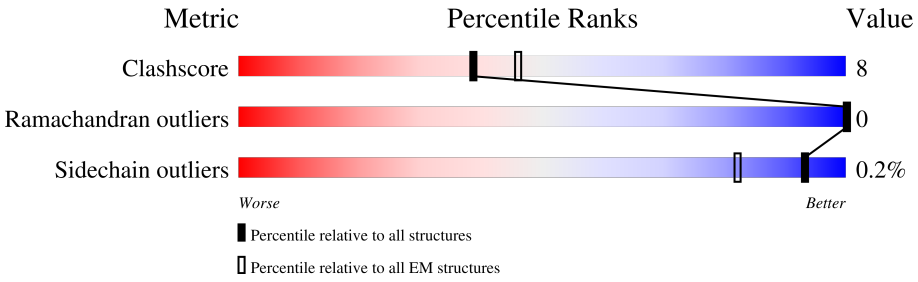
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	E	12	33% 50% 8% 42%
1	F	12	42% 58% 42%
2	A	3184	25% 68% 18% 14%
2	B	3184	24% 69% 18% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 44174 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	7	Total	C	N	O	0	0
			53	33	8	12		
1	F	7	Total	C	N	O	0	0
			53	33	8	12		

- Molecule 2 is a protein called Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2748	Total	C	N	O	S	0	0
			22001	14066	3738	4046	151		
2	B	2748	Total	C	N	O	S	0	0
			22001	14066	3738	4046	151		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP Q13315
A	-126	ASP	-	expression tag	UNP Q13315
A	-125	TYR	-	expression tag	UNP Q13315
A	-124	LYS	-	expression tag	UNP Q13315
A	-123	ASP	-	expression tag	UNP Q13315
A	-122	ASP	-	expression tag	UNP Q13315
A	-121	ASP	-	expression tag	UNP Q13315
A	-120	ASP	-	expression tag	UNP Q13315
A	-119	LYS	-	expression tag	UNP Q13315
A	-118	HIS	-	expression tag	UNP Q13315
A	-117	MET	-	expression tag	UNP Q13315
A	-116	GLY	-	expression tag	UNP Q13315
A	-115	VAL	-	expression tag	UNP Q13315
A	-114	GLN	-	expression tag	UNP Q13315
A	-113	VAL	-	expression tag	UNP Q13315
A	-112	GLU	-	expression tag	UNP Q13315
A	-111	THR	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-110	ILE	-	expression tag	UNP Q13315
A	-109	SER	-	expression tag	UNP Q13315
A	-108	PRO	-	expression tag	UNP Q13315
A	-107	GLY	-	expression tag	UNP Q13315
A	-106	ASP	-	expression tag	UNP Q13315
A	-105	GLY	-	expression tag	UNP Q13315
A	-104	ARG	-	expression tag	UNP Q13315
A	-103	THR	-	expression tag	UNP Q13315
A	-102	PHE	-	expression tag	UNP Q13315
A	-101	PRO	-	expression tag	UNP Q13315
A	-100	LYS	-	expression tag	UNP Q13315
A	-99	ARG	-	expression tag	UNP Q13315
A	-98	GLY	-	expression tag	UNP Q13315
A	-97	GLN	-	expression tag	UNP Q13315
A	-96	THR	-	expression tag	UNP Q13315
A	-95	CYS	-	expression tag	UNP Q13315
A	-94	VAL	-	expression tag	UNP Q13315
A	-93	VAL	-	expression tag	UNP Q13315
A	-92	HIS	-	expression tag	UNP Q13315
A	-91	TYR	-	expression tag	UNP Q13315
A	-90	THR	-	expression tag	UNP Q13315
A	-89	GLY	-	expression tag	UNP Q13315
A	-88	MET	-	expression tag	UNP Q13315
A	-87	LEU	-	expression tag	UNP Q13315
A	-86	GLU	-	expression tag	UNP Q13315
A	-85	ASP	-	expression tag	UNP Q13315
A	-84	GLY	-	expression tag	UNP Q13315
A	-83	LYS	-	expression tag	UNP Q13315
A	-82	LYS	-	expression tag	UNP Q13315
A	-81	PHE	-	expression tag	UNP Q13315
A	-80	ASP	-	expression tag	UNP Q13315
A	-79	SER	-	expression tag	UNP Q13315
A	-78	SER	-	expression tag	UNP Q13315
A	-77	ARG	-	expression tag	UNP Q13315
A	-76	ASP	-	expression tag	UNP Q13315
A	-75	ARG	-	expression tag	UNP Q13315
A	-74	ASN	-	expression tag	UNP Q13315
A	-73	LYS	-	expression tag	UNP Q13315
A	-72	PRO	-	expression tag	UNP Q13315
A	-71	PHE	-	expression tag	UNP Q13315
A	-70	LYS	-	expression tag	UNP Q13315
A	-69	PHE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-68	MET	-	expression tag	UNP Q13315
A	-67	LEU	-	expression tag	UNP Q13315
A	-66	GLY	-	expression tag	UNP Q13315
A	-65	LYS	-	expression tag	UNP Q13315
A	-64	GLN	-	expression tag	UNP Q13315
A	-63	GLU	-	expression tag	UNP Q13315
A	-62	VAL	-	expression tag	UNP Q13315
A	-61	ILE	-	expression tag	UNP Q13315
A	-60	ARG	-	expression tag	UNP Q13315
A	-59	GLY	-	expression tag	UNP Q13315
A	-58	TRP	-	expression tag	UNP Q13315
A	-57	GLU	-	expression tag	UNP Q13315
A	-56	GLU	-	expression tag	UNP Q13315
A	-55	GLY	-	expression tag	UNP Q13315
A	-54	VAL	-	expression tag	UNP Q13315
A	-53	ALA	-	expression tag	UNP Q13315
A	-52	GLN	-	expression tag	UNP Q13315
A	-51	MET	-	expression tag	UNP Q13315
A	-50	SER	-	expression tag	UNP Q13315
A	-49	VAL	-	expression tag	UNP Q13315
A	-48	GLY	-	expression tag	UNP Q13315
A	-47	GLN	-	expression tag	UNP Q13315
A	-46	ARG	-	expression tag	UNP Q13315
A	-45	ALA	-	expression tag	UNP Q13315
A	-44	LYS	-	expression tag	UNP Q13315
A	-43	LEU	-	expression tag	UNP Q13315
A	-42	THR	-	expression tag	UNP Q13315
A	-41	ILE	-	expression tag	UNP Q13315
A	-40	SER	-	expression tag	UNP Q13315
A	-39	PRO	-	expression tag	UNP Q13315
A	-38	ASP	-	expression tag	UNP Q13315
A	-37	TYR	-	expression tag	UNP Q13315
A	-36	ALA	-	expression tag	UNP Q13315
A	-35	TYR	-	expression tag	UNP Q13315
A	-34	GLY	-	expression tag	UNP Q13315
A	-33	ALA	-	expression tag	UNP Q13315
A	-32	THR	-	expression tag	UNP Q13315
A	-31	GLY	-	expression tag	UNP Q13315
A	-30	HIS	-	expression tag	UNP Q13315
A	-29	PRO	-	expression tag	UNP Q13315
A	-28	GLY	-	expression tag	UNP Q13315
A	-27	ILE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	ILE	-	expression tag	UNP Q13315
A	-25	PRO	-	expression tag	UNP Q13315
A	-24	PRO	-	expression tag	UNP Q13315
A	-23	HIS	-	expression tag	UNP Q13315
A	-22	ALA	-	expression tag	UNP Q13315
A	-21	THR	-	expression tag	UNP Q13315
A	-20	LEU	-	expression tag	UNP Q13315
A	-19	VAL	-	expression tag	UNP Q13315
A	-18	PHE	-	expression tag	UNP Q13315
A	-17	ASP	-	expression tag	UNP Q13315
A	-16	VAL	-	expression tag	UNP Q13315
A	-15	GLU	-	expression tag	UNP Q13315
A	-14	LEU	-	expression tag	UNP Q13315
A	-13	LEU	-	expression tag	UNP Q13315
A	-12	LYS	-	expression tag	UNP Q13315
A	-11	LEU	-	expression tag	UNP Q13315
A	-10	GLU	-	expression tag	UNP Q13315
A	-9	GLY	-	expression tag	UNP Q13315
A	-8	GLY	-	expression tag	UNP Q13315
A	-7	SER	-	expression tag	UNP Q13315
A	-6	ALA	-	expression tag	UNP Q13315
A	-5	GLY	-	expression tag	UNP Q13315
A	-4	SER	-	expression tag	UNP Q13315
A	-3	GLY	-	expression tag	UNP Q13315
A	-2	SER	-	expression tag	UNP Q13315
A	-1	ALA	-	expression tag	UNP Q13315
A	0	SER	-	expression tag	UNP Q13315
A	2971	ALA	GLN	engineered mutation	UNP Q13315
B	-127	MET	-	initiating methionine	UNP Q13315
B	-126	ASP	-	expression tag	UNP Q13315
B	-125	TYR	-	expression tag	UNP Q13315
B	-124	LYS	-	expression tag	UNP Q13315
B	-123	ASP	-	expression tag	UNP Q13315
B	-122	ASP	-	expression tag	UNP Q13315
B	-121	ASP	-	expression tag	UNP Q13315
B	-120	ASP	-	expression tag	UNP Q13315
B	-119	LYS	-	expression tag	UNP Q13315
B	-118	HIS	-	expression tag	UNP Q13315
B	-117	MET	-	expression tag	UNP Q13315
B	-116	GLY	-	expression tag	UNP Q13315
B	-115	VAL	-	expression tag	UNP Q13315
B	-114	GLN	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-113	VAL	-	expression tag	UNP Q13315
B	-112	GLU	-	expression tag	UNP Q13315
B	-111	THR	-	expression tag	UNP Q13315
B	-110	ILE	-	expression tag	UNP Q13315
B	-109	SER	-	expression tag	UNP Q13315
B	-108	PRO	-	expression tag	UNP Q13315
B	-107	GLY	-	expression tag	UNP Q13315
B	-106	ASP	-	expression tag	UNP Q13315
B	-105	GLY	-	expression tag	UNP Q13315
B	-104	ARG	-	expression tag	UNP Q13315
B	-103	THR	-	expression tag	UNP Q13315
B	-102	PHE	-	expression tag	UNP Q13315
B	-101	PRO	-	expression tag	UNP Q13315
B	-100	LYS	-	expression tag	UNP Q13315
B	-99	ARG	-	expression tag	UNP Q13315
B	-98	GLY	-	expression tag	UNP Q13315
B	-97	GLN	-	expression tag	UNP Q13315
B	-96	THR	-	expression tag	UNP Q13315
B	-95	CYS	-	expression tag	UNP Q13315
B	-94	VAL	-	expression tag	UNP Q13315
B	-93	VAL	-	expression tag	UNP Q13315
B	-92	HIS	-	expression tag	UNP Q13315
B	-91	TYR	-	expression tag	UNP Q13315
B	-90	THR	-	expression tag	UNP Q13315
B	-89	GLY	-	expression tag	UNP Q13315
B	-88	MET	-	expression tag	UNP Q13315
B	-87	LEU	-	expression tag	UNP Q13315
B	-86	GLU	-	expression tag	UNP Q13315
B	-85	ASP	-	expression tag	UNP Q13315
B	-84	GLY	-	expression tag	UNP Q13315
B	-83	LYS	-	expression tag	UNP Q13315
B	-82	LYS	-	expression tag	UNP Q13315
B	-81	PHE	-	expression tag	UNP Q13315
B	-80	ASP	-	expression tag	UNP Q13315
B	-79	SER	-	expression tag	UNP Q13315
B	-78	SER	-	expression tag	UNP Q13315
B	-77	ARG	-	expression tag	UNP Q13315
B	-76	ASP	-	expression tag	UNP Q13315
B	-75	ARG	-	expression tag	UNP Q13315
B	-74	ASN	-	expression tag	UNP Q13315
B	-73	LYS	-	expression tag	UNP Q13315
B	-72	PRO	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-71	PHE	-	expression tag	UNP Q13315
B	-70	LYS	-	expression tag	UNP Q13315
B	-69	PHE	-	expression tag	UNP Q13315
B	-68	MET	-	expression tag	UNP Q13315
B	-67	LEU	-	expression tag	UNP Q13315
B	-66	GLY	-	expression tag	UNP Q13315
B	-65	LYS	-	expression tag	UNP Q13315
B	-64	GLN	-	expression tag	UNP Q13315
B	-63	GLU	-	expression tag	UNP Q13315
B	-62	VAL	-	expression tag	UNP Q13315
B	-61	ILE	-	expression tag	UNP Q13315
B	-60	ARG	-	expression tag	UNP Q13315
B	-59	GLY	-	expression tag	UNP Q13315
B	-58	TRP	-	expression tag	UNP Q13315
B	-57	GLU	-	expression tag	UNP Q13315
B	-56	GLU	-	expression tag	UNP Q13315
B	-55	GLY	-	expression tag	UNP Q13315
B	-54	VAL	-	expression tag	UNP Q13315
B	-53	ALA	-	expression tag	UNP Q13315
B	-52	GLN	-	expression tag	UNP Q13315
B	-51	MET	-	expression tag	UNP Q13315
B	-50	SER	-	expression tag	UNP Q13315
B	-49	VAL	-	expression tag	UNP Q13315
B	-48	GLY	-	expression tag	UNP Q13315
B	-47	GLN	-	expression tag	UNP Q13315
B	-46	ARG	-	expression tag	UNP Q13315
B	-45	ALA	-	expression tag	UNP Q13315
B	-44	LYS	-	expression tag	UNP Q13315
B	-43	LEU	-	expression tag	UNP Q13315
B	-42	THR	-	expression tag	UNP Q13315
B	-41	ILE	-	expression tag	UNP Q13315
B	-40	SER	-	expression tag	UNP Q13315
B	-39	PRO	-	expression tag	UNP Q13315
B	-38	ASP	-	expression tag	UNP Q13315
B	-37	TYR	-	expression tag	UNP Q13315
B	-36	ALA	-	expression tag	UNP Q13315
B	-35	TYR	-	expression tag	UNP Q13315
B	-34	GLY	-	expression tag	UNP Q13315
B	-33	ALA	-	expression tag	UNP Q13315
B	-32	THR	-	expression tag	UNP Q13315
B	-31	GLY	-	expression tag	UNP Q13315
B	-30	HIS	-	expression tag	UNP Q13315

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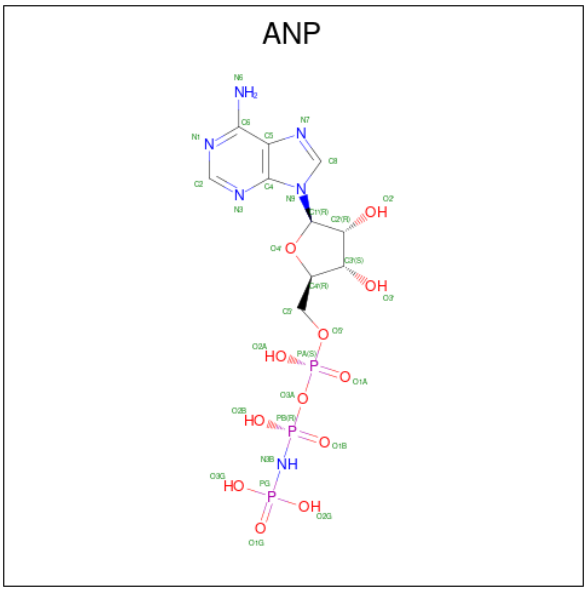
Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	PRO	-	expression tag	UNP Q13315
B	-28	GLY	-	expression tag	UNP Q13315
B	-27	ILE	-	expression tag	UNP Q13315
B	-26	ILE	-	expression tag	UNP Q13315
B	-25	PRO	-	expression tag	UNP Q13315
B	-24	PRO	-	expression tag	UNP Q13315
B	-23	HIS	-	expression tag	UNP Q13315
B	-22	ALA	-	expression tag	UNP Q13315
B	-21	THR	-	expression tag	UNP Q13315
B	-20	LEU	-	expression tag	UNP Q13315
B	-19	VAL	-	expression tag	UNP Q13315
B	-18	PHE	-	expression tag	UNP Q13315
B	-17	ASP	-	expression tag	UNP Q13315
B	-16	VAL	-	expression tag	UNP Q13315
B	-15	GLU	-	expression tag	UNP Q13315
B	-14	LEU	-	expression tag	UNP Q13315
B	-13	LEU	-	expression tag	UNP Q13315
B	-12	LYS	-	expression tag	UNP Q13315
B	-11	LEU	-	expression tag	UNP Q13315
B	-10	GLU	-	expression tag	UNP Q13315
B	-9	GLY	-	expression tag	UNP Q13315
B	-8	GLY	-	expression tag	UNP Q13315
B	-7	SER	-	expression tag	UNP Q13315
B	-6	ALA	-	expression tag	UNP Q13315
B	-5	GLY	-	expression tag	UNP Q13315
B	-4	SER	-	expression tag	UNP Q13315
B	-3	GLY	-	expression tag	UNP Q13315
B	-2	SER	-	expression tag	UNP Q13315
B	-1	ALA	-	expression tag	UNP Q13315
B	0	SER	-	expression tag	UNP Q13315
B	2971	ALA	GLN	engineered mutation	UNP Q13315

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

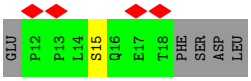
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

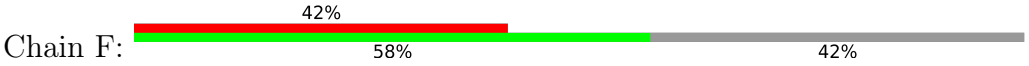
• Molecule 1: Cellular tumor antigen p53

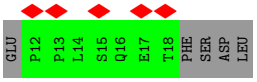
Chain E:



• Molecule 1: Cellular tumor antigen p53

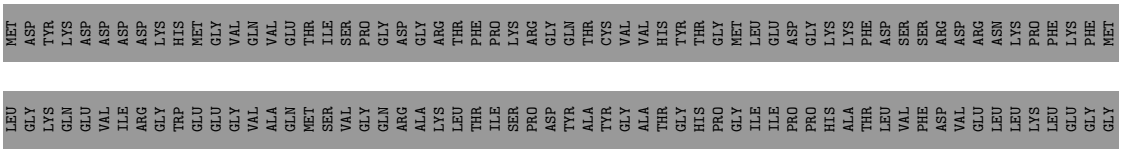
Chain F:

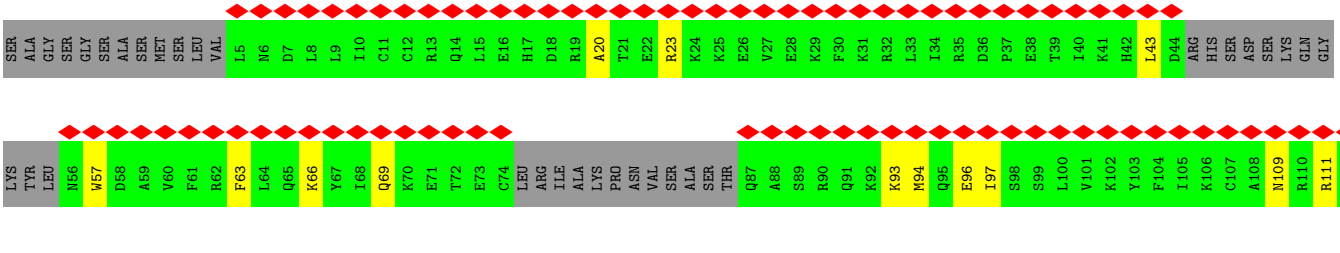


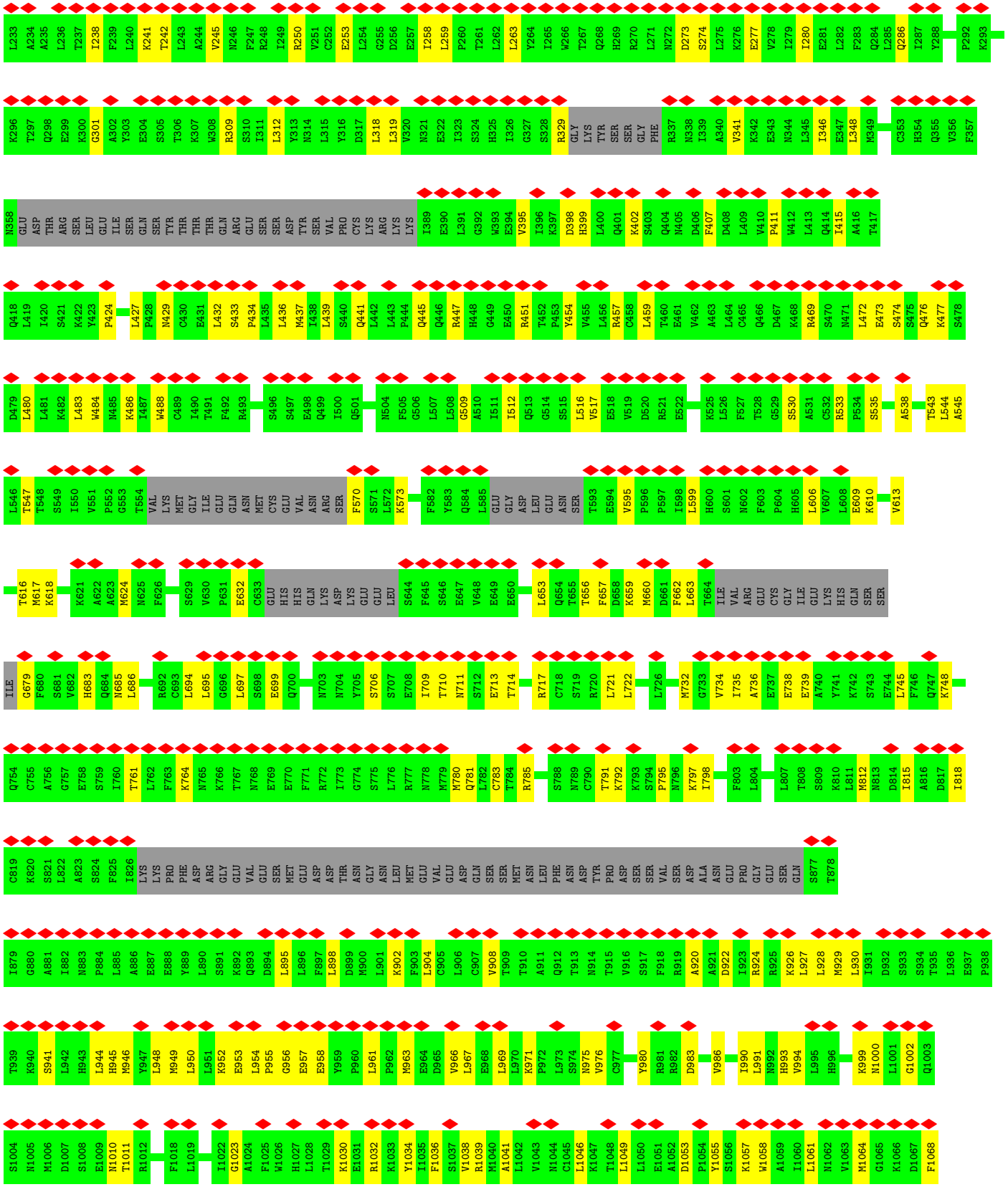


• Molecule 2: Serine-protein kinase ATM

Chain A:






L233 A234 A235 L236 T237 I238 F239 L240 K241 T242 L243 A244 V245 N246 F247 R248 I249 R250 V251 C252 E253 L254 G255 D256 E257 I258 L259 P260 T261 L262 L263 Y264 I265 W266 T267 Q268 H269 R270 L271 N272 D273 S274 L275 K276 E277 V278 I279 I280 E281 L282 F283 Q284 L285 Q286 I287 Y288 P292 K293
K296 T297 Q298 E299 K300 G301 A302 Y303 E304 S305 T306 K307 W308 R309 S310 I311 L312 Y313 N314 L315 Y316 D317 L318 L319 V320 N321 E322 I323 S324 H325 I326 G327 S328 R329 GLY LYS TYR SER SER GLY PHE R337 N338 I339 A340 V341 K342 E343 N344 L345 I346 E347 L348 M349 C353 H354 Q355 V356 F357
N358 GLU ASP THR ARG SER LEU GLU ILE SER GLN SER TYR THR THR THR GLN ARG GLU SER SER ASP TYR SER VAL PRO CYS LYS ARG LYS LYS I389 E390 L391 G392 W393 E394 V395 I396 K397 D398 H399 L400 Q401 K402 S403 Q404 N405 D406 F407 D408 L409 V410 P411 W412 L413 Q414 I415 A416 T417
Q418 L419 I420 S421 K422 Y423 P424 L427 P428 N429 C430 E431 L432 S433 P434 L435 L436 M437 I438 L439 S440 Q441 L442 L443 P444 Q445 Q446 R447 H448 G449 E450 R451 T452 P453 Y454 V455 L456 R457 C458 L459 T460 E461 V462 A463 L464 C465 Q466 D467 K468 R469 S470 N471 I472 E473 S474 S475 Q476 K477 S478
D479 L480 L481 K482 L483 W484 N485 K486 I487 W488 C489 I490 T491 F492 R493 S496 S497 E498 Q499 I500 Q501 N504 F505 G506 L507 L508 G509 A510 I511 I512 Q513 G514 S515 L516 V517 E518 V519 D520 R521 E522 K525 L526 F527 T528 G529 S530 A531 C532 R533 P534 S535 A538 T543 L544 A545
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T616 M617 K618 K621 A622 A623 M624 N625 F626 S629 V630 P631 E632 G633 GLU HIS HIS GLN LYS ASP LYS GLU GLU LEU S644 F645 S646 E647 V648 E649 E650 L653 Q654 T655 T656 F657 D658 K659 M660 D661 F662 L663 T664 ILE VAL ARG GLU CYS GLY ILE GLU LYS HIS GLN SER SER
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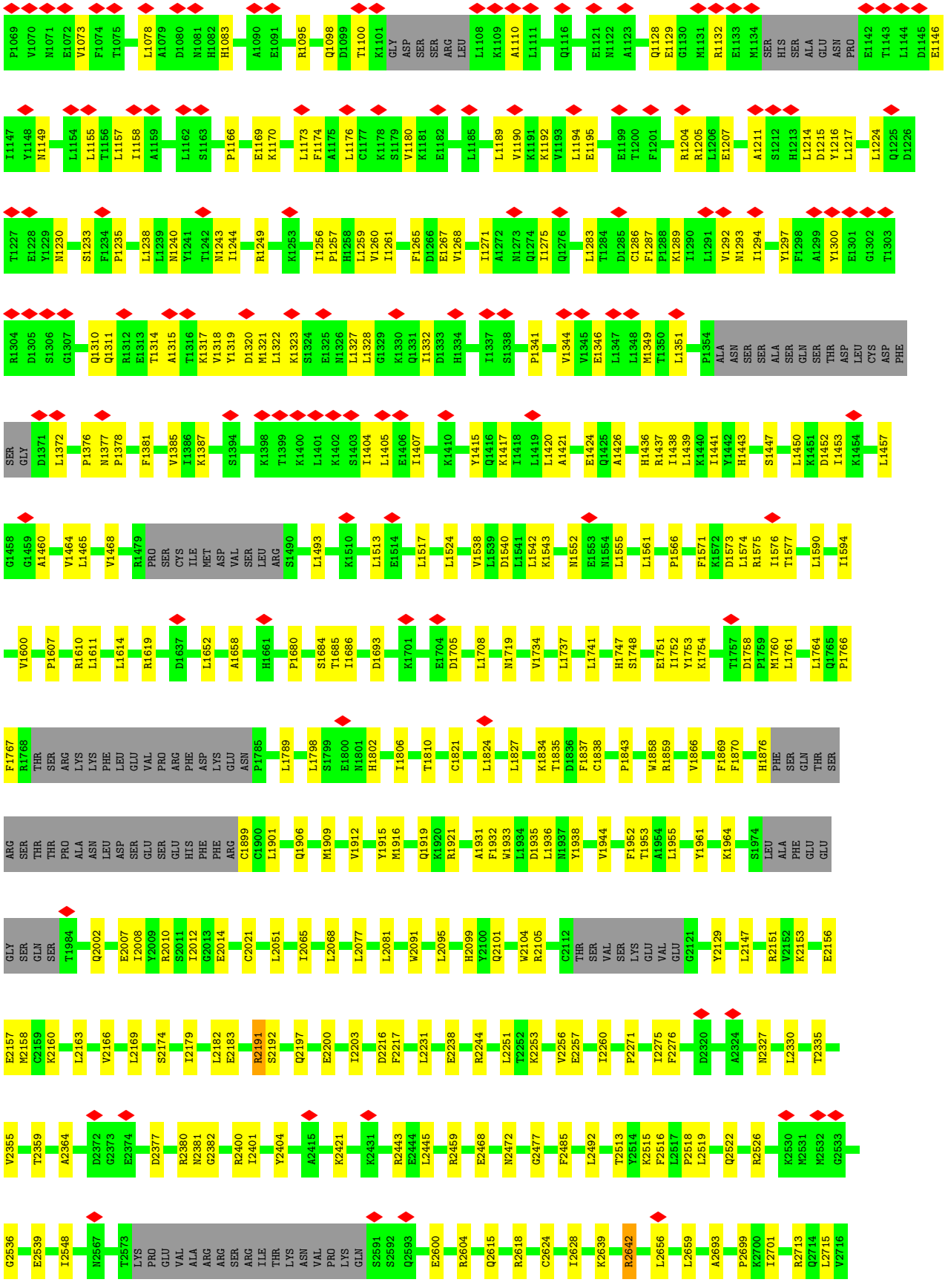
S1004 N1005 M1006 D1007 S1008 E1009 N1010 T1011 R1012 F1018 L1019 I1022 G1023 A1024 F1025 W1026 H1027 L1028 T1029 K1030 E1031 R1032 K1033 Y1034 I1035 F1036 S1037 V1038 R1039 M1040 A1041 L1042 V1043 N1044 C1045 L1046 K1047 T1048 L1049 L1050 E1051 A1052 D1053 P1054 Y1055 S1056 K1057 W1058 A1059 I1060 L1061 N1062 V1063 M1064 G1065 K1066 D1067 F1068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SER GLY D1371 L1372 P1376 N1377 P1378 F1381 V1385 I1386 K1387 S1394 K1398 T1399 K1400 L1401 K1402 S1403 I1404 L1405 E1406 I1407 K1410 Y1415 Q1416 K1417 I1418 L1419 L1420 A1421 E1424 Q1425 A1426 H1436 R1437 I1438 L1439 K1440 I1441 Y1442 H1443 S1447 L1450 K1451 D1452 I1453 K1454 L1457
G1458 G1459 A1460 V1464 L1465 V1468 R1479 PRO SER CYS ILE MET ASP VAL SER LEU ARG S1490 L1493 K1510 L1513 E1514 L1517 L1524 V1538 L1539 D1540 L1541 L1542 K1543 N1552 E1553 N1554 L1555 L1561 P1566 F1571 K1572 D1573 L1574 R1575 I1576 T1577 L1590 I1594
V1600 P1607 R1610 L1611 L1614 R1619 D1637 L1652 A1658 H1661 P1680 S1684 T1685 I1686 D1693 K1701 E1704 D1705 L1708 N1719 V1734 L1737 L1741 H1747 S1748 E1751 I1752 Y1753 K1754 T1757 D1758 P1759 M1760 L1761 L1764 Q1765 P1766
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ARG SER THR THR PRO ALA ASN LEU ASP SER GLU SER GLU GLU HIS PHE PHE ARG C1899 C1900 L1901 Q1906 M1909 V1912 Y1915 M1916 Q1919 K1920 R1921 A1931 F1932 W1933 L1934 D1935 L1936 N1937 Y1938 V1944 F1952 T1953 A1954 L1955 Y1961 K1964 S1974 LEU ALA PHE GLU GLU
GLY SER GLN SER T1984 Q2002 E2007 I2008 Y2009 R2010 S2011 I2012 G2013 E2014 C2021 L2051 I2065 L2068 L2077 L2081 W2091 L2095 H2099 Y2100 Q2101 W2104 R2105 C2112 THR SER VAL SER LYS GLU VAL GLU G2121 Y2129 L2147 R2151 V2152 K2153 E2156
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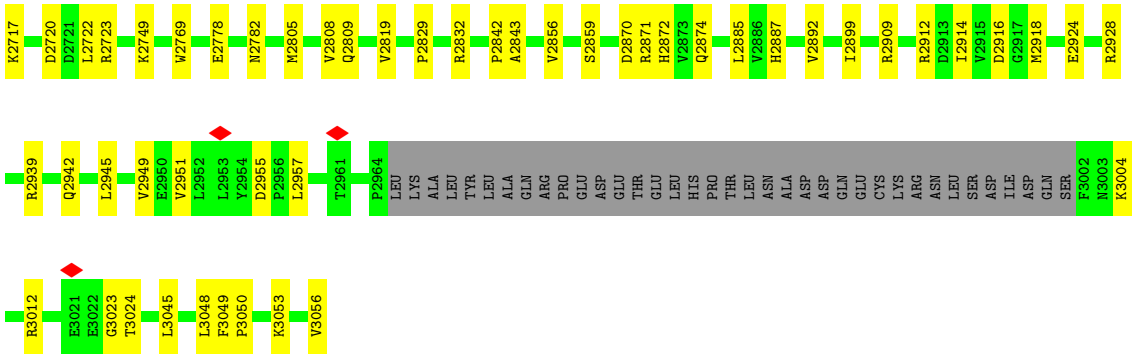
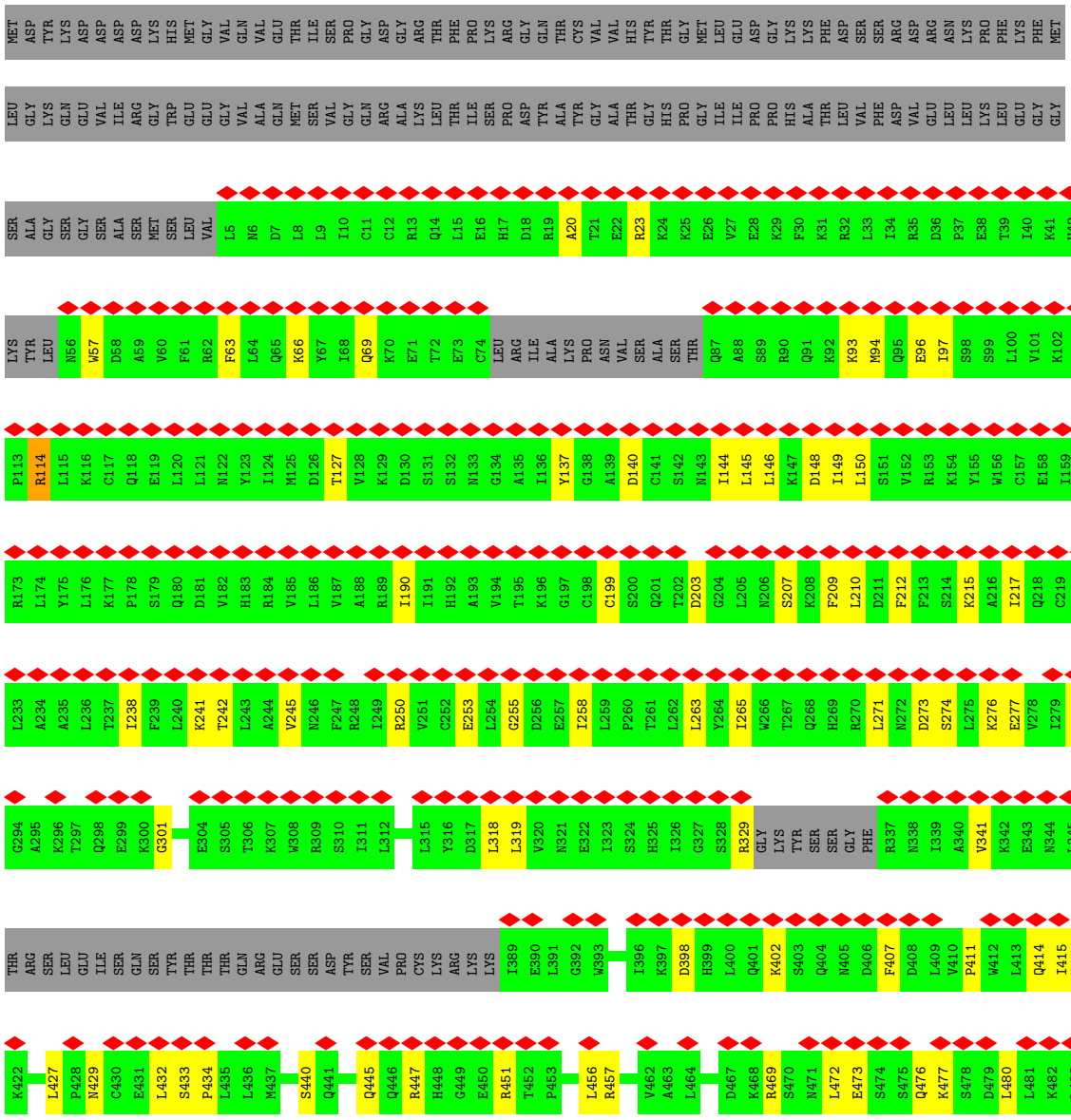
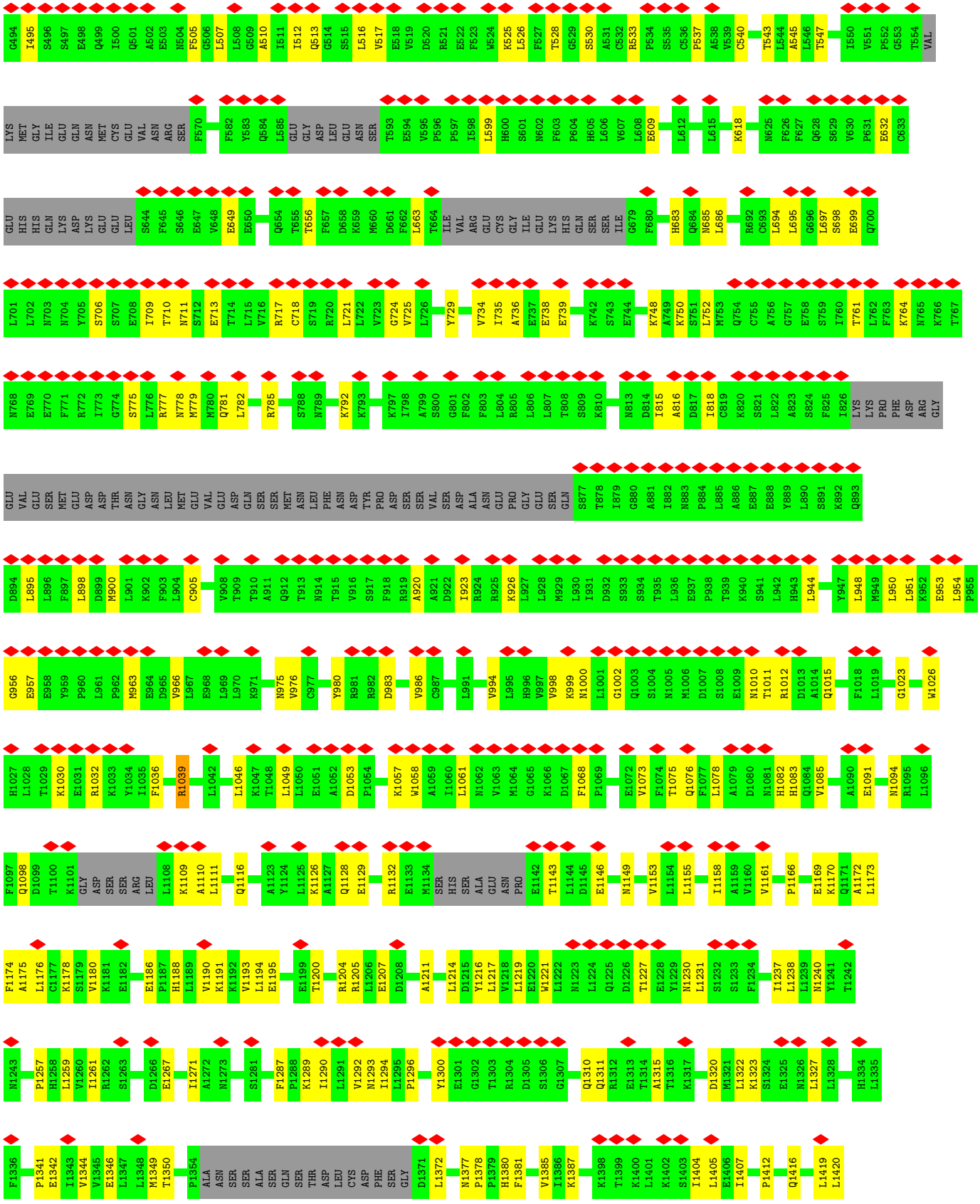
V2355 T2359 A2364 D2372 G2373 E2374 D2377 R2380 N2381 G2382 R2400 I2401 Y2404 A2415 K2421 K2431 R2443 E2444 L2445 R2459 E2468 N2472 G2477 F2485 L2492 T2513 Y2514 K2515 F2516 L2517 P2518 L2519 Q2522 R2526 K2530 M2531 M2532 G2533
G2536 E2539 I2548 N2567 T2573 LYS PRO GLU VAL ALA ARG ARG SER ARG ILE THR LYS ASN VAL PRO LYS GLN S2591 S2592 Q2593 E2600 R2604 Q2615 R2618 C2624 I2628 K2639 R2642 L2656 L2659 A2693 P2699 K2700 I2701 R2713 Q2714 L2715 V2716



• Molecule 2: Serine-protein kinase ATM

Chain B:

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LYS MET GLY ILE GLU GLN ASN MET CYS GLU VAL ASN ARG SER F570 F582 Y583 Q584 L585 GLU GLY ASP LEU GLU ASN SER T593 E594 V595 P596 P597 I598 L599 H600 S601 N602 F603 P604 H605 L606 V607 L608 E609 L612 L615 K618 N625 F626 F627 Q628 S629 V630 P631 E632 C633
GLU HIS HIS GLN LYS ASP LYS GLU GLU LEU S644 F645 S646 E647 V648 E649 E650 Q654 T655 T656 F657 D658 K659 M660 D661 F662 L663 T664 ILE VAL ARG GLU CYS GLY ILE GLU LYS HIS GLN SER SER ILE G679 F680 H683 Q684 N685 L686 R692 C693 L694 L695 G696 L697 S698 E699 Q700
L701 L702 N703 N704 Y705 S706 S707 E708 I709 T710 N711 S712 E713 T714 L715 V716 R717 C718 S719 R720 L721 L722 V723 G724 V725 L726 Y729 V734 I735 A736 E737 E738 E739 K742 S743 E744 K748 A749 K750 S751 L752 M753 Q754 C755 A756 G757 E758 S759 I760 T761 L762 F763 K764 N765 K766 T767
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GLU VAL GLU SER MET GLU ASP ASP THR ASN GLY ASN LEU MET GLU VAL GLU ASP GLN SER SER MET ASN LEU PHE ASN ASP TYR PRO ASP SER SER VAL SER ASP ALA ASN GLU PRO GLY GLU SER GLN S877 T878 I879 G880 A881 I882 N883 P884 L885 A886 E887 E888 Y889 L890 S891 K892 Q893
D894 L895 L896 F897 L898 D899 M900 L901 K902 F903 L904 C905 V908 T909 T910 A911 Q912 T913 N914 T915 V916 S917 F918 R919 A920 A921 D922 I923 R924 R925 K926 L927 L928 M929 L930 I931 D932 S933 S934 T935 L936 E937 P938 T939 K940 S941 L942 H943 L944 Y947 L948 M949 L950 L951 K952 E953 L954 P955
G956 E957 E958 Y959 P960 L961 P962 M963 E964 D965 V966 L967 E968 L969 L970 K971 N975 V976 C977 Y980 R981 R982 D983 V986 C987 L991 V994 L995 H996 V997 V998 K999 N1000 L1001 G1002 Q1003 S1004 N1005 M1006 D1007 S1008 E1009 N1010 T1011 R1012 D1013 A1014 Q1015 F1018 L1019 G1023 W1026
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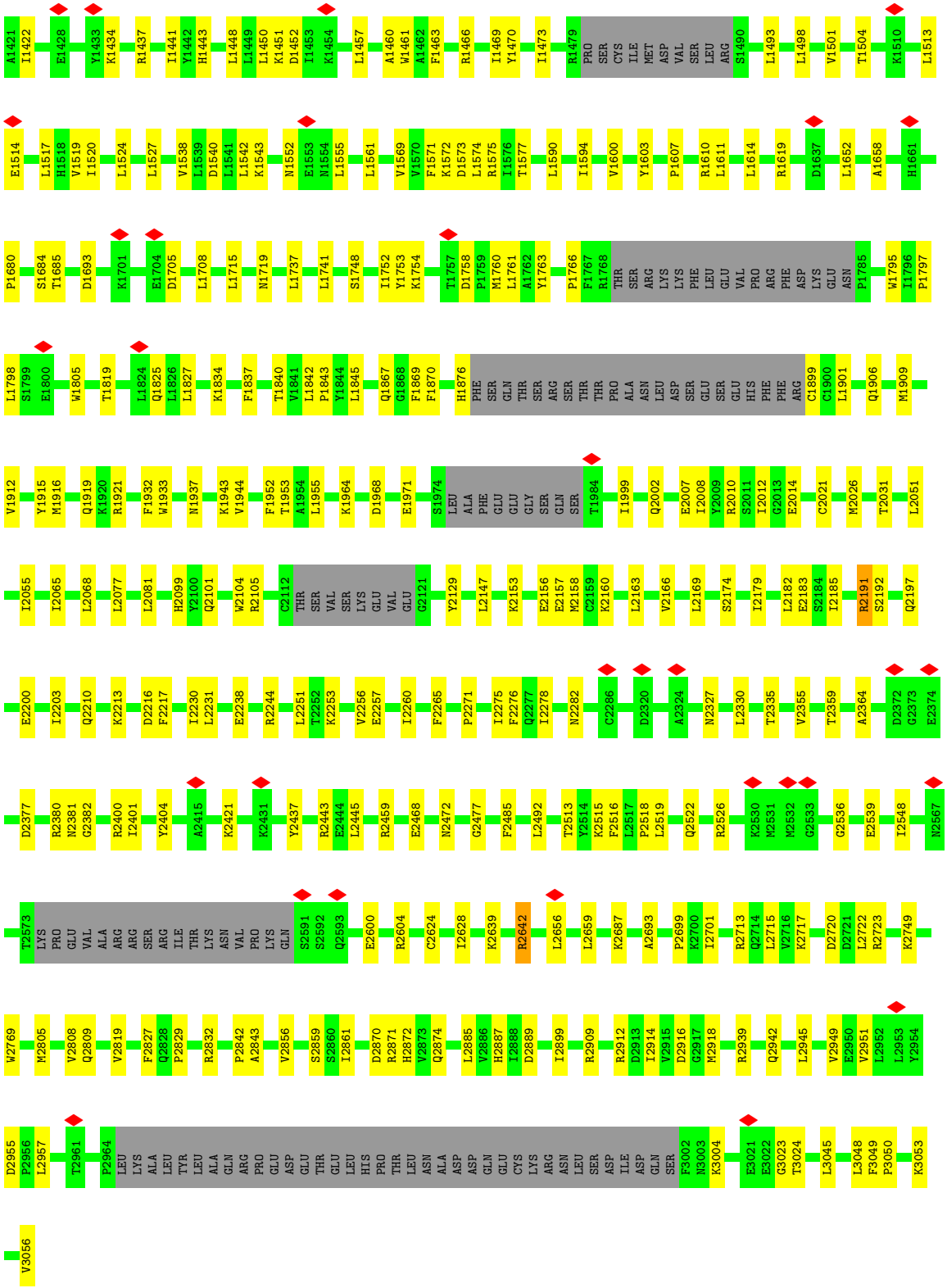
F1097 Q1098 D1099 T1100 K1101 GLY ASP SER SER ARG LEU L1108 K1109 A1110 L1111 Q1116 A1123 Y1124 L1125 K1126 A1127 Q1128 E1129 R1132 E1133 M1134 SER HIS SER ALA GLU ASN PRO E1142 T1143 L1144 D1145 E1146 N1149 V1153 L1154 L1155 I1158 A1159 V1160 V1161 P1166 E1169 K1170 Q1171 A1172 L1173
F1174 A1175 L1176 C1177 K1178 S1179 V1180 K1181 E1182 E1186 P1187 H1188 L1189 V1190 K1191 K1192 V1193 L1194 E1195 E1199 T1200 R1204 R1205 L1206 E1207 D1208 A1211 L1214 D1215 Y1216 L1217 V1218 L1219 E1220 W1221 L1222 N1223 L1224 Q1225 D1226 T1227 E1228 Y1229 N1230 L1231 S1232 S1233 F1234 I1237 L1238 L1239 N1240 Y1241 T1242
N1243 P1257 H1258 L1259 V1260 I1261 R1262 S1263 D1266 E1267 I1271 A1272 N1273 S1281 F1287 P1288 K1289 I1290 L1291 V1292 N1293 I1294 L1295 P1296 Y1300 E1301 G1302 T1303 R1304 D1305 S1306 G1307 Q1310 Q1311 R1312 E1313 T1314 A1315 T1316 K1317 D1320 M1321 L1322 K1323 S1324 E1325 N1326 L1327 L1328 H1334 L1335
F1336 P1341 E1342 I1343 V1344 V1345 E1346 L1347 L1348 M1349 T1350 P1354 ALA ASN SER SER ALA SER GLN SER THR ASP LEU CYS ASP PHE SER GLY D1371 L1372 N1377 P1378 P1379 H1380 F1381 V1385 I1386 K1387 K1398 T1399 K1400 L1401 K1402 S1403 I1404 L1405 E1406 I1407 P1412 Q1416 L1419 L1420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E1514 L1517 H1518 V1519 I1520 L1524 L1527 V1538 L1539 D1540 L1541 L1542 K1543 N1552 E1553 N1554 L1555 L1561 V1569 V1570 F1571 K1572 D1573 L1574 R1575 I1576 T1577 L1590 I1594 V1600 Y1603 P1607 R1610 L1611 L1614 R1619 D1637 L1652 A1658 H1661
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E2200 I2203 Q2210 K2213 D2216 F2217 I2230 L2231 E2238 R2244 L2251 T2252 K2253 V2256 E2257 I2260 F2265 P2271 I2275 F2276 Q2277 I2278 N2282 C2286 D2320 A2324 N2327 L2330 T2335 V2355 T2359 A2364 D2372 G2373 E2374
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V3056

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.537	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	330.4, 330.4, 330.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, 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	E	0.22	0/54	0.45	0/73
1	F	0.24	0/54	0.48	0/73
2	A	0.24	0/22409	0.45	0/30274
2	B	0.24	0/22409	0.45	0/30274
All	All	0.24	0/44926	0.45	0/60694

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	53	0	51	1	0
1	F	53	0	51	0	0
2	A	22001	0	22171	366	0
2	B	22001	0	22171	342	0
3	A	31	0	13	1	0
3	B	31	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
All	All	44174	0	44470	702	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 8.

All (702) 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:B:1876:HIS:CE1	2:B:1899:CYS:SG	2.73	0.76
2:A:259:LEU:HD21	2:A:286:GLN:HE22	1.51	0.76
2:B:718:CYS:SG	2:B:748:LYS:NZ	2.59	0.76
2:A:954:LEU:HD23	2:A:969:LEU:HD22	1.69	0.75
2:A:1249:ARG:HE	2:A:1275:ILE:HG13	1.54	0.71
2:B:1175:ALA:HA	2:B:1178:LYS:HE2	1.73	0.70
2:A:991:LEU:HD22	2:A:1041:ALA:HB1	1.73	0.70
2:B:1111:LEU:HB2	2:B:1116:GLN:HE21	1.57	0.70
2:A:301:GLY:HA2	2:A:656:THR:HG21	1.73	0.69
2:A:1289:LYS:O	2:A:1293:ASN:ND2	2.24	0.69
2:B:957:GLU:HB2	2:B:999:LYS:HD3	1.74	0.69
2:A:1158:ILE:HG21	2:A:1176:LEU:HD13	1.73	0.69
2:B:1737:LEU:O	2:B:1741:LEU:HB2	1.93	0.69
2:A:2231:LEU:HB3	2:A:2251:LEU:HD12	1.75	0.69
2:B:1158:ILE:HG21	2:B:1176:LEU:HD13	1.74	0.68
2:A:1211:ALA:HA	2:A:1214:LEU:HD23	1.76	0.68
2:B:2231:LEU:HB3	2:B:2251:LEU:HD12	1.75	0.68
2:A:1719:ASN:ND2	2:A:1760:MET:SD	2.66	0.68
2:A:217:ILE:HG21	2:A:258:ILE:HG23	1.74	0.67
2:B:301:GLY:HA2	2:B:656:THR:HG21	1.75	0.67
2:A:927:LEU:HD12	2:A:950:LEU:HD11	1.77	0.67
2:A:1257:PRO:HG2	2:A:1289:LYS:HD3	1.78	0.66
2:A:1292:VAL:HG11	2:A:1346:GLU:HB2	1.78	0.66
2:B:1158:ILE:HG12	2:B:1176:LEU:HB2	1.77	0.66
2:B:1754:LYS:HA	2:B:1761:LEU:HD21	1.77	0.66
2:A:1341:PRO:HA	2:A:1344:VAL:HG12	1.78	0.65
2:A:2147:LEU:HD21	2:A:2182:LEU:HD23	1.78	0.65
2:A:2477:GLY:O	2:A:2515:LYS:NZ	2.30	0.65
2:A:1953:THR:HG22	2:A:2842:PRO:HG2	1.77	0.65
2:B:1953:THR:HG22	2:B:2842:PRO:HG2	1.78	0.64
2:B:2147:LEU:HD21	2:B:2182:LEU:HD23	1.79	0.64
2:A:395:VAL:O	2:A:399:HIS:ND1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2443:ARG:NH1	2:B:2899:ILE:O	2.30	0.64
2:B:1091:GLU:O	2:B:1094:ASN:ND2	2.30	0.64
2:B:485:ASN:OD1	2:B:486:LYS:N	2.31	0.64
2:A:2899:ILE:O	2:B:2443:ARG:NH1	2.31	0.64
2:B:2477:GLY:O	2:B:2515:LYS:NZ	2.30	0.64
2:A:957:GLU:HB2	2:A:999:LYS:HD3	1.78	0.63
2:B:473:GLU:OE1	2:B:476:GLN:NE2	2.31	0.63
2:A:1652:LEU:HD21	2:A:2163:LEU:HG	1.81	0.63
2:B:495:ILE:HG21	2:B:526:LEU:HD11	1.80	0.63
2:B:1652:LEU:HD21	2:B:2163:LEU:HG	1.81	0.63
2:A:1190:VAL:O	2:A:1194:LEU:HG	1.98	0.62
2:B:273:ASP:OD1	2:B:274:SER:N	2.32	0.62
2:A:473:GLU:OE1	2:A:476:GLN:NE2	2.33	0.62
2:A:653:LEU:HD13	2:A:659:LYS:HD3	1.81	0.62
2:A:1322:LEU:HD13	2:A:1327:LEU:HD13	1.80	0.62
2:A:1320:ASP:HA	2:A:1323:LYS:HD3	1.82	0.62
2:B:1901:LEU:HB2	2:B:1906:GLN:HE22	1.64	0.62
2:A:908:VAL:HG23	2:A:920:ALA:HB1	1.80	0.62
2:B:980:TYR:HB3	2:B:986:VAL:HG11	1.82	0.62
2:B:895:LEU:HD23	2:B:898:LEU:HD21	1.81	0.62
2:B:1036:PHE:HA	2:B:1039:ARG:HE	1.65	0.62
2:A:273:ASP:OD1	2:A:274:SER:N	2.33	0.62
2:A:2693:ALA:HB3	2:A:2699:PRO:HG2	1.82	0.61
2:A:2859:SER:HB2	2:A:2887:HIS:HE2	1.64	0.61
2:B:512:ILE:HG21	2:B:545:ALA:HA	1.83	0.61
2:A:695:LEU:O	2:A:699:GLU:HG2	2.01	0.60
2:A:1405:LEU:HD12	2:A:1452:ASP:HB3	1.82	0.60
2:A:1876:HIS:CE1	2:A:1899:CYS:SG	2.93	0.60
2:B:2238:GLU:O	2:B:2244:ARG:NH2	2.35	0.60
2:B:2693:ALA:HB3	2:B:2699:PRO:HG2	1.82	0.60
2:A:952:LYS:HD3	2:A:993:HIS:CD2	2.37	0.60
2:B:698:SER:HB2	2:B:748:LYS:HG3	1.83	0.60
2:B:1180:VAL:HG11	2:B:1238:LEU:HD21	1.84	0.59
2:A:2238:GLU:O	2:A:2244:ARG:NH2	2.35	0.59
2:B:445:GLN:NE2	2:B:447:ARG:O	2.35	0.59
2:A:445:GLN:NE2	2:A:447:ARG:O	2.35	0.59
2:A:1095:ARG:HE	2:A:1100:THR:HG21	1.66	0.59
2:B:329:ARG:NH2	2:B:407:PHE:O	2.34	0.59
2:A:2870:ASP:O	2:A:2871:ARG:NH1	2.35	0.59
2:B:695:LEU:O	2:B:699:GLU:HG2	2.03	0.59
2:A:1806:ILE:HD11	2:A:1835:THR:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:983:ASP:HB3	2:A:986:VAL:HG12	1.85	0.59
2:B:1294:ILE:HG23	2:B:1315:ALA:HB1	1.84	0.59
2:B:1443:HIS:HB2	2:B:1493:LEU:HD21	1.84	0.59
2:B:1190:VAL:O	2:B:1194:LEU:HD23	2.03	0.59
2:B:217:ILE:HG21	2:B:258:ILE:HG23	1.83	0.59
2:B:2101:GLN:HA	2:B:2104:TRP:CD1	2.38	0.59
2:A:483:LEU:HA	2:A:486:LYS:HD2	1.84	0.58
2:A:509:GLY:HA2	2:A:544:LEU:HD11	1.84	0.58
2:A:2101:GLN:HA	2:A:2104:TRP:CD1	2.38	0.58
2:A:1257:PRO:HG3	2:A:1286:CYS:HB3	1.85	0.58
2:A:1513:LEU:HB3	2:A:1517:LEU:HD22	1.85	0.58
2:B:1524:LEU:HD12	2:B:1538:VAL:HG22	1.85	0.58
2:A:2717:LYS:HD2	2:A:2722:LEU:HD21	1.86	0.58
2:B:2909:ARG:NH2	2:B:3056:VAL:O	2.36	0.58
2:B:618:LYS:HG2	2:B:683:HIS:HD2	1.68	0.58
2:A:2909:ARG:NH2	2:A:3056:VAL:O	2.36	0.58
2:B:1211:ALA:HA	2:B:1214:LEU:HD23	1.85	0.58
2:B:1867:GLN:NE2	2:B:1937:ASN:OD1	2.37	0.58
2:A:226:SER:HA	2:A:229:LEU:HD23	1.86	0.57
2:A:1053:ASP:OD1	2:A:1057:LYS:NZ	2.37	0.57
2:B:1600:VAL:HG13	2:B:1610:ARG:HH12	1.69	0.57
2:B:618:LYS:HG2	2:B:683:HIS:CD2	2.39	0.57
2:B:1155:LEU:HD11	2:B:1193:VAL:HG21	1.86	0.57
2:A:1834:LYS:HG3	2:A:1837:PHE:H	1.68	0.57
2:B:1404:ILE:HD12	2:B:1407:ILE:HD11	1.86	0.57
2:A:1600:VAL:HG13	2:A:1610:ARG:HH12	1.69	0.57
2:A:547:THR:HG22	2:A:624:MET:HB3	1.87	0.57
2:A:1314:THR:HA	2:A:1317:LYS:HG2	1.86	0.57
2:B:2717:LYS:HD2	2:B:2722:LEU:HD21	1.87	0.57
2:A:941:SER:O	2:A:945:HIS:ND1	2.30	0.57
2:B:1207:GLU:OE2	2:B:1240:ASN:ND2	2.38	0.57
2:A:2717:LYS:HG2	2:A:2720:ASP:HB2	1.85	0.57
2:B:1460:ALA:HA	2:B:1766:PRO:HB3	1.85	0.57
2:B:2717:LYS:HG2	2:B:2720:ASP:HB2	1.87	0.57
2:A:212:PHE:HD1	2:A:215:LYS:HZ1	1.51	0.57
2:A:1460:ALA:HB2	2:A:1766:PRO:HB3	1.87	0.56
2:B:146:LEU:HA	2:B:150:LEU:HB2	1.87	0.56
2:B:1053:ASP:OD1	2:B:1057:LYS:NZ	2.36	0.56
2:B:456:LEU:HB3	2:B:507:LEU:HD11	1.87	0.56
2:B:2832:ARG:NH1	2:B:2916:ASP:OD2	2.37	0.56
2:A:199:CYS:HB2	2:A:242:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ASP:HB3	2:B:986:VAL:HG12	1.87	0.56
2:B:1463:PHE:HE1	2:B:1466:ARG:HH21	1.52	0.56
2:B:1191:LYS:NZ	2:B:1237:ILE:O	2.31	0.56
2:B:663:LEU:HB2	2:B:1200:THR:HG21	1.87	0.56
2:B:1110:ALA:HB3	2:B:1372:LEU:HD21	1.88	0.56
2:A:1046:LEU:HD23	2:A:1049:LEU:HD21	1.87	0.56
2:A:1180:VAL:HG11	2:A:1238:LEU:HD21	1.87	0.56
2:A:1443:HIS:HB2	2:A:1493:LEU:HD21	1.88	0.56
2:B:609:GLU:HG2	2:B:724:GLY:HA3	1.87	0.56
2:A:679:GLY:N	2:A:732:MET:SD	2.78	0.55
2:A:1753:TYR:OH	2:A:1758:ASP:OD2	2.23	0.55
2:B:1513:LEU:HB3	2:B:1517:LEU:HD22	1.89	0.55
2:A:606:LEU:HB3	2:A:610:LYS:HE3	1.86	0.55
2:B:609:GLU:HG3	2:B:721:LEU:HD12	1.88	0.55
2:A:146:LEU:HD11	2:A:190:ILE:HG13	1.89	0.55
2:A:1235:PRO:HB2	2:A:1238:LEU:HD23	1.89	0.55
2:A:1243:ASN:OD1	2:A:1244:ILE:N	2.38	0.55
2:B:1075:THR:HA	2:B:1078:LEU:HD13	1.89	0.55
2:B:1292:VAL:HG11	2:B:1346:GLU:HB2	1.89	0.55
2:B:2639:LYS:O	2:B:2642:ARG:NH1	2.40	0.55
2:B:1542:LEU:HB3	2:B:1574:LEU:HD21	1.88	0.55
2:A:991:LEU:HA	2:A:994:VAL:HG12	1.89	0.54
2:B:1540:ASP:HA	2:B:1543:LYS:HE3	1.89	0.54
2:A:1098:GLN:HG3	2:A:1100:THR:HG23	1.89	0.54
2:A:2639:LYS:O	2:A:2642:ARG:NH1	2.40	0.54
2:B:226:SER:HA	2:B:229:LEU:HD23	1.88	0.54
2:B:2468:GLU:OE2	2:B:2472:ASN:ND2	2.39	0.54
2:A:2832:ARG:NH1	2:A:2916:ASP:OD2	2.37	0.54
2:B:341:VAL:HB	2:B:346:ILE:HD11	1.89	0.54
2:A:2377:ASP:HA	2:A:2380:ARG:HG2	1.90	0.54
2:A:2468:GLU:OE2	2:A:2472:ASN:ND2	2.40	0.54
2:B:1753:TYR:OH	2:B:1758:ASP:OD2	2.25	0.54
2:A:66:LYS:HA	2:A:69:GLN:HG2	1.88	0.54
2:A:2401:ILE:HG21	2:A:2459:ARG:HB2	1.90	0.54
2:B:66:LYS:HA	2:B:69:GLN:HG2	1.89	0.54
2:A:1524:LEU:HD12	2:A:1538:VAL:HG22	1.89	0.54
2:B:140:ASP:O	2:B:144:ILE:HD12	2.07	0.54
2:A:329:ARG:NH2	2:A:407:PHE:O	2.36	0.54
2:A:895:LEU:HD23	2:A:898:LEU:HD21	1.90	0.54
2:A:2656:LEU:HD21	2:A:2659:LEU:HD11	1.90	0.54
2:B:146:LEU:HD11	2:B:190:ILE:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2401:ILE:HG21	2:B:2459:ARG:HB2	1.89	0.54
2:B:212:PHE:HD1	2:B:215:LYS:HZ1	1.54	0.54
2:A:2699:PRO:HB2	2:A:2715:LEU:HD11	1.90	0.54
2:B:818:ILE:HG13	2:B:900:MET:HE3	1.90	0.54
2:B:2191:ARG:NH1	2:B:2192:SER:O	2.41	0.54
2:B:1524:LEU:HA	2:B:1527:LEU:HD13	1.90	0.53
2:B:1719:ASN:ND2	2:B:1760:MET:SD	2.79	0.53
2:A:1287:PHE:HZ	2:A:1332:ILE:HG13	1.73	0.53
2:A:2516:PHE:HD1	2:A:2519:LEU:HD11	1.73	0.53
2:B:2600:GLU:OE2	2:B:2604:ARG:NE	2.41	0.53
2:A:1421:ALA:O	2:A:1424:GLU:HG2	2.08	0.53
2:B:1419:LEU:HD13	2:B:1422:ILE:HD11	1.89	0.53
2:B:1843:PRO:HD3	2:B:1912:VAL:HG22	1.89	0.53
2:A:1128:GLN:HB3	2:A:1132:ARG:HH21	1.74	0.53
2:B:1289:LYS:O	2:B:1293:ASN:ND2	2.38	0.53
2:A:140:ASP:O	2:A:144:ILE:HD12	2.08	0.53
2:A:695:LEU:HD13	2:A:748:LYS:HD3	1.90	0.53
2:B:2516:PHE:HD1	2:B:2519:LEU:HD11	1.73	0.53
2:A:1158:ILE:HG12	2:A:1176:LEU:HB2	1.91	0.53
2:B:1320:ASP:HA	2:B:1323:LYS:HD3	1.91	0.53
2:A:146:LEU:HA	2:A:150:LEU:HB2	1.90	0.53
2:A:2600:GLU:OE2	2:A:2604:ARG:NE	2.42	0.53
2:B:319:LEU:HD21	2:B:348:LEU:HD23	1.91	0.53
2:B:1046:LEU:HD23	2:B:1049:LEU:HD21	1.90	0.53
2:B:2327:ASN:HB3	2:B:2330:LEU:HD23	1.91	0.53
2:A:902:LYS:HZ3	2:A:953:GLU:HG2	1.74	0.53
2:A:1540:ASP:HA	2:A:1543:LYS:HE3	1.91	0.53
2:B:2256:VAL:O	2:B:2260:ILE:HD12	2.09	0.53
2:B:2723:ARG:HH21	2:B:2957:LEU:HA	1.74	0.53
2:A:1173:LEU:HG	2:A:1217:LEU:HD21	1.90	0.52
2:B:445:GLN:HB3	2:B:451:ARG:HH21	1.74	0.52
2:B:2693:ALA:HB2	2:B:2701:ILE:HD11	1.91	0.52
2:A:530:SER:HA	2:A:533:ARG:HH22	1.74	0.52
2:A:1194:LEU:HD11	2:A:1238:LEU:HD12	1.90	0.52
2:A:2939:ARG:O	2:A:2942:GLN:NE2	2.24	0.52
2:B:2656:LEU:HD21	2:B:2659:LEU:HD11	1.91	0.52
2:B:2699:PRO:HB2	2:B:2715:LEU:HD11	1.91	0.52
2:A:1404:ILE:HD12	2:A:1407:ILE:HD11	1.90	0.52
2:A:2492:LEU:HD22	2:A:2526:ARG:HG3	1.92	0.52
2:B:280:ILE:HG23	2:B:348:LEU:HD22	1.90	0.52
2:A:975:ASN:OD1	2:A:976:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1023:GLY:HA2	2:B:1061:LEU:HD12	1.91	0.52
2:B:2377:ASP:HA	2:B:2380:ARG:HG2	1.90	0.52
2:A:1351:LEU:HB3	2:A:1441:ILE:HG12	1.92	0.52
2:A:1754:LYS:HA	2:A:1761:LEU:HD21	1.90	0.52
2:A:341:VAL:HB	2:A:346:ILE:HD11	1.91	0.52
2:A:2421:LYS:HD2	2:A:2445:LEU:HD11	1.92	0.52
2:B:2200:GLU:HA	2:B:2203:ILE:HG12	1.91	0.52
2:B:2421:LYS:HD2	2:B:2445:LEU:HD11	1.91	0.52
2:A:280:ILE:HG23	2:A:348:LEU:HD22	1.90	0.52
2:B:1346:GLU:HA	2:B:1349:MET:HG3	1.92	0.52
2:A:1207:GLU:OE2	2:A:1240:ASN:ND2	2.42	0.52
2:B:2492:LEU:HD22	2:B:2526:ARG:HG3	1.92	0.52
2:A:2327:ASN:HB3	2:A:2330:LEU:HD23	1.90	0.52
2:B:63:PHE:HD1	2:B:66:LYS:HZ3	1.58	0.52
2:B:221:ARG:HA	2:B:265:ILE:HD11	1.92	0.52
2:B:975:ASN:OD1	2:B:976:VAL:N	2.42	0.52
2:A:1259:LEU:HD11	2:A:1268:VAL:HB	1.91	0.51
2:B:510:ALA:O	2:B:513:GLN:HB3	2.09	0.51
2:B:781:GLN:HB3	2:B:785:ARG:HH12	1.74	0.51
2:A:1265:PHE:HA	2:A:1268:VAL:HG12	1.91	0.51
2:A:1349:MET:HA	2:A:1441:ILE:HD13	1.91	0.51
2:A:2693:ALA:HB2	2:A:2701:ILE:HD11	1.92	0.51
2:B:2007:GLU:OE1	2:B:2010:ARG:NH2	2.39	0.51
2:A:484:TRP:CD1	2:A:516:LEU:HD23	2.46	0.51
2:A:2200:GLU:HA	2:A:2203:ILE:HG12	1.90	0.51
2:B:1216:TYR:HA	2:B:1378:PRO:HG3	1.91	0.51
2:A:1955:LEU:HB2	2:A:2008:ILE:HG21	1.93	0.51
2:A:2007:GLU:OE1	2:A:2010:ARG:NH2	2.38	0.51
2:B:1571:PHE:HD2	2:B:1574:LEU:HD22	1.76	0.51
2:A:309:ARG:HA	2:A:312:LEU:HD12	1.92	0.51
2:A:599:LEU:HD21	2:A:714:THR:HB	1.92	0.51
2:A:2400:ARG:HD2	2:B:3024:THR:HA	1.91	0.51
2:A:3024:THR:HA	2:B:2400:ARG:HD2	1.91	0.51
2:A:1843:PRO:HD3	2:A:1912:VAL:HG22	1.93	0.51
2:B:2829:PRO:HG3	2:B:2912:ARG:HB3	1.93	0.51
2:A:1061:LEU:HD21	2:A:1073:VAL:HG21	1.91	0.51
2:B:1341:PRO:HA	2:B:1344:VAL:HG22	1.93	0.51
2:A:1110:ALA:HB3	2:A:1372:LEU:HD21	1.93	0.51
2:B:1346:GLU:O	2:B:1350:THR:HG23	2.11	0.51
2:B:199:CYS:HB2	2:B:242:THR:HG21	1.93	0.51
2:B:414:GLN:HG2	2:B:457:ARG:HH22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1552:ASN:HB2	2:B:1555:LEU:HB2	1.93	0.51
2:A:436:LEU:HD22	2:A:483:LEU:HB3	1.93	0.51
2:B:1955:LEU:HB2	2:B:2008:ILE:HG21	1.93	0.51
2:A:2256:VAL:O	2:A:2260:ILE:HD12	2.10	0.50
2:B:775:SER:O	2:B:779:MET:HG2	2.12	0.50
2:A:1685:THR:HG23	2:A:2166:VAL:HG21	1.94	0.50
2:A:2872:HIS:CE1	2:A:2874:GLN:HB2	2.46	0.50
2:B:440:SER:HB3	2:B:487:ILE:HD11	1.94	0.50
2:B:2381:ASN:OD1	2:B:2382:GLY:N	2.44	0.50
2:A:145:LEU:HA	2:A:149:ILE:HD13	1.93	0.50
2:A:424:PRO:O	2:A:469:ARG:NH2	2.44	0.50
2:A:2147:LEU:HD22	2:A:2179:ILE:HG23	1.92	0.50
2:A:2723:ARG:HH21	2:A:2957:LEU:HA	1.76	0.50
2:B:1267:GLU:O	2:B:1271:ILE:HG12	2.10	0.50
2:A:955:PRO:HA	2:A:961:LEU:HD11	1.94	0.50
2:A:1170:LYS:HE2	2:A:1377:ASN:HA	1.93	0.50
2:A:927:LEU:HD13	2:A:930:LEU:HD12	1.94	0.50
2:A:1215:ASP:OD1	2:A:1216:TYR:N	2.45	0.50
2:A:1901:LEU:HB2	2:A:1906:GLN:HE22	1.77	0.50
2:A:111:ARG:HB2	2:A:114:ARG:HH12	1.77	0.49
2:A:451:ARG:HA	2:A:454:TYR:HD2	1.76	0.49
2:A:2381:ASN:OD1	2:A:2382:GLY:N	2.44	0.49
2:A:445:GLN:HB3	2:A:451:ARG:HH21	1.76	0.49
2:A:1216:TYR:HA	2:A:1378:PRO:HG3	1.92	0.49
2:A:1552:ASN:HB2	2:A:1555:LEU:HB2	1.93	0.49
2:A:1590:LEU:O	2:A:1594:ILE:HG12	2.12	0.49
2:A:781:GLN:HB3	2:A:785:ARG:HH12	1.76	0.49
2:B:920:ALA:HA	2:B:923:ILE:HD12	1.94	0.49
2:A:1078:LEU:HD11	2:A:1157:LEU:HD11	1.94	0.49
2:B:1412:PRO:HB3	2:B:1460:ALA:HB2	1.93	0.49
2:A:1420:LEU:HG	2:A:1734:VAL:HG11	1.95	0.49
2:A:259:LEU:HD21	2:A:286:GLN:NE2	2.22	0.49
2:A:657:PHE:CE2	2:A:1155:LEU:HD23	2.48	0.49
2:B:1837:PHE:HA	2:B:1840:THR:HG22	1.95	0.49
2:B:2859:SER:HB2	2:B:2887:HIS:HE2	1.78	0.49
2:B:2872:HIS:CE1	2:B:2874:GLN:HB2	2.47	0.49
2:A:1256:ILE:O	2:A:1260:VAL:HG23	2.13	0.49
2:A:1294:ILE:HG23	2:A:1315:ALA:HB1	1.94	0.49
2:B:1204:ARG:HG2	2:B:1205:ARG:HG3	1.94	0.49
2:A:2485:PHE:HZ	2:A:2518:PRO:HB2	1.79	0.48
2:A:3004:LYS:NZ	2:B:2437:TYR:OH	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:SER:O	2:B:710:THR:OG1	2.31	0.48
2:A:319:LEU:HD21	2:A:348:LEU:HD23	1.95	0.48
2:A:1230:ASN:H	2:A:1233:SER:HG	1.61	0.48
2:A:1680:PRO:HG3	2:A:2174:SER:HB2	1.96	0.48
2:A:1764:LEU:HA	2:A:1767:PHE:HD2	1.78	0.48
2:A:2870:ASP:HB2	2:A:2892:VAL:HG22	1.95	0.48
2:B:1261:ILE:HG22	2:B:1294:ILE:HD11	1.95	0.48
2:A:245:VAL:HG22	2:A:1083:HIS:HB3	1.95	0.48
2:A:815:ILE:HA	2:A:818:ILE:HG12	1.95	0.48
2:B:1685:THR:HG23	2:B:2166:VAL:HG21	1.95	0.48
2:A:2051:LEU:HD21	2:B:2276:PHE:HB2	1.94	0.48
2:B:1590:LEU:O	2:B:1594:ILE:HG12	2.13	0.48
2:B:1760:MET:HA	2:B:1763:TYR:HD2	1.78	0.48
2:B:2068:LEU:HB2	2:B:2077:LEU:HD12	1.95	0.48
2:A:1346:GLU:HA	2:A:1349:MET:HG3	1.94	0.48
2:B:145:LEU:HA	2:B:149:ILE:HD13	1.95	0.48
2:B:1457:LEU:H	2:B:1461:TRP:HB3	1.78	0.48
2:A:1318:VAL:HG22	2:A:1321:MET:HE2	1.95	0.48
2:A:1436:HIS:HA	2:A:1439:LEU:HG	1.96	0.48
2:B:1387:LYS:O	2:B:1387:LYS:NZ	2.41	0.48
2:B:1416:GLN:HE22	2:B:1420:LEU:HD12	1.79	0.48
2:A:599:LEU:O	2:A:717:ARG:NE	2.47	0.48
2:A:791:THR:HG21	2:A:958:GLU:HG2	1.95	0.48
2:A:948:LEU:HB3	2:A:993:HIS:ND1	2.28	0.48
2:A:432:LEU:HD21	2:A:472:LEU:HD21	1.96	0.48
2:A:812:MET:HA	2:A:815:ILE:HG22	1.95	0.48
2:A:1055:TYR:HB2	2:A:1057:LYS:HZ1	1.79	0.48
2:B:111:ARG:HB2	2:B:114:ARG:HH12	1.79	0.48
2:B:230:ASN:OD1	2:B:231:HIS:N	2.46	0.48
2:B:815:ILE:HA	2:B:818:ILE:HG12	1.96	0.48
2:B:1219:LEU:HD23	2:B:1378:PRO:HB2	1.95	0.48
2:A:411:PRO:O	2:A:415:ILE:HG12	2.14	0.48
2:A:488:TRP:CG	2:A:517:VAL:HG11	2.49	0.48
2:A:1405:LEU:O	2:A:1415:TYR:OH	2.32	0.48
2:A:2081:LEU:HD21	2:A:2099:HIS:HA	1.96	0.48
2:A:2276:PHE:HB2	2:B:2051:LEU:HD21	1.95	0.48
2:B:250:ARG:HH11	2:B:253:GLU:HG3	1.79	0.48
2:A:230:ASN:OD1	2:A:231:HIS:N	2.46	0.47
2:A:780:MET:HA	2:A:783:CYS:SG	2.54	0.47
2:A:2012:ILE:HG23	2:A:2014:GLU:H	1.79	0.47
2:A:2829:PRO:HG3	2:A:2912:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1932:PHE:CZ	2:B:1964:LYS:HB2	2.49	0.47
2:B:543:THR:O	2:B:547:THR:HG23	2.14	0.47
2:B:721:LEU:O	2:B:725:VAL:HG23	2.15	0.47
2:B:1498:LEU:HA	2:B:1501:VAL:HG22	1.96	0.47
2:B:2713:ARG:HB3	2:B:2769:TRP:HB3	1.97	0.47
2:A:109:ASN:ND2	2:A:148:ASP:OD2	2.47	0.47
2:A:1129:GLU:HA	2:A:1132:ARG:HG2	1.96	0.47
2:A:1513:LEU:HD22	2:A:1517:LEU:HD13	1.96	0.47
2:A:2335:THR:HG23	2:A:2364:ALA:HB1	1.96	0.47
2:B:209:PHE:O	2:B:212:PHE:HB2	2.14	0.47
2:B:427:LEU:O	2:B:469:ARG:NH2	2.45	0.47
2:B:2253:LYS:O	2:B:2257:GLU:HG2	2.14	0.47
2:A:63:PHE:HD1	2:A:66:LYS:HZ3	1.62	0.47
2:B:1342:GLU:N	2:B:1342:GLU:OE1	2.45	0.47
2:B:1680:PRO:HG3	2:B:2174:SER:HB2	1.96	0.47
2:A:963:MET:HA	2:A:966:VAL:HG22	1.97	0.47
2:B:2485:PHE:HZ	2:B:2518:PRO:HB2	1.78	0.47
2:A:1030:LYS:O	2:A:1032:ARG:NH1	2.48	0.47
2:A:1870:PHE:HD1	2:A:1944:VAL:HG21	1.77	0.47
2:B:1129:GLU:HA	2:B:1132:ARG:HG2	1.97	0.47
2:B:1819:THR:OG1	2:B:1825:GLN:OE1	2.30	0.47
2:B:2012:ILE:HG23	2:B:2014:GLU:H	1.80	0.47
2:B:2147:LEU:HD13	2:B:2183:GLU:HG2	1.97	0.47
2:A:512:ILE:HG21	2:A:545:ALA:HA	1.97	0.47
2:A:2147:LEU:HD13	2:A:2183:GLU:HG2	1.95	0.47
2:B:1834:LYS:HG3	2:B:1837:PHE:H	1.80	0.47
2:B:1921:ARG:HA	2:B:1933:TRP:HZ3	1.80	0.47
2:A:94:MET:HA	2:A:97:ILE:HG12	1.97	0.47
2:A:1921:ARG:HA	2:A:1933:TRP:HZ3	1.78	0.47
3:A:3101:ANP:O2A	3:A:3101:ANP:H8	2.15	0.47
2:B:2870:ASP:O	2:B:2871:ARG:NE	2.48	0.47
2:A:127:THR:HB	2:A:137:TYR:HE2	1.80	0.47
2:A:2713:ARG:HB3	2:A:2769:TRP:HB3	1.96	0.47
2:B:1098:GLN:NE2	2:B:1109:LYS:O	2.45	0.47
2:B:1513:LEU:HD22	2:B:1517:LEU:HD13	1.96	0.47
2:A:2068:LEU:HB2	2:A:2077:LEU:HD12	1.96	0.46
2:B:414:GLN:HG2	2:B:457:ARG:NH2	2.30	0.46
2:B:2081:LEU:HD21	2:B:2099:HIS:HA	1.96	0.46
2:B:2914:ILE:O	2:B:2918:MET:HG3	2.16	0.46
2:A:948:LEU:HD21	2:A:990:ILE:HG22	1.97	0.46
2:B:127:THR:HB	2:B:137:TYR:HE2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:ALA:HA	2:A:23:ARG:HE	1.80	0.46
2:A:685:ASN:OD1	2:A:686:LEU:N	2.49	0.46
2:A:1426:ALA:HB2	2:A:1438:ILE:HD13	1.96	0.46
2:B:951:LEU:HD21	2:B:994:VAL:HG12	1.96	0.46
2:B:1870:PHE:HD1	2:B:1944:VAL:HG21	1.81	0.46
2:A:1023:GLY:HA2	2:A:1061:LEU:HD12	1.98	0.46
2:A:1267:GLU:O	2:A:1271:ILE:HG12	2.15	0.46
2:A:2536:GLY:O	2:A:2539:GLU:HG3	2.15	0.46
2:A:1034:TYR:HB3	2:A:1038:VAL:HB	1.97	0.46
2:B:293:LYS:HG2	2:B:649:GLU:HB3	1.98	0.46
2:B:2216:ASP:OD1	2:B:2217:PHE:N	2.48	0.46
2:B:1466:ARG:O	2:B:1469:ILE:HG22	2.15	0.46
2:B:2805:MET:O	2:B:2809:GLN:HG2	2.16	0.46
2:B:2945:LEU:O	2:B:2949:VAL:HG23	2.15	0.46
2:A:238:ILE:HD12	2:A:241:LYS:HE2	1.97	0.46
2:A:3049:PHE:CD1	2:A:3050:PRO:HD2	2.51	0.46
2:B:1470:TYR:O	2:B:1473:ILE:HG22	2.16	0.46
2:B:2939:ARG:O	2:B:2942:GLN:NE2	2.24	0.46
2:A:2216:ASP:OD1	2:A:2217:PHE:N	2.49	0.46
2:B:537:PRO:HA	2:B:540:CYS:SG	2.56	0.46
2:B:729:TYR:HB3	2:B:735:ILE:HG12	1.98	0.46
2:B:1173:LEU:HG	2:B:1217:LEU:HD21	1.98	0.46
2:B:1287:PHE:HD1	2:B:1290:ILE:HD11	1.81	0.46
2:B:1434:LYS:HA	2:B:1437:ARG:HG2	1.97	0.46
2:B:1705:ASP:HB3	2:B:1708:LEU:HD23	1.98	0.46
2:A:2191:ARG:NH1	2:A:2192:SER:O	2.48	0.46
2:A:3045:LEU:HA	2:A:3048:LEU:HD12	1.97	0.46
2:B:599:LEU:O	2:B:717:ARG:NE	2.43	0.46
2:B:1797:PRO:HD2	2:B:1805:TRP:CD1	2.51	0.46
2:B:3045:LEU:HA	2:B:3048:LEU:HD12	1.98	0.46
2:A:902:LYS:HE3	2:A:949:MET:CE	2.46	0.46
2:B:1561:LEU:HD21	2:B:1600:VAL:HA	1.98	0.46
2:B:2065:ILE:HG23	2:B:2077:LEU:HD11	1.98	0.46
2:B:2147:LEU:HD22	2:B:2179:ILE:HG23	1.98	0.46
2:B:2957:LEU:HD23	2:B:2957:LEU:H	1.81	0.46
2:A:146:LEU:HG	2:A:150:LEU:HD12	1.98	0.45
2:A:1166:PRO:HA	2:A:1169:GLU:HG2	1.98	0.45
2:B:255:GLY:HA3	2:B:286:GLN:NE2	2.31	0.45
2:B:2717:LYS:NZ	3:B:3101:ANP:O2A	2.41	0.45
2:A:1802:HIS:O	2:A:1806:ILE:HG12	2.15	0.45
2:B:2808:VAL:HG21	2:B:2819:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:706:SER:O	2:A:710:THR:OG1	2.34	0.45
2:A:780:MET:HB2	2:A:780:MET:HE2	1.74	0.45
2:A:2253:LYS:O	2:A:2257:GLU:HG2	2.16	0.45
2:A:2914:ILE:O	2:A:2918:MET:HG3	2.17	0.45
2:B:998:VAL:HG11	2:B:1049:LEU:HA	1.97	0.45
2:B:2522:GLN:O	2:B:2526:ARG:HG2	2.16	0.45
2:A:454:TYR:HD1	2:A:457:ARG:HH21	1.63	0.45
2:A:1573:ASP:HA	2:A:1576:ILE:HG12	1.99	0.45
2:B:238:ILE:HD12	2:B:241:LYS:HE2	1.97	0.45
2:B:816:ALA:HB1	2:B:926:LYS:HD3	1.98	0.45
2:B:1349:MET:HA	2:B:1441:ILE:HD13	1.97	0.45
2:B:1574:LEU:HA	2:B:1577:THR:HG22	1.98	0.45
2:B:1684:SER:HB2	2:B:2749:LYS:HD3	1.99	0.45
2:B:2485:PHE:CE1	2:B:2519:LEU:HB3	2.52	0.45
2:B:2522:GLN:HE21	2:B:2951:VAL:HB	1.81	0.45
2:B:2536:GLY:O	2:B:2539:GLU:HG3	2.15	0.45
2:A:924:ARG:CZ	2:A:954:LEU:HD13	2.46	0.45
2:B:1061:LEU:HD21	2:B:1073:VAL:HG21	1.98	0.45
2:B:1076:GLN:HA	2:B:1126:LYS:HE3	1.99	0.45
2:B:3049:PHE:CD1	2:B:3050:PRO:HD2	2.52	0.45
2:A:209:PHE:O	2:A:212:PHE:HB2	2.17	0.45
2:A:761:THR:O	2:A:764:LYS:HG2	2.16	0.45
2:A:791:THR:HA	2:A:797:LYS:HE2	1.98	0.45
2:B:734:VAL:HG12	2:B:735:ILE:HG23	1.98	0.45
2:B:944:LEU:O	2:B:948:LEU:HG	2.16	0.45
2:B:1010:ASN:OD1	2:B:1011:THR:N	2.49	0.45
2:B:1405:LEU:HD12	2:B:1452:ASP:HB3	1.98	0.45
2:B:1450:LEU:HD23	2:B:1504:THR:HG21	1.97	0.45
2:B:2158:MET:HE1	2:B:2169:LEU:HA	1.98	0.45
2:A:433:SER:HB3	2:A:434:PRO:HD3	1.99	0.45
2:A:2945:LEU:O	2:A:2949:VAL:HG23	2.16	0.45
2:B:2955:ASP:OD1	2:B:2955:ASP:N	2.50	0.45
2:A:926:LYS:O	2:A:930:LEU:HG	2.17	0.45
2:A:1600:VAL:HG13	2:A:1610:ARG:HH22	1.82	0.45
2:A:1748:SER:O	2:A:1752:ILE:HG12	2.17	0.45
2:A:3053:LYS:HB3	2:A:3056:VAL:HB	1.99	0.45
2:B:484:TRP:CD1	2:B:516:LEU:HD23	2.51	0.45
2:A:543:THR:O	2:A:547:THR:HG23	2.16	0.45
2:A:657:PHE:HD1	2:A:660:MET:HE1	1.82	0.45
2:A:902:LYS:NZ	2:A:949:MET:O	2.44	0.45
2:A:1002:GLY:HA2	2:A:1058:TRP:HZ2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:MET:HB3	2:B:415:ILE:HD12	1.99	0.45
2:B:530:SER:O	2:B:530:SER:OG	2.32	0.45
2:B:1572:LYS:O	2:B:1575:ARG:HB2	2.17	0.45
2:A:736:ALA:HB3	2:A:739:GLU:HG2	1.99	0.45
2:A:945:HIS:O	2:A:949:MET:HG3	2.17	0.45
2:A:2522:GLN:O	2:A:2526:ARG:HG2	2.17	0.45
2:A:2957:LEU:H	2:A:2957:LEU:HD23	1.82	0.45
2:A:250:ARG:HH11	2:A:253:GLU:HG3	1.82	0.44
2:A:613:VAL:O	2:A:617:MET:HG2	2.17	0.44
2:A:1693:ASP:OD1	2:A:1693:ASP:N	2.49	0.44
2:B:736:ALA:HB3	2:B:739:GLU:HG2	1.99	0.44
2:B:2827:PHE:O	2:B:2912:ARG:NH1	2.50	0.44
2:A:1318:VAL:O	2:A:1322:LEU:HD23	2.17	0.44
2:A:1798:LEU:HD12	2:A:1901:LEU:HD13	1.99	0.44
2:B:274:SER:O	2:B:277:GLU:HG3	2.18	0.44
2:B:1191:LYS:O	2:B:1195:GLU:OE1	2.35	0.44
2:B:1259:LEU:HD23	2:B:1267:GLU:HB3	1.99	0.44
2:B:1693:ASP:OD1	2:B:1693:ASP:N	2.50	0.44
3:B:3101:ANP:N3B	3:B:3101:ANP:O1A	2.50	0.44
2:A:163:GLN:HA	2:A:166:GLU:HG2	1.98	0.44
2:A:662:PHE:CE2	2:A:663:LEU:HD23	2.52	0.44
2:A:1297:TYR:HD2	2:A:1315:ALA:HB2	1.83	0.44
2:A:2808:VAL:HG21	2:A:2819:VAL:HG11	1.99	0.44
2:B:2856:VAL:HG22	2:B:2885:LEU:HD12	1.97	0.44
2:A:926:LYS:HA	2:A:929:MET:HG2	2.00	0.44
2:A:1734:VAL:HG23	2:A:1767:PHE:HE1	1.83	0.44
2:A:1859:ARG:HE	2:A:1935:ASP:H	1.65	0.44
2:B:20:ALA:HA	2:B:23:ARG:HE	1.83	0.44
2:B:1322:LEU:HD13	2:B:1327:LEU:HD13	1.99	0.44
2:A:738:GLU:HG2	2:A:739:GLU:N	2.32	0.44
2:A:952:LYS:HD3	2:A:993:HIS:CG	2.53	0.44
2:A:980:TYR:HB3	2:A:986:VAL:HG11	2.00	0.44
2:B:432:LEU:HD21	2:B:472:LEU:HD21	1.99	0.44
2:A:274:SER:O	2:A:277:GLU:HG3	2.18	0.44
2:A:1319:TYR:CE2	2:A:1323:LYS:HD2	2.52	0.44
2:B:94:MET:HA	2:B:97:ILE:HG12	2.00	0.44
2:B:411:PRO:O	2:B:415:ILE:HG12	2.18	0.44
2:B:1463:PHE:HB2	2:B:1763:TYR:HD1	1.83	0.44
2:B:1573:ASP:OD1	2:B:1573:ASP:N	2.51	0.44
2:B:1748:SER:O	2:B:1752:ILE:HG12	2.17	0.44
2:A:437:MET:SD	2:A:441:GLN:NE2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:616:THR:HA	2:A:686:LEU:HD23	2.00	0.44
2:A:1261:ILE:HD13	2:A:1294:ILE:HG13	1.99	0.44
2:A:1827:LEU:HD23	2:A:1827:LEU:H	1.83	0.44
2:B:694:LEU:O	2:B:697:LEU:HG	2.17	0.44
2:B:1061:LEU:HD23	2:B:1068:PHE:O	2.17	0.44
2:B:1466:ARG:HA	2:B:1469:ILE:HG22	2.00	0.44
2:B:3053:LYS:HB3	2:B:3056:VAL:HB	1.99	0.44
2:A:711:ASN:ND2	2:A:713:GLU:OE2	2.51	0.44
2:A:1931:ALA:O	2:A:1938:TYR:OH	2.29	0.44
2:A:2101:GLN:HE21	2:A:2105:ARG:HH21	1.64	0.44
2:A:2485:PHE:CE1	2:A:2519:LEU:HB3	2.52	0.44
2:A:2805:MET:O	2:A:2809:GLN:HG2	2.17	0.44
2:B:433:SER:HB3	2:B:434:PRO:HD3	2.00	0.44
2:B:1300:TYR:HB2	2:B:1385:VAL:HG13	1.99	0.44
2:B:2210:GLN:HA	2:B:2213:LYS:HG2	1.99	0.44
2:A:1439:LEU:HD13	2:A:1493:LEU:HD22	1.99	0.43
2:A:1932:PHE:CZ	2:A:1964:LYS:HB2	2.53	0.43
2:A:2158:MET:HE1	2:A:2169:LEU:HA	2.00	0.43
2:B:163:GLN:HA	2:B:166:GLU:HG2	1.99	0.43
2:B:245:VAL:HG22	2:B:1083:HIS:HB3	2.00	0.43
3:B:3101:ANP:O2A	3:B:3101:ANP:H8	2.18	0.43
2:A:694:LEU:HD23	2:A:697:LEU:HD21	2.00	0.43
2:A:2856:VAL:HG22	2:A:2885:LEU:HD12	1.99	0.43
2:B:477:LYS:HA	2:B:480:LEU:HG	2.01	0.43
2:B:1149:ASN:O	2:B:1153:VAL:HG23	2.18	0.43
2:B:1176:LEU:O	2:B:1180:VAL:HG23	2.18	0.43
2:B:2101:GLN:HE21	2:B:2105:ARG:HH21	1.64	0.43
2:A:1176:LEU:O	2:A:1180:VAL:HG23	2.17	0.43
2:A:1453:ILE:O	2:A:1453:ILE:HG13	2.18	0.43
2:A:1561:LEU:HD21	2:A:1600:VAL:HA	1.99	0.43
2:A:1705:ASP:HB3	2:A:1708:LEU:HD23	2.00	0.43
2:B:271:LEU:HB3	2:B:276:LYS:HD2	2.01	0.43
2:B:711:ASN:ND2	2:B:713:GLU:OE2	2.51	0.43
2:B:777:ARG:NH1	2:B:778:ASN:OD1	2.41	0.43
2:B:782:LEU:HD23	2:B:785:ARG:HH21	1.83	0.43
2:B:1843:PRO:HB2	2:B:1915:TYR:CD2	2.53	0.43
2:A:1061:LEU:HD23	2:A:1068:PHE:O	2.19	0.43
2:A:1573:ASP:N	2:A:1573:ASP:OD1	2.51	0.43
2:A:1607:PRO:HG2	2:A:1658:ALA:HB2	1.99	0.43
2:A:1789:LEU:HD12	2:A:1858:TRP:HZ3	1.83	0.43
2:B:346:ILE:HG23	2:B:415:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:905:CYS:HB3	2:B:953:GLU:HB3	2.00	0.43
2:B:2624:CYS:O	2:B:2628:ILE:HG12	2.18	0.43
2:B:1158:ILE:HA	2:B:1161:VAL:HG12	1.99	0.43
2:B:2026:MET:SD	2:B:2031:THR:OG1	2.66	0.43
2:A:595:VAL:HB	2:A:599:LEU:HD23	2.00	0.43
2:A:898:LEU:HA	2:A:949:MET:HE3	1.99	0.43
2:A:1204:ARG:HG2	2:A:1205:ARG:HG3	2.01	0.43
2:B:761:THR:O	2:B:764:LYS:HG2	2.18	0.43
2:B:2335:THR:HG23	2:B:2364:ALA:HB1	1.99	0.43
2:B:2829:PRO:O	2:B:2832:ARG:NH1	2.52	0.43
2:A:657:PHE:HD2	2:A:1189:LEU:HD22	1.83	0.43
2:A:904:LEU:HD13	2:A:927:LEU:HD21	2.00	0.43
2:A:1300:TYR:CG	2:A:1385:VAL:HG22	2.54	0.43
2:A:2002:GLN:NE2	2:A:2021:CYS:O	2.52	0.43
2:A:2153:LYS:O	2:A:2156:GLU:HG3	2.19	0.43
2:B:1310:GLN:HE21	2:B:1311:GLN:NE2	2.17	0.43
2:B:1380:HIS:ND1	2:B:1380:HIS:O	2.52	0.43
2:B:2104:TRP:HB3	2:B:2129:TYR:HB2	2.01	0.43
2:B:2153:LYS:O	2:B:2156:GLU:HG3	2.19	0.43
2:B:2157:GLU:HA	2:B:2160:LYS:HE2	2.01	0.43
2:A:530:SER:O	2:A:530:SER:OG	2.33	0.43
2:A:1465:LEU:HA	2:A:1468:VAL:HG22	2.00	0.43
2:A:474:SER:HA	2:A:477:LYS:HG2	2.00	0.43
2:A:1417:LYS:HA	2:A:1420:LEU:HB2	2.00	0.43
2:A:1457:LEU:HD12	2:A:1464:VAL:HG21	2.00	0.43
2:A:2065:ILE:HG23	2:A:2077:LEU:HD11	1.99	0.43
2:A:2829:PRO:O	2:A:2832:ARG:NH1	2.51	0.43
2:A:2955:ASP:N	2:A:2955:ASP:OD1	2.51	0.43
2:B:1869:PHE:CE2	2:B:1909:MET:HG3	2.53	0.43
1:E:15:SER:HB3	2:A:2872:HIS:HE2	1.83	0.43
2:A:944:LEU:O	2:A:948:LEU:HG	2.18	0.43
2:A:1283:LEU:HD23	2:A:1328:LEU:HD23	2.01	0.43
2:A:1821:CYS:HB2	2:A:1824:LEU:HB2	2.00	0.43
2:A:2404:TYR:HB2	2:B:3023:GLY:HA3	2.01	0.43
2:B:93:LYS:HA	2:B:96:GLU:CD	2.39	0.43
2:B:748:LYS:HZ3	2:B:752:LEU:HD21	1.84	0.43
2:B:750:LYS:HB2	2:B:750:LYS:HE3	1.86	0.43
2:B:1082:HIS:HB3	2:B:1085:VAL:HG23	2.00	0.43
2:A:445:GLN:HB3	2:A:451:ARG:NH2	2.34	0.42
2:A:795:PRO:HA	2:A:798:ILE:HD12	2.01	0.42
2:A:946:MET:HA	2:A:949:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1952:PHE:CD1	2:A:2843:ALA:HA	2.54	0.42
2:B:685:ASN:OD1	2:B:686:LEU:N	2.52	0.42
2:B:1952:PHE:CD1	2:B:2843:ALA:HA	2.54	0.42
2:A:618:LYS:HA	2:A:683:HIS:NE2	2.35	0.42
2:A:662:PHE:O	2:A:663:LEU:HG	2.20	0.42
2:A:1571:PHE:HD2	2:A:1574:LEU:HD22	1.84	0.42
2:A:1938:TYR:HB2	2:A:1961:TYR:HB2	2.01	0.42
2:A:2624:CYS:O	2:A:2628:ILE:HG12	2.19	0.42
2:A:3012:ARG:HD2	2:A:3012:ARG:HA	1.91	0.42
2:B:109:ASN:ND2	2:B:148:ASP:OD2	2.51	0.42
2:B:709:ILE:HG13	2:B:710:THR:N	2.35	0.42
2:B:956:GLY:N	2:B:1000:ASN:OD1	2.53	0.42
2:A:535:SER:H	2:A:538:ALA:HB3	1.84	0.42
2:A:1192:LYS:HA	2:A:1195:GLU:CD	2.39	0.42
2:A:1310:GLN:HE21	2:A:1311:GLN:NE2	2.17	0.42
2:A:2104:TRP:HB3	2:A:2129:TYR:HB2	2.02	0.42
2:B:146:LEU:HG	2:B:150:LEU:HD12	2.01	0.42
2:B:525:LYS:O	2:B:528:THR:OG1	2.29	0.42
2:B:1827:LEU:HD23	2:B:1827:LEU:H	1.84	0.42
2:B:1932:PHE:HZ	2:B:1964:LYS:HB2	1.85	0.42
2:A:570:PHE:N	2:A:573:LYS:HZ3	2.18	0.42
2:A:1174:PHE:HZ	2:A:1224:LEU:HD11	1.85	0.42
2:A:1566:PRO:HA	2:A:1575:ARG:HH21	1.84	0.42
2:A:1737:LEU:O	2:A:1741:LEU:HB2	2.19	0.42
2:B:1174:PHE:HE1	2:B:1221:TRP:CD1	2.38	0.42
2:B:1519:VAL:HG13	2:B:1520:ILE:HD12	2.02	0.42
2:A:609:GLU:HG3	2:A:721:LEU:HD12	2.01	0.42
2:A:632:GLU:HA	2:A:792:LYS:HE3	2.01	0.42
2:A:924:ARG:O	2:A:928:LEU:HG	2.20	0.42
2:A:1010:ASN:OD1	2:A:1011:THR:N	2.53	0.42
2:A:2522:GLN:HE21	2:A:2951:VAL:HB	1.84	0.42
2:B:398:ASP:O	2:B:402:LYS:HG2	2.20	0.42
2:B:1227:THR:O	2:B:1230:ASN:ND2	2.53	0.42
2:B:1611:LEU:HA	2:B:1614:LEU:HD12	2.02	0.42
2:A:439:LEU:HB3	2:A:459:LEU:HD21	2.02	0.42
2:A:472:LEU:HD13	2:A:480:LEU:HD21	2.02	0.42
2:B:505:PHE:HD2	2:B:537:PRO:HB2	1.84	0.42
2:B:1170:LYS:HE2	2:B:1377:ASN:HA	2.01	0.42
2:B:2271:PRO:O	2:B:2275:ILE:HG12	2.18	0.42
2:A:1916:MET:HA	2:A:1919:GLN:HG2	2.02	0.42
2:B:429:ASN:HA	2:B:432:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1030:LYS:O	2:B:1032:ARG:NH1	2.53	0.42
2:B:2002:GLN:NE2	2:B:2021:CYS:O	2.52	0.42
2:A:93:LYS:HA	2:A:96:GLU:CD	2.39	0.42
2:A:1684:SER:HB2	2:A:2749:LYS:HD3	2.01	0.42
2:A:2091:TRP:HZ3	2:A:2095:LEU:HD23	1.85	0.42
2:B:1257:PRO:O	2:B:1261:ILE:HG23	2.20	0.42
2:B:1448:LEU:O	2:B:1451:LYS:HG2	2.20	0.42
2:A:429:ASN:HA	2:A:432:LEU:HD23	2.00	0.41
2:A:1869:PHE:CE2	2:A:1909:MET:HG3	2.55	0.41
2:A:2197:GLN:O	2:A:2200:GLU:HG2	2.20	0.41
2:B:263:LEU:HD12	2:B:318:LEU:HD22	2.02	0.41
2:B:1012:ARG:HA	2:B:1015:GLN:HG2	2.02	0.41
2:B:1143:THR:HA	2:B:1146:GLU:OE2	2.19	0.41
2:B:1569:VAL:O	2:B:1572:LYS:HG3	2.19	0.41
2:B:1715:LEU:HD23	2:B:1715:LEU:HA	1.88	0.41
2:B:2197:GLN:O	2:B:2200:GLU:HG2	2.20	0.41
2:B:2278:ILE:O	2:B:2282:ASN:N	2.52	0.41
2:B:3004:LYS:H	2:B:3004:LYS:HG3	1.72	0.41
2:B:950:LEU:HD12	2:B:954:LEU:HD11	2.03	0.41
2:B:1514:GLU:O	2:B:1603:TYR:OH	2.38	0.41
2:B:1607:PRO:HG2	2:B:1658:ALA:HB2	2.02	0.41
2:B:2513:THR:HB	2:B:2548:ILE:HG12	2.03	0.41
2:A:709:ILE:HG13	2:A:710:THR:N	2.34	0.41
2:A:1574:LEU:HA	2:A:1577:THR:HG22	2.02	0.41
2:A:1843:PRO:HB2	2:A:1915:TYR:CD2	2.55	0.41
2:B:207:SER:HA	2:B:210:LEU:HD23	2.02	0.41
2:B:1469:ILE:HD13	2:B:1501:VAL:HG21	2.03	0.41
2:B:1600:VAL:HG13	2:B:1610:ARG:HH22	1.85	0.41
2:B:1916:MET:HA	2:B:1919:GLN:HG2	2.02	0.41
2:A:20:ALA:HB2	2:A:23:ARG:HH21	1.85	0.41
2:A:1447:SER:HA	2:A:1450:LEU:HG	2.02	0.41
2:A:2271:PRO:O	2:A:2275:ILE:HG12	2.20	0.41
2:B:1231:LEU:HD11	2:B:1259:LEU:HD11	2.02	0.41
2:B:1795:TRP:O	2:B:1805:TRP:NE1	2.53	0.41
2:A:207:SER:HA	2:A:210:LEU:HD23	2.03	0.41
2:A:2157:GLU:HA	2:A:2160:LYS:HE2	2.01	0.41
2:A:2615:GLN:HA	2:A:2618:ARG:HG2	2.03	0.41
2:B:2355:VAL:O	2:B:2359:THR:OG1	2.29	0.41
2:B:2871:ARG:HH22	2:B:2889:ASP:HB3	1.85	0.41
2:A:2859:SER:HB2	2:A:2887:HIS:NE2	2.33	0.41
2:A:3023:GLY:HA3	2:B:2404:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:632:GLU:HA	2:B:792:LYS:HE3	2.03	0.41
2:B:738:GLU:OE1	2:B:738:GLU:N	2.53	0.41
2:B:1128:GLN:HB3	2:B:1132:ARG:HH21	1.84	0.41
2:A:1460:ALA:O	2:A:1464:VAL:HG13	2.21	0.41
2:A:1611:LEU:HA	2:A:1614:LEU:HD12	2.01	0.41
2:A:734:VAL:HG12	2:A:735:ILE:HG23	2.03	0.41
2:B:43:LEU:HD23	2:B:57:TRP:HZ2	1.86	0.41
2:B:963:MET:HA	2:B:966:VAL:HG22	2.02	0.41
2:B:1158:ILE:HD11	2:B:1172:ALA:O	2.21	0.41
2:B:1520:ILE:HD12	2:B:1520:ILE:H	1.86	0.41
2:B:2217:PHE:HB2	2:B:2265:PHE:CG	2.55	0.41
2:A:812:MET:O	2:A:815:ILE:HG22	2.20	0.41
2:A:967:LEU:O	2:A:971:LYS:HG3	2.21	0.41
2:A:1542:LEU:HB3	2:A:1574:LEU:HD21	2.02	0.41
2:A:1747:HIS:O	2:A:1751:GLU:HG2	2.21	0.41
2:A:1859:ARG:HE	2:A:1935:ASP:N	2.19	0.41
2:A:2151:ARG:HG3	2:A:2179:ILE:HG21	2.03	0.41
2:A:2513:THR:HB	2:A:2548:ILE:HG12	2.03	0.41
2:A:2778:GLU:O	2:A:2782:ASN:HB2	2.21	0.41
2:B:1026:TRP:CZ2	2:B:1030:LYS:HD3	2.56	0.41
2:B:1842:LEU:HD12	2:B:1845:LEU:HD11	2.03	0.41
2:B:1943:LYS:HD2	2:B:1999:ILE:HG21	2.03	0.41
2:B:2185:ILE:HG13	2:B:2230:ILE:HG21	2.03	0.41
2:B:2687:LYS:HA	2:B:2687:LYS:HD2	1.90	0.41
2:A:1146:GLU:HA	2:A:1149:ASN:HD22	1.87	0.40
2:A:1866:VAL:HG11	2:A:1936:LEU:HD21	2.03	0.40
2:B:1798:LEU:HD12	2:B:1901:LEU:HD13	2.03	0.40
2:A:43:LEU:HD23	2:A:57:TRP:HZ2	1.86	0.40
2:A:722:LEU:HG	2:A:745:LEU:HD12	2.03	0.40
2:A:922:ASP:OD1	2:A:926:LYS:HE3	2.21	0.40
2:A:1036:PHE:HA	2:A:1039:ARG:HD3	2.02	0.40
2:B:488:TRP:CG	2:B:517:VAL:HG11	2.56	0.40
2:B:1002:GLY:HA2	2:B:1058:TRP:HZ2	1.86	0.40
2:B:2055:ILE:H	2:B:2055:ILE:HD12	1.87	0.40
2:B:2861:ILE:HD13	2:B:2861:ILE:HA	1.91	0.40
2:A:427:LEU:O	2:A:469:ARG:NH2	2.55	0.40
2:A:1297:TYR:HE1	2:A:1381:PHE:HZ	1.68	0.40
2:A:1376:PRO:HB3	2:A:1437:ARG:HD2	2.04	0.40
2:A:1810:THR:HG21	2:A:1838:CYS:HB3	2.03	0.40
2:A:2924:GLU:HG3	2:A:2928:ARG:HH21	1.85	0.40
2:B:161:GLN:NE2	2:B:203:ASP:OD1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1166:PRO:HA	2:B:1169:GLU:HG2	2.02	0.40
2:B:1296:PRO:HB2	2:B:1381:PHE:HE2	1.85	0.40
2:B:1473:ILE:HD12	2:B:1473:ILE:HA	1.95	0.40
2:A:263:LEU:HD12	2:A:318:LEU:HD22	2.03	0.40
2:A:398:ASP:O	2:A:402:LYS:HG2	2.21	0.40
2:A:439:LEU:HD13	2:A:459:LEU:HD22	2.04	0.40
2:A:956:GLY:N	2:A:1000:ASN:OD1	2.52	0.40
2:B:530:SER:HA	2:B:533:ARG:HH22	1.87	0.40
2:B:1968:ASP:O	2:B:1971:GLU:HG3	2.22	0.40
2:A:1155:LEU:HD13	2:A:1190:VAL:HG12	2.02	0.40
2:A:1387:LYS:HD3	2:A:1387:LYS:HA	1.87	0.40
2:A:1686:ILE:HG22	2:A:1952:PHE:HZ	1.86	0.40
2:A:2355:VAL:O	2:A:2359:THR:OG1	2.29	0.40
2:B:1186:GLU:HB3	2:B:1188:HIS:CE1	2.57	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	E	5/12 (42%)	5 (100%)	0	0	100	100
1	F	5/12 (42%)	5 (100%)	0	0	100	100
2	A	2708/3184 (85%)	2652 (98%)	56 (2%)	0	100	100
2	B	2708/3184 (85%)	2651 (98%)	57 (2%)	0	100	100
All	All	5426/6392 (85%)	5313 (98%)	113 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	E	7/12 (58%)	7 (100%)	0	100 100
1	F	7/12 (58%)	7 (100%)	0	100 100
2	A	2444/2883 (85%)	2439 (100%)	5 (0%)	93 97
2	B	2444/2883 (85%)	2439 (100%)	5 (0%)	93 97
All	All	4902/5790 (85%)	4892 (100%)	10 (0%)	93 97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	114	ARG
2	A	1064	MET
2	A	1619	ARG
2	A	2191	ARG
2	A	2642	ARG
2	B	114	ARG
2	B	1039	ARG
2	B	1619	ARG
2	B	2191	ARG
2	B	2642	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1083	HIS
2	A	1149	ASN
2	A	1310	GLN
2	A	2177	GLN
2	A	2208	HIS
2	B	286	GLN
2	B	683	HIS
2	B	1116	GLN
2	B	1310	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1416	GLN
2	B	1867	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
3	ANP	B	3101	4	29,33,33	1.09	4 (13%)	31,52,52	1.10	2 (6%)
3	ANP	A	3101	4	29,33,33	1.08	4 (13%)	31,52,52	1.08	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	B	3101	4	-	6/14/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	3101	4	-	6/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3101	ANP	PG-O1G	2.46	1.50	1.46
3	A	3101	ANP	PG-O1G	2.46	1.50	1.46
3	B	3101	ANP	PG-N3B	2.43	1.69	1.63
3	A	3101	ANP	PG-N3B	2.43	1.69	1.63
3	B	3101	ANP	PB-O1B	2.33	1.49	1.46
3	A	3101	ANP	PB-O1B	2.33	1.49	1.46
3	B	3101	ANP	PB-O3A	-2.28	1.56	1.59
3	A	3101	ANP	PB-O3A	-2.26	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3101	ANP	PB-O3A-PA	-3.75	119.42	132.62
3	A	3101	ANP	PB-O3A-PA	-3.66	119.71	132.62
3	B	3101	ANP	C5-C6-N6	2.27	123.80	120.35
3	A	3101	ANP	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PB-N3B-PG-O1G
3	A	3101	ANP	C5'-O5'-PA-O1A
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	A	3101	ANP	C3'-C4'-C5'-O5'
3	B	3101	ANP	PB-N3B-PG-O1G
3	B	3101	ANP	C5'-O5'-PA-O1A
3	B	3101	ANP	O4'-C4'-C5'-O5'
3	B	3101	ANP	C3'-C4'-C5'-O5'
3	A	3101	ANP	C5'-O5'-PA-O3A
3	B	3101	ANP	C5'-O5'-PA-O3A
3	A	3101	ANP	C5'-O5'-PA-O2A
3	B	3101	ANP	C5'-O5'-PA-O2A

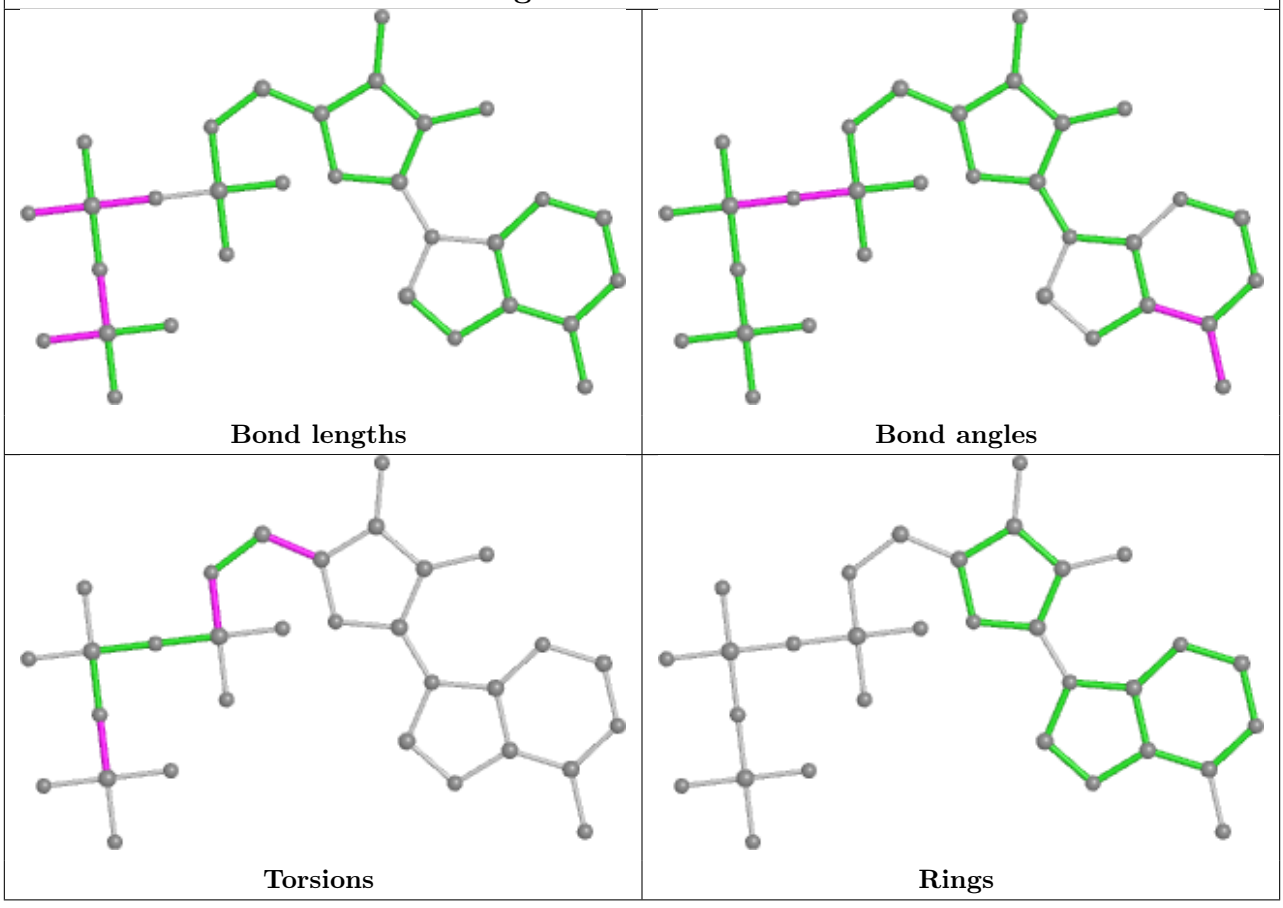
There are no ring outliers.

2 monomers are involved in 4 short contacts:

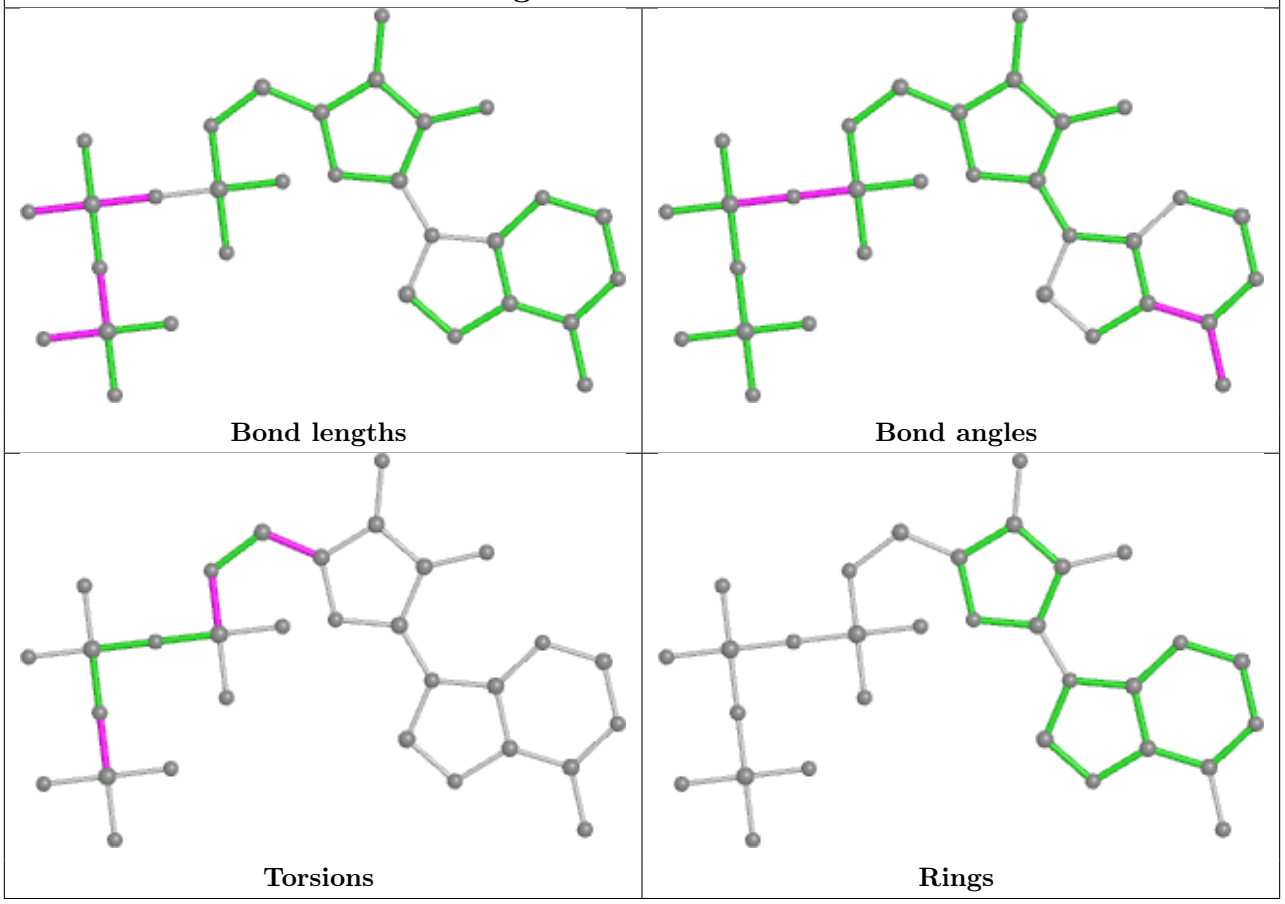
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3101	ANP	3	0
3	A	3101	ANP	1	0

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

Ligand ANP B 3101



Ligand ANP A 3101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

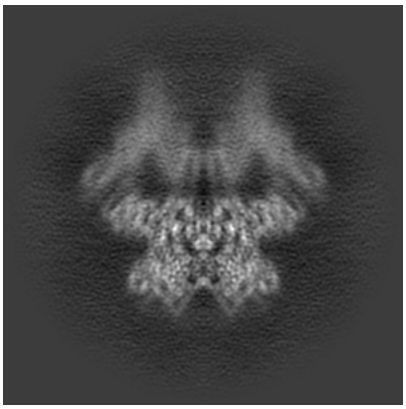
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17265. These allow visual inspection of the internal detail of the map and identification of artifacts.

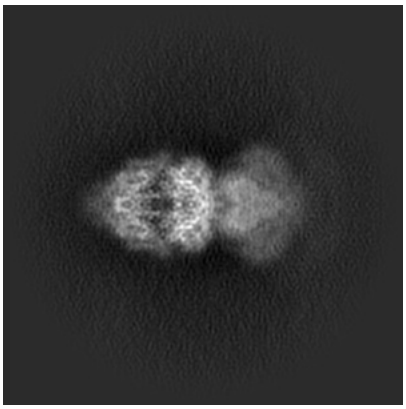
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

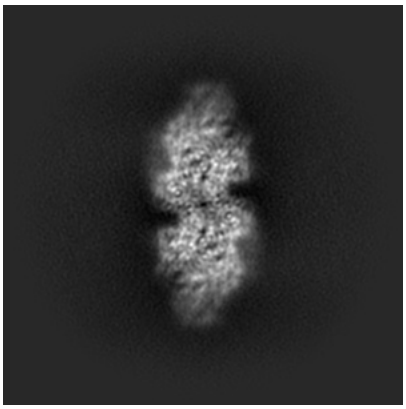
6.1.1 Primary map



X

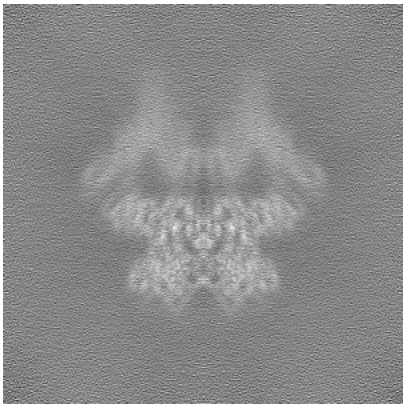


Y

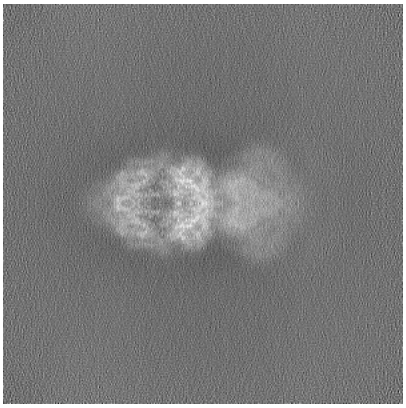


Z

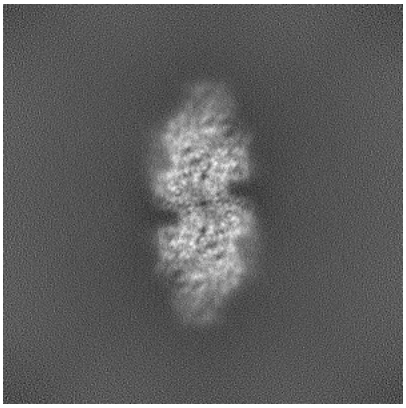
6.1.2 Raw map



X



Y

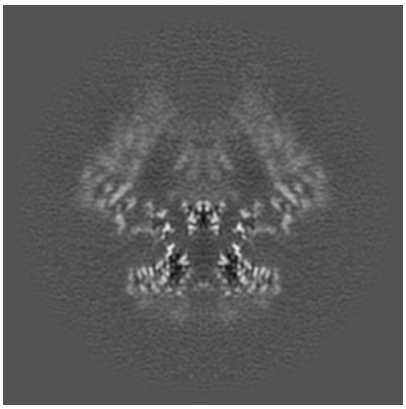


Z

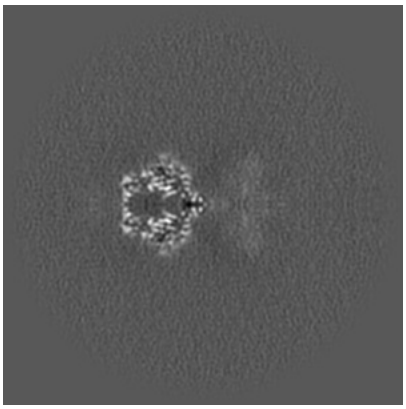
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

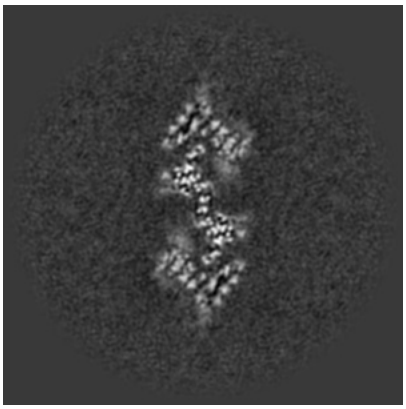
6.2.1 Primary map



X Index: 200

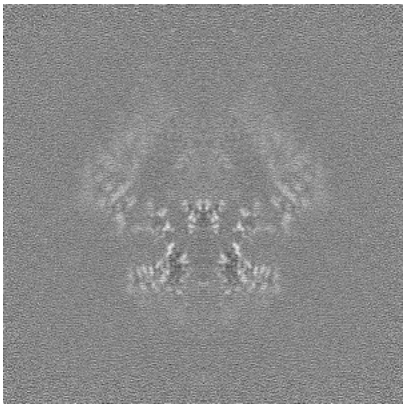


Y Index: 200

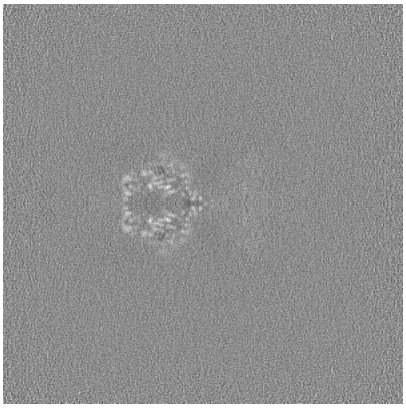


Z Index: 200

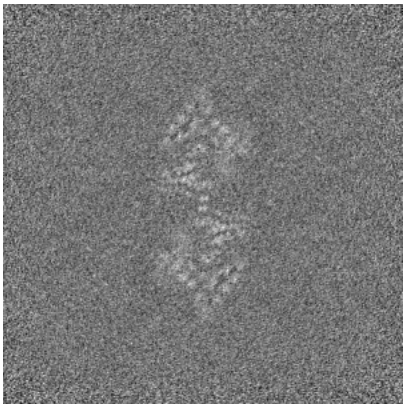
6.2.2 Raw map



X Index: 200



Y Index: 200

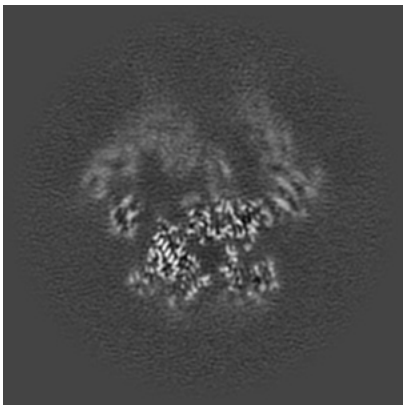


Z Index: 200

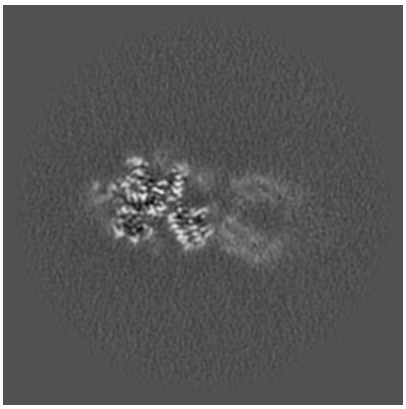
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

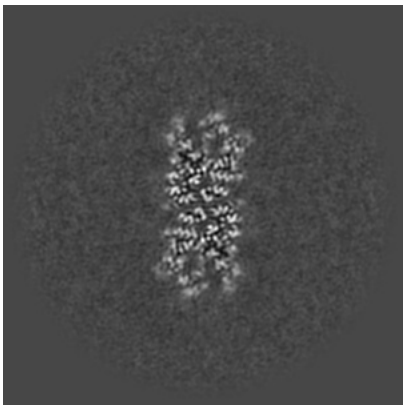
6.3.1 Primary map



X Index: 191

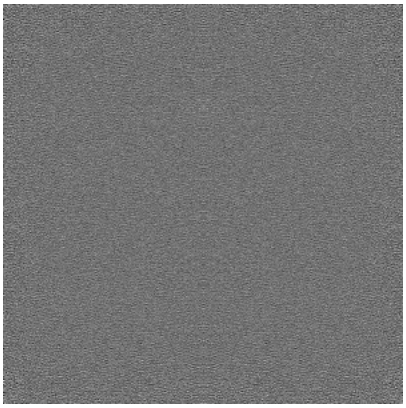


Y Index: 229

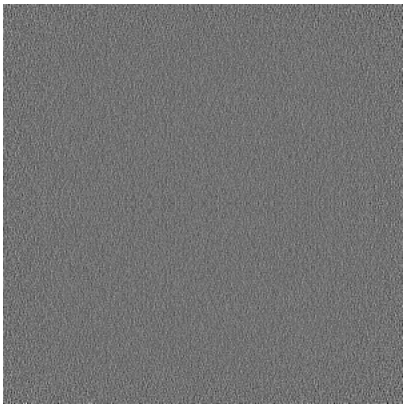


Z Index: 177

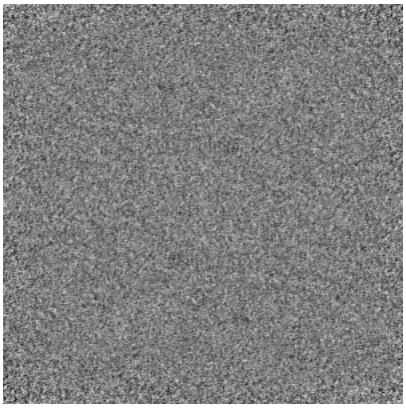
6.3.2 Raw map



X Index: 0



Y Index: 0

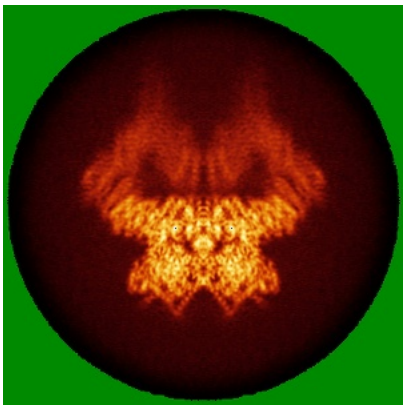


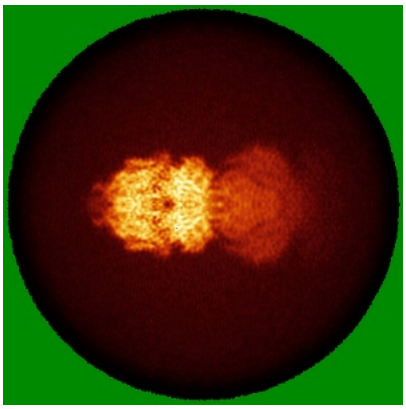
Z Index: 0

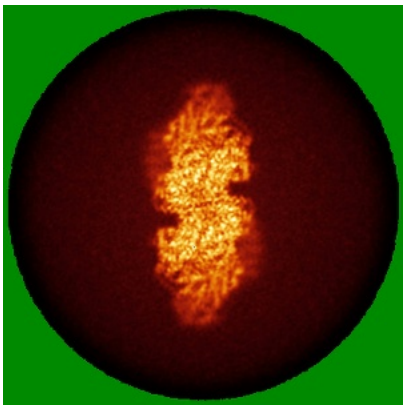
The images above show the largest variance slices of the map in three orthogonal directions.

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

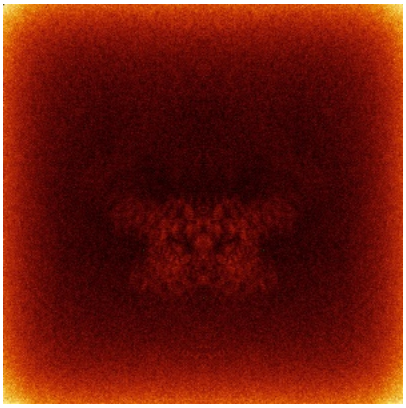
6.4.1 Primary map

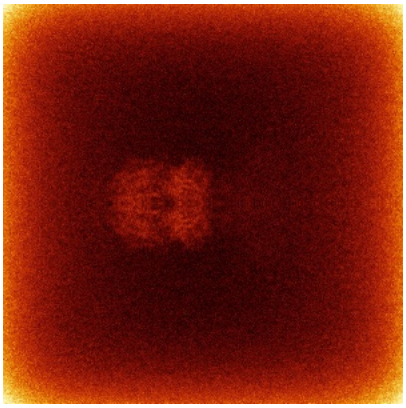

X

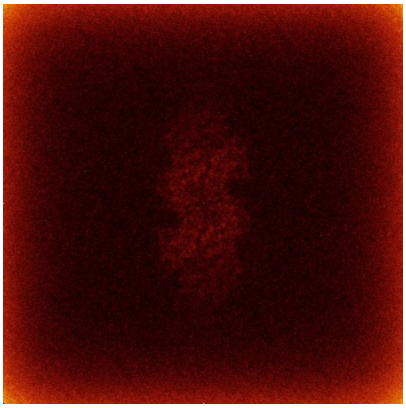

Y


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.

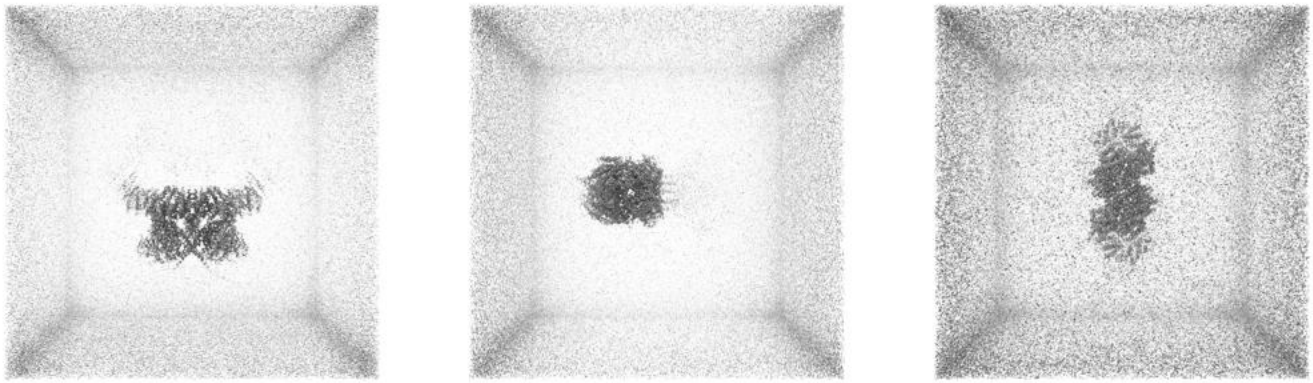
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

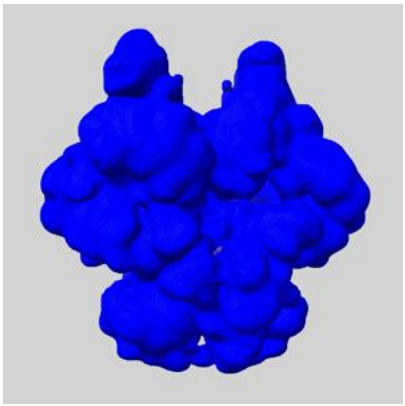
6.6 Mask visualisation

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

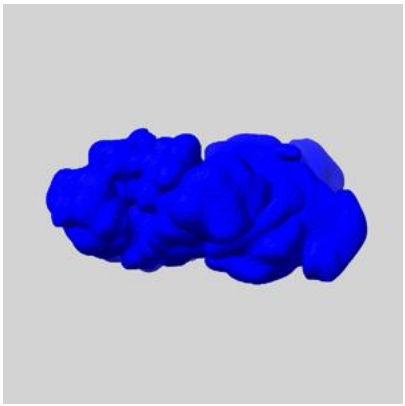
A mask typically either:

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

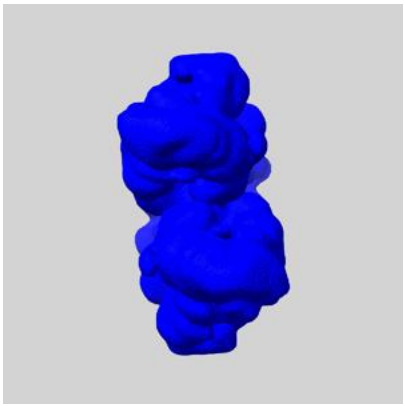
6.6.1 emd_17265_msk_1.map



X



Y

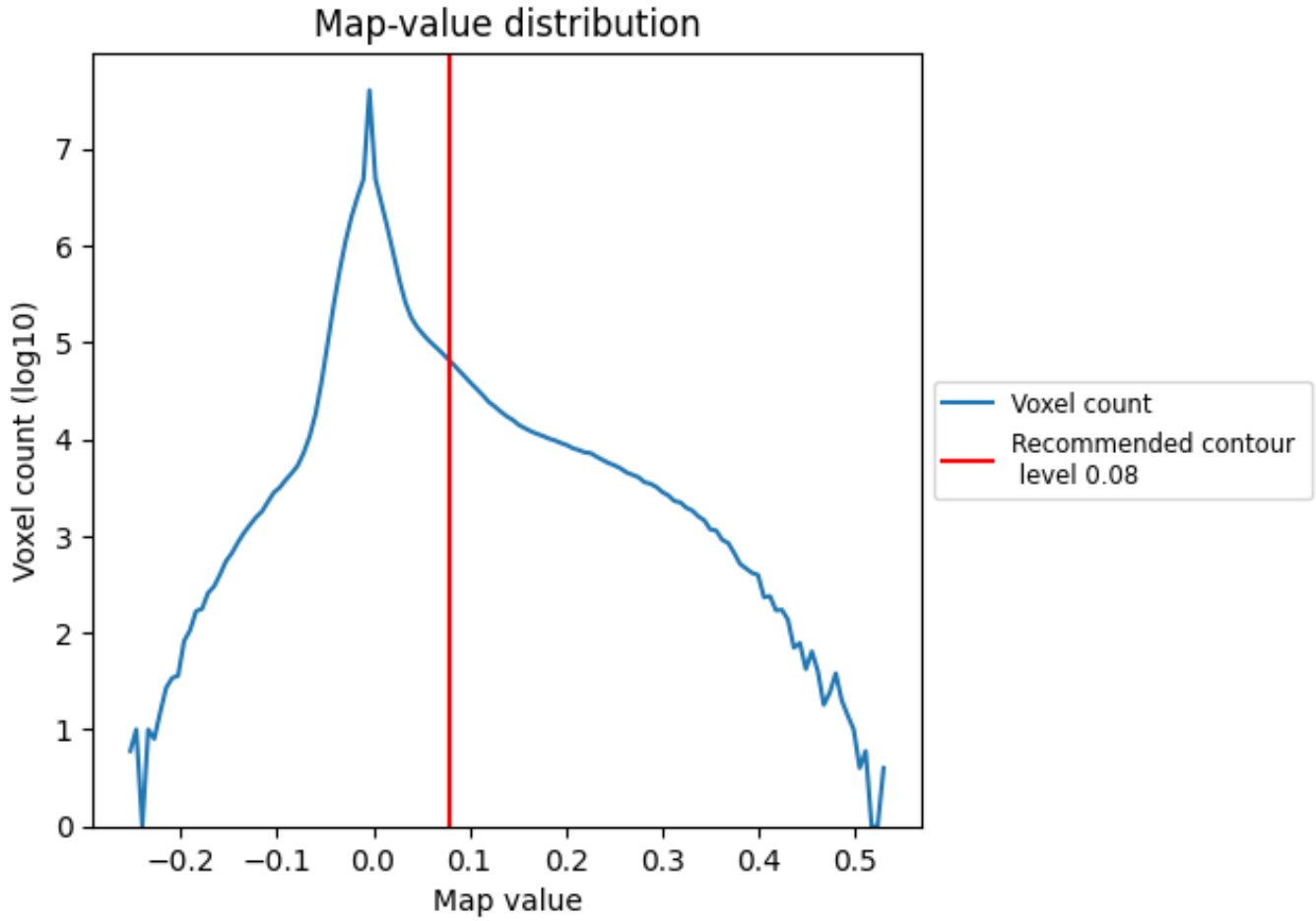


Z

7 Map analysis

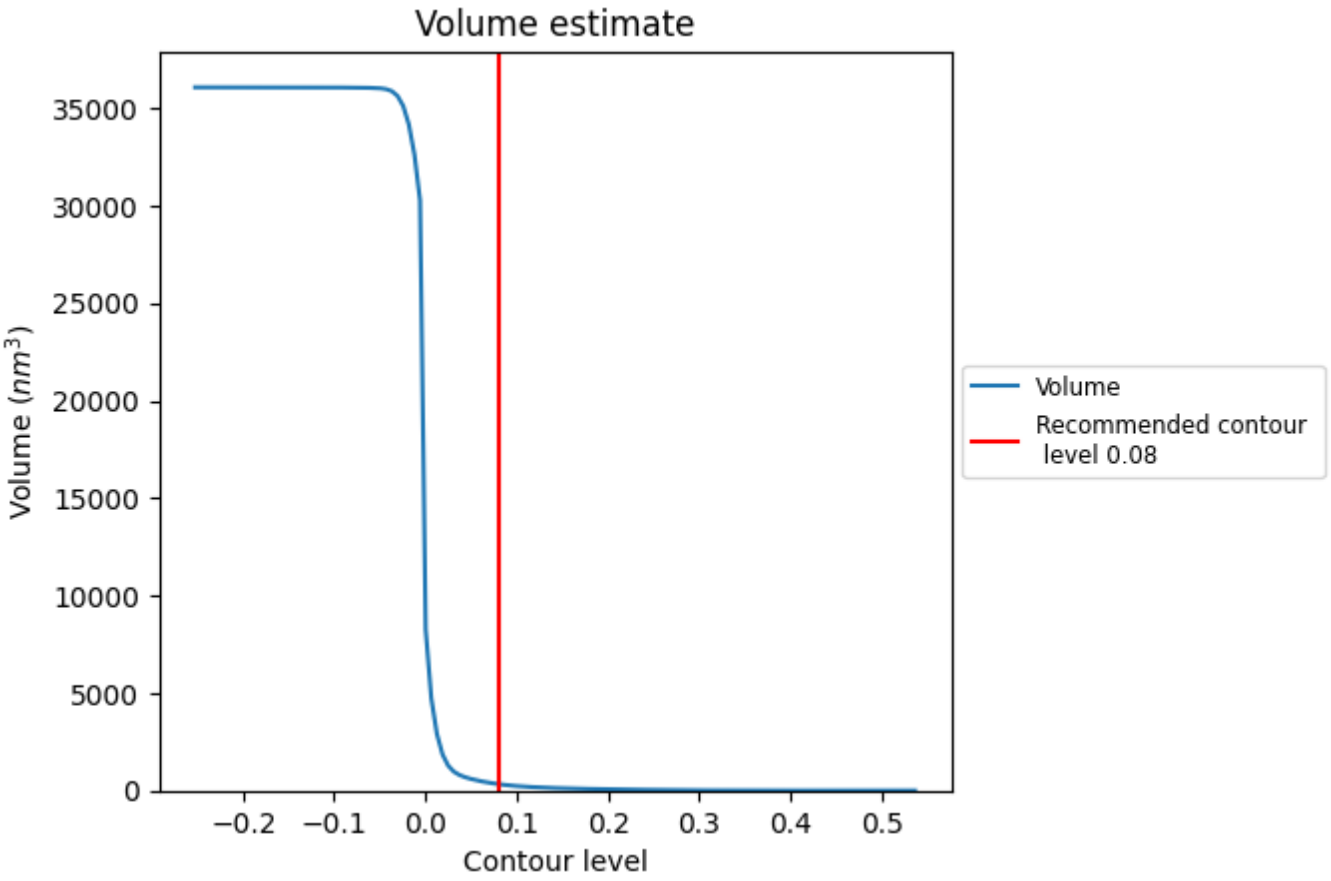
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

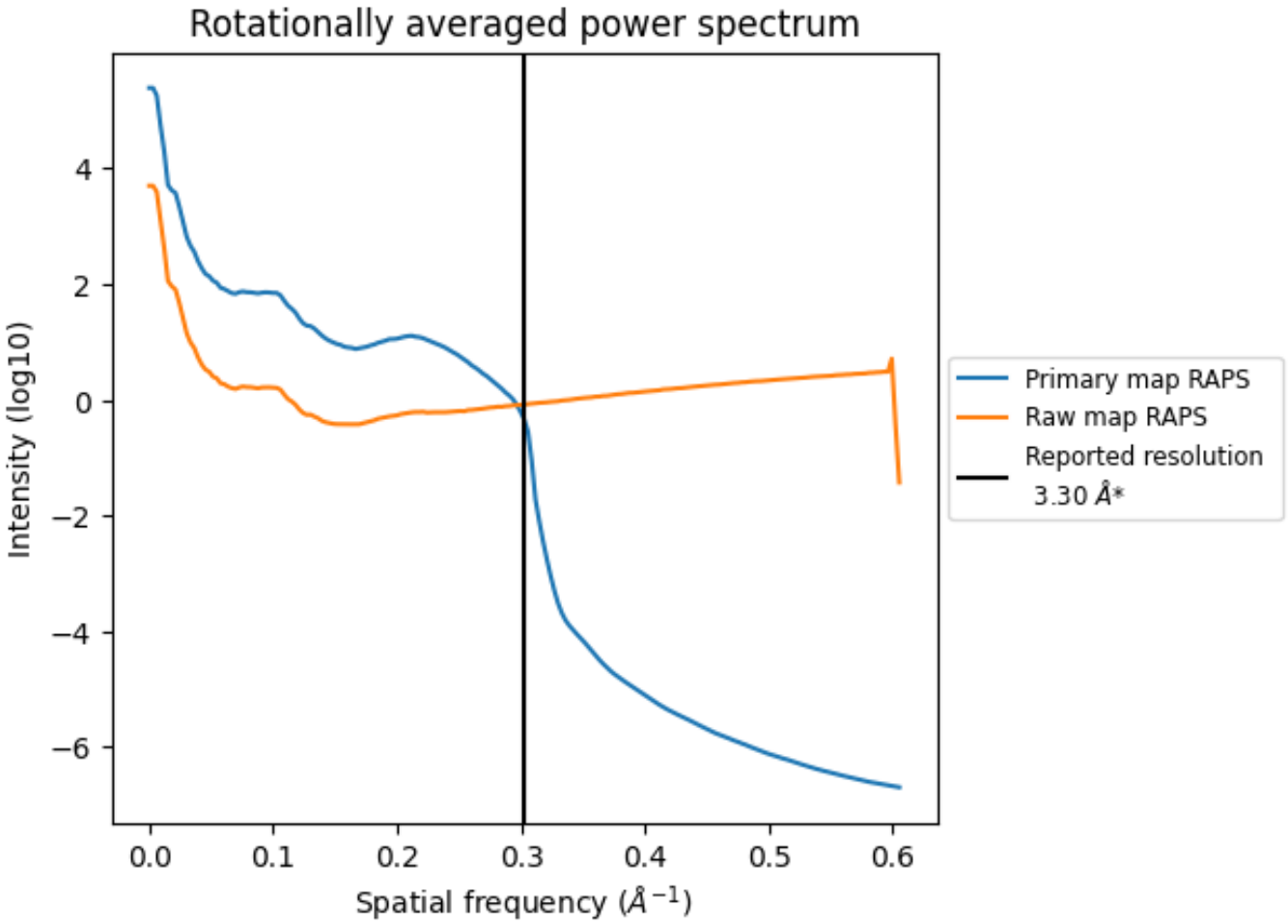
7.2 Volume estimate



The volume at the recommended contour level is 331 nm^3; this corresponds to an approximate mass of 299 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)

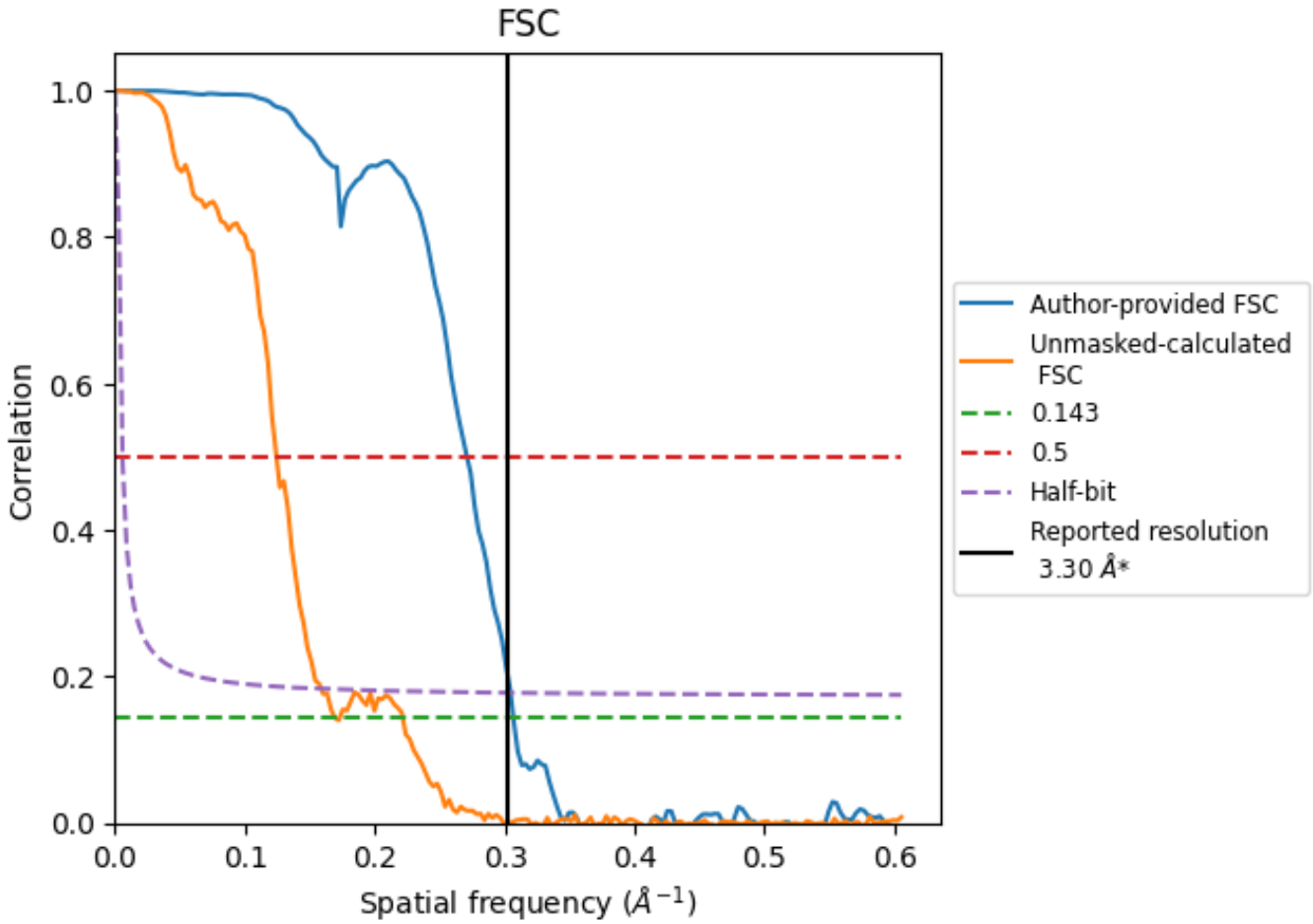


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8.2 Resolution estimates (i)

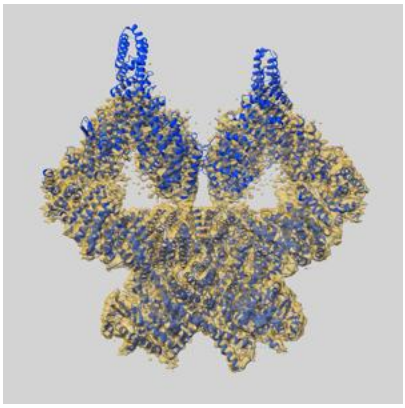
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.69	3.28
Unmasked-calculated*	5.90	8.04	6.29

*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 5.90 differs from the reported value 3.3 by more than 10 %

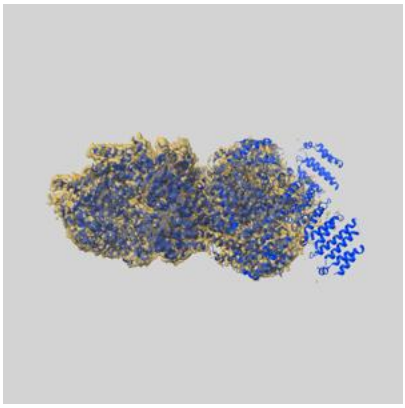
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17265 and PDB model 8OXM. Per-residue inclusion information can be found in section 3 on page 11.

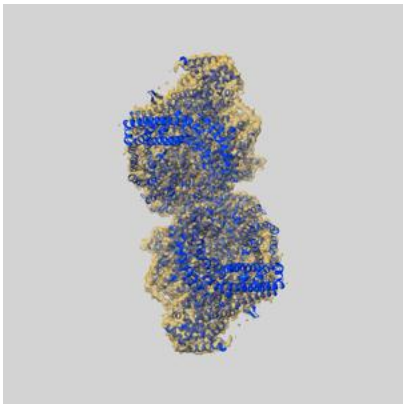
9.1 Map-model overlay



X



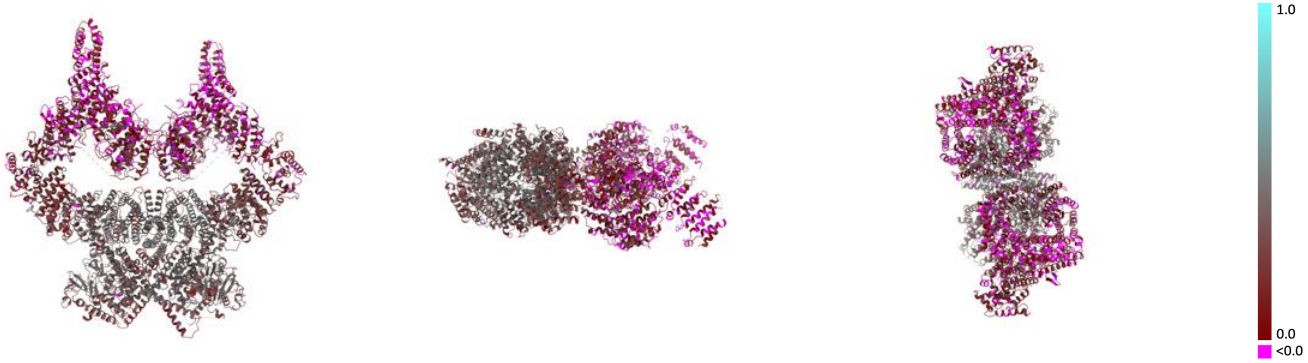
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

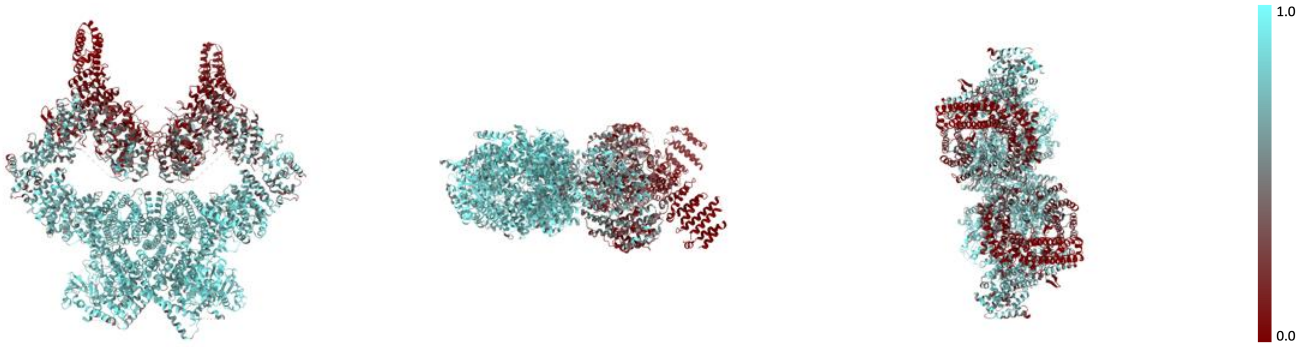
9.2 Q-score mapped to coordinate model



X Y Z

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

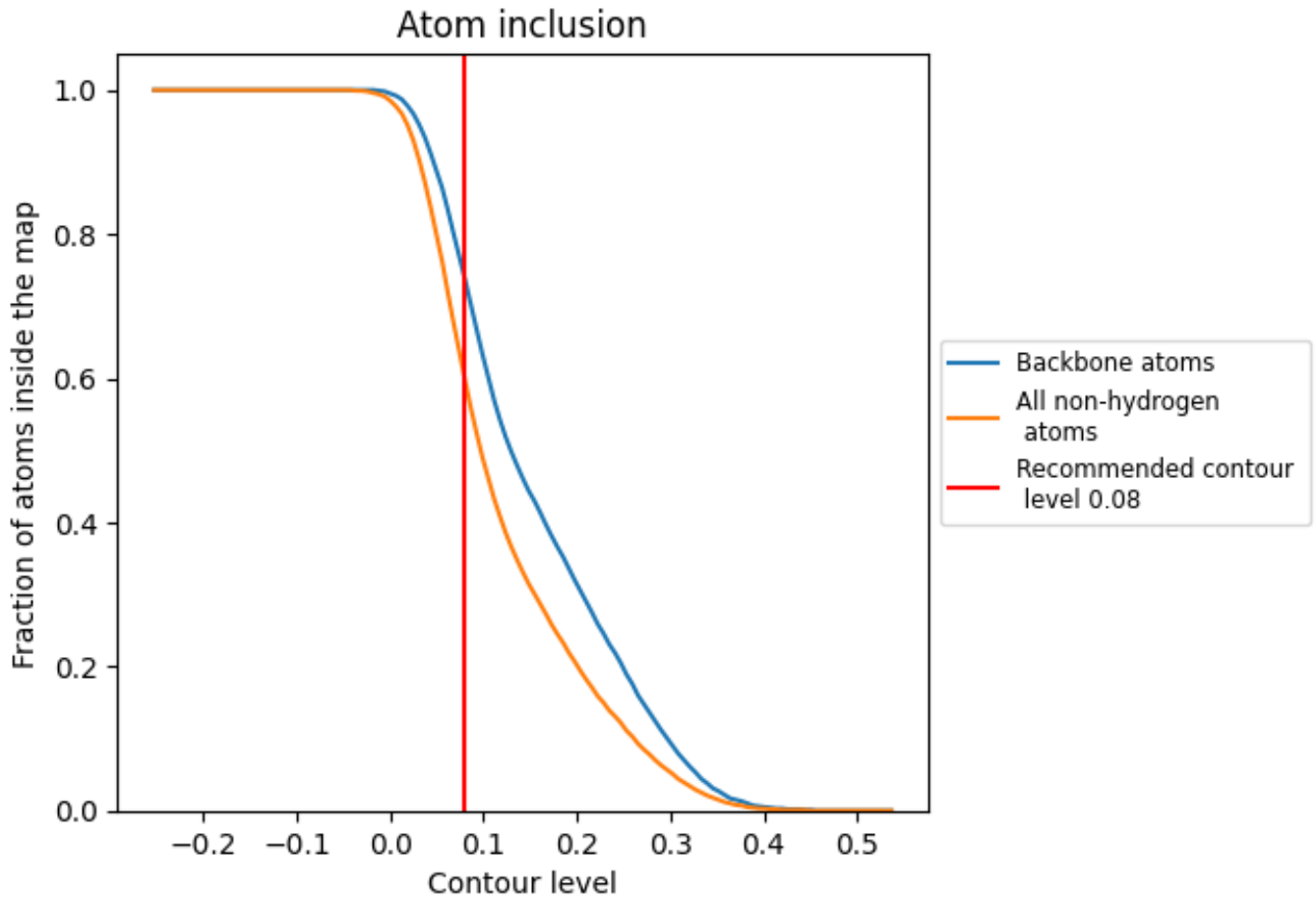
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.2450
A	0.5960	0.2410
B	0.6020	0.2480
E	0.2830	0.2750
F	0.2830	0.2820