Full wwPDB EM Validation Report

Nov 19, 2022 – 06:42 pm GMT

PDB ID	:	5OG1
EMDB ID	:	EMD-3777
Title	:	Cryo EM structure of the E. coli disaggregase ClpB (BAP form, DWB mutant), in the ATPgammaS state
Authors	:	Deville, C.; Carroni, M.; Franke, K.B.; Topf, M.; Bukau, B.; Mogk, A.; Saibil, H.R.
Deposited on	:	2017-07-11
Resolution	:	4.50 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 (1)) were used in the production of this report:

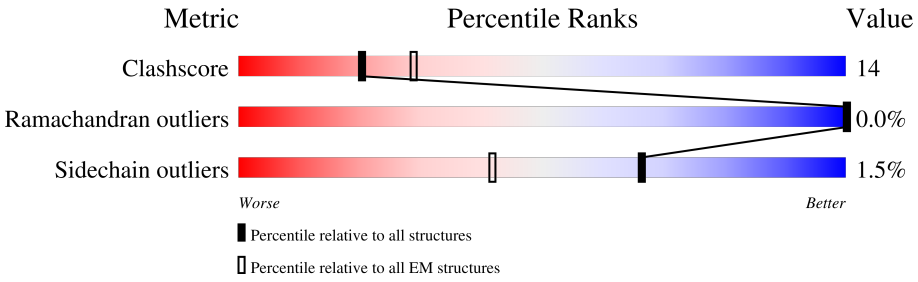
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	871	68% 68% 25% · 6%
1	B	871	42% 45% 21% · 34%
1	C	871	45% 45% 26% 28%
1	D	871	46% 49% 22% 28%
1	E	871	51% 56% 22% 21%
1	F	871	55% 53% 26% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31380 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 Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	624	Total	C	N	O	S	0	0
			4960	3101	900	941	18		
1	F	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	E	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	D	624	Total	C	N	O	S	0	0
			4960	3101	900	941	18		
1	B	572	Total	C	N	O	S	0	0
			4518	2834	823	845	16		
1	A	819	Total	C	N	O	S	0	0
			5841	3667	1118	1037	19		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	MET	-	initiating methionine	UNP P63284
C	-2	ARG	-	expression tag	UNP P63284
C	-1	GLY	-	expression tag	UNP P63284
C	0	SER	-	expression tag	UNP P63284
C	279	ALA	GLU	engineered mutation	UNP P63284
C	678	ALA	GLU	engineered mutation	UNP P63284
C	745	ILE	ILE	linker	UNP P0ABH9
C	746	LYS	LYS	linker	UNP P0ABH9
C	747	LYS	LYS	linker	UNP P0ABH9
C	748	ILE	ILE	linker	UNP P0ABH9
C	858	GLY	-	expression tag	UNP P63284
C	859	SER	-	expression tag	UNP P63284
C	860	ARG	-	expression tag	UNP P63284
C	861	SER	-	expression tag	UNP P63284
C	862	HIS	-	expression tag	UNP P63284
C	863	HIS	-	expression tag	UNP P63284
C	864	HIS	-	expression tag	UNP P63284

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Chain	Residue	Modelled	Actual	Comment	Reference
C	865	HIS	-	expression tag	UNP P63284
C	866	HIS	-	expression tag	UNP P63284
C	867	HIS	-	expression tag	UNP P63284
F	-3	MET	-	initiating methionine	UNP P63284
F	-2	ARG	-	expression tag	UNP P63284
F	-1	GLY	-	expression tag	UNP P63284
F	0	SER	-	expression tag	UNP P63284
F	279	ALA	GLU	engineered mutation	UNP P63284
F	678	ALA	GLU	engineered mutation	UNP P63284
F	745	ILE	ILE	linker	UNP P0ABH9
F	746	LYS	LYS	linker	UNP P0ABH9
F	747	LYS	LYS	linker	UNP P0ABH9
F	748	ILE	ILE	linker	UNP P0ABH9
F	858	GLY	-	expression tag	UNP P63284
F	859	SER	-	expression tag	UNP P63284
F	860	ARG	-	expression tag	UNP P63284
F	861	SER	-	expression tag	UNP P63284
F	862	HIS	-	expression tag	UNP P63284
F	863	HIS	-	expression tag	UNP P63284
F	864	HIS	-	expression tag	UNP P63284
F	865	HIS	-	expression tag	UNP P63284
F	866	HIS	-	expression tag	UNP P63284
F	867	HIS	-	expression tag	UNP P63284
E	-3	MET	-	initiating methionine	UNP P63284
E	-2	ARG	-	expression tag	UNP P63284
E	-1	GLY	-	expression tag	UNP P63284
E	0	SER	-	expression tag	UNP P63284
E	279	ALA	GLU	engineered mutation	UNP P63284
E	678	ALA	GLU	engineered mutation	UNP P63284
E	745	ILE	ILE	linker	UNP P0ABH9
E	746	LYS	LYS	linker	UNP P0ABH9
E	747	LYS	LYS	linker	UNP P0ABH9
E	748	ILE	ILE	linker	UNP P0ABH9
E	858	GLY	-	expression tag	UNP P63284
E	859	SER	-	expression tag	UNP P63284
E	860	ARG	-	expression tag	UNP P63284
E	861	SER	-	expression tag	UNP P63284
E	862	HIS	-	expression tag	UNP P63284
E	863	HIS	-	expression tag	UNP P63284
E	864	HIS	-	expression tag	UNP P63284
E	865	HIS	-	expression tag	UNP P63284
E	866	HIS	-	expression tag	UNP P63284

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Chain	Residue	Modelled	Actual	Comment	Reference
E	867	HIS	-	expression tag	UNP P63284
D	-3	MET	-	initiating methionine	UNP P63284
D	-2	ARG	-	expression tag	UNP P63284
D	-1	GLY	-	expression tag	UNP P63284
D	0	SER	-	expression tag	UNP P63284
D	279	ALA	GLU	engineered mutation	UNP P63284
D	678	ALA	GLU	engineered mutation	UNP P63284
D	745	ILE	ILE	linker	UNP P0ABH9
D	746	LYS	LYS	linker	UNP P0ABH9
D	747	LYS	LYS	linker	UNP P0ABH9
D	748	ILE	ILE	linker	UNP P0ABH9
D	858	GLY	-	expression tag	UNP P63284
D	859	SER	-	expression tag	UNP P63284
D	860	ARG	-	expression tag	UNP P63284
D	861	SER	-	expression tag	UNP P63284
D	862	HIS	-	expression tag	UNP P63284
D	863	HIS	-	expression tag	UNP P63284
D	864	HIS	-	expression tag	UNP P63284
D	865	HIS	-	expression tag	UNP P63284
D	866	HIS	-	expression tag	UNP P63284
D	867	HIS	-	expression tag	UNP P63284
B	-3	MET	-	initiating methionine	UNP P63284
B	-2	ARG	-	expression tag	UNP P63284
B	-1	GLY	-	expression tag	UNP P63284
B	0	SER	-	expression tag	UNP P63284
B	279	ALA	GLU	engineered mutation	UNP P63284
B	678	ALA	GLU	engineered mutation	UNP P63284
B	745	ILE	ILE	linker	UNP P0ABH9
B	746	LYS	LYS	linker	UNP P0ABH9
B	747	LYS	LYS	linker	UNP P0ABH9
B	748	ILE	ILE	linker	UNP P0ABH9
B	858	GLY	-	expression tag	UNP P63284
B	859	SER	-	expression tag	UNP P63284
B	860	ARG	-	expression tag	UNP P63284
B	861	SER	-	expression tag	UNP P63284
B	862	HIS	-	expression tag	UNP P63284
B	863	HIS	-	expression tag	UNP P63284
B	864	HIS	-	expression tag	UNP P63284
B	865	HIS	-	expression tag	UNP P63284
B	866	HIS	-	expression tag	UNP P63284
B	867	HIS	-	expression tag	UNP P63284
A	-3	MET	-	initiating methionine	UNP P63284

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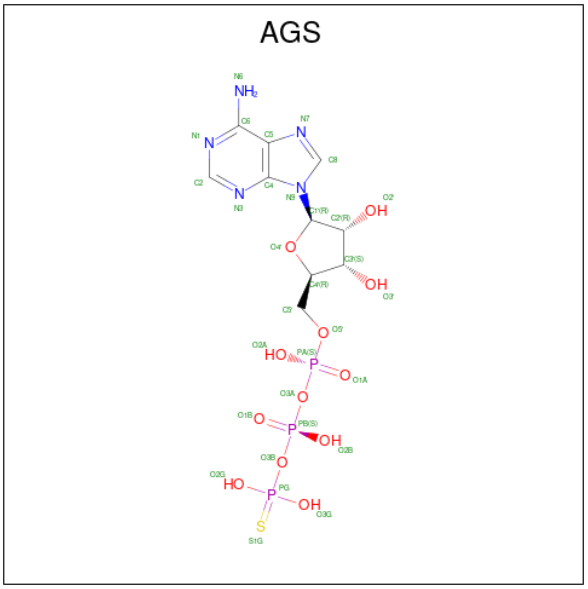
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ARG	-	expression tag	UNP P63284
A	-1	GLY	-	expression tag	UNP P63284
A	0	SER	-	expression tag	UNP P63284
A	279	ALA	GLU	engineered mutation	UNP P63284
A	678	ALA	GLU	engineered mutation	UNP P63284
A	745	ILE	ILE	linker	UNP P0ABH9
A	746	LYS	LYS	linker	UNP P0ABH9
A	747	LYS	LYS	linker	UNP P0ABH9
A	748	ILE	ILE	linker	UNP P0ABH9
A	858	GLY	-	expression tag	UNP P63284
A	859	SER	-	expression tag	UNP P63284
A	860	ARG	-	expression tag	UNP P63284
A	861	SER	-	expression tag	UNP P63284
A	862	HIS	-	expression tag	UNP P63284
A	863	HIS	-	expression tag	UNP P63284
A	864	HIS	-	expression tag	UNP P63284
A	865	HIS	-	expression tag	UNP P63284
A	866	HIS	-	expression tag	UNP P63284
A	867	HIS	-	expression tag	UNP P63284

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

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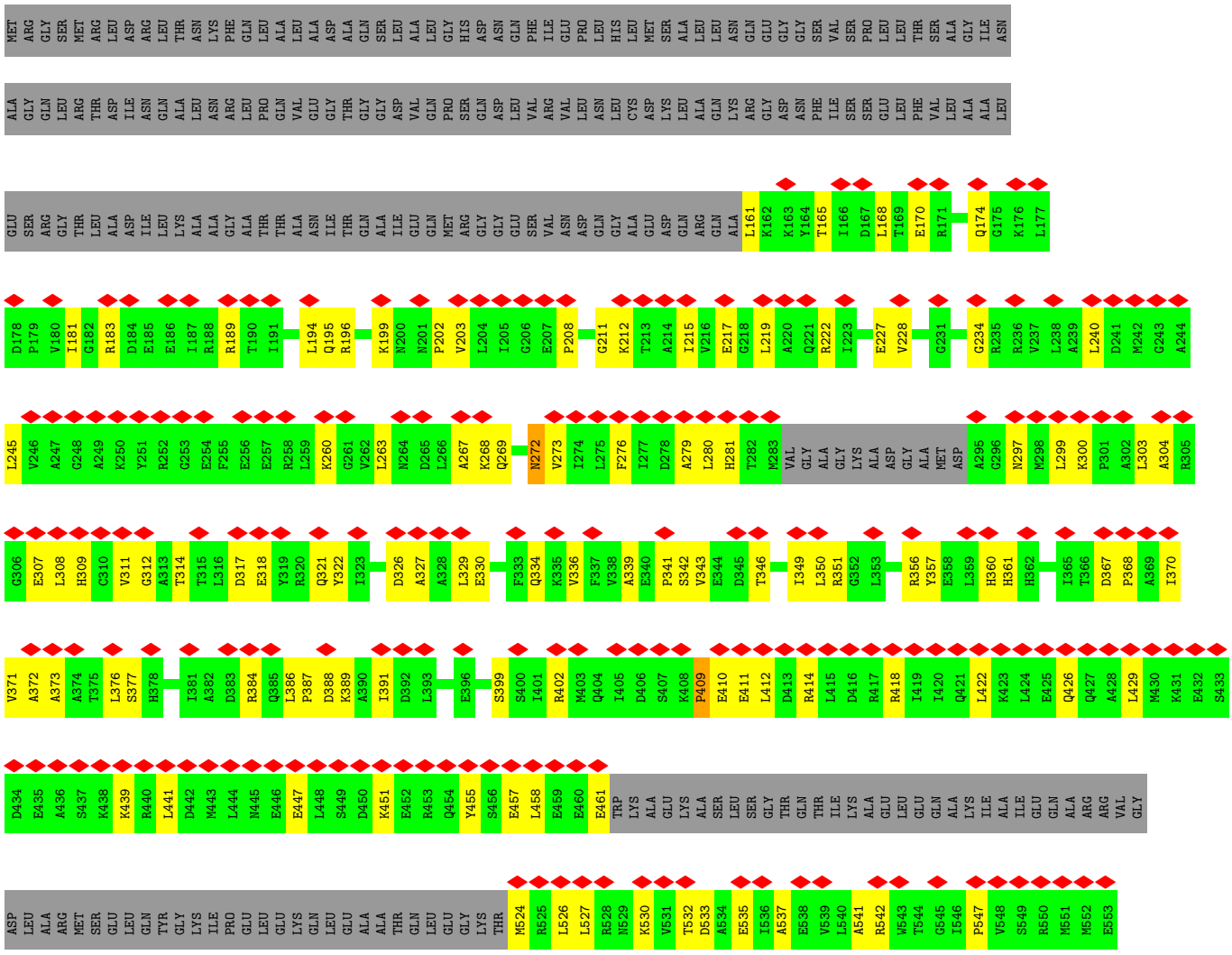
Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

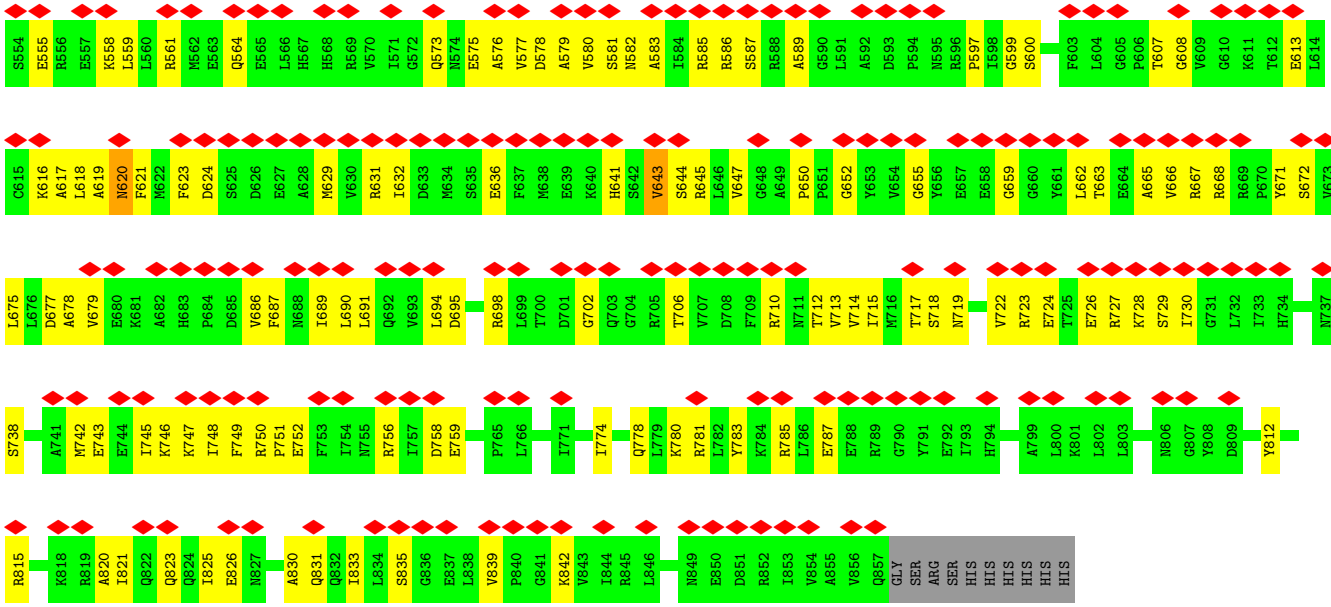
3 Residue-property plots (i)

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.

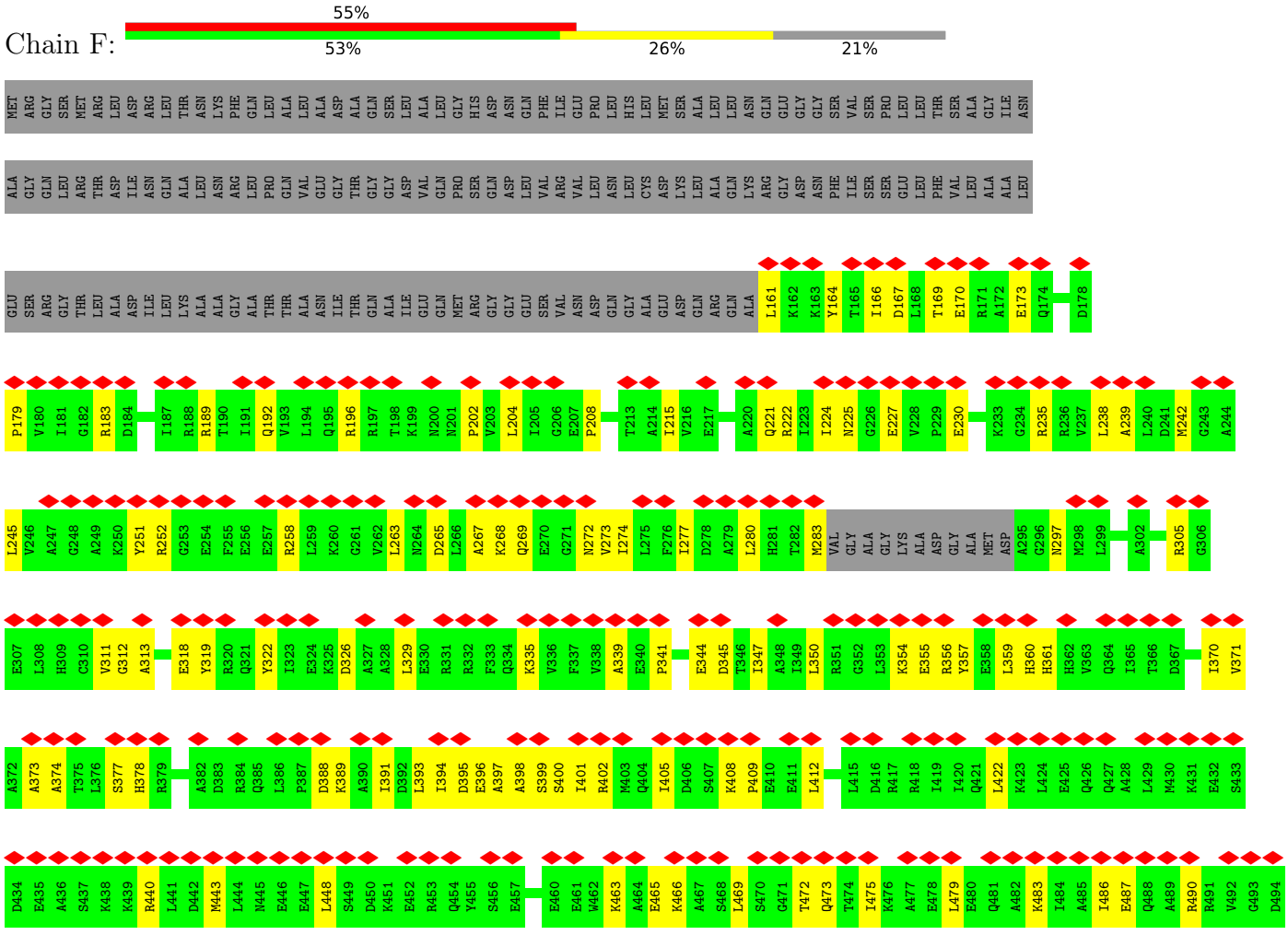
• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

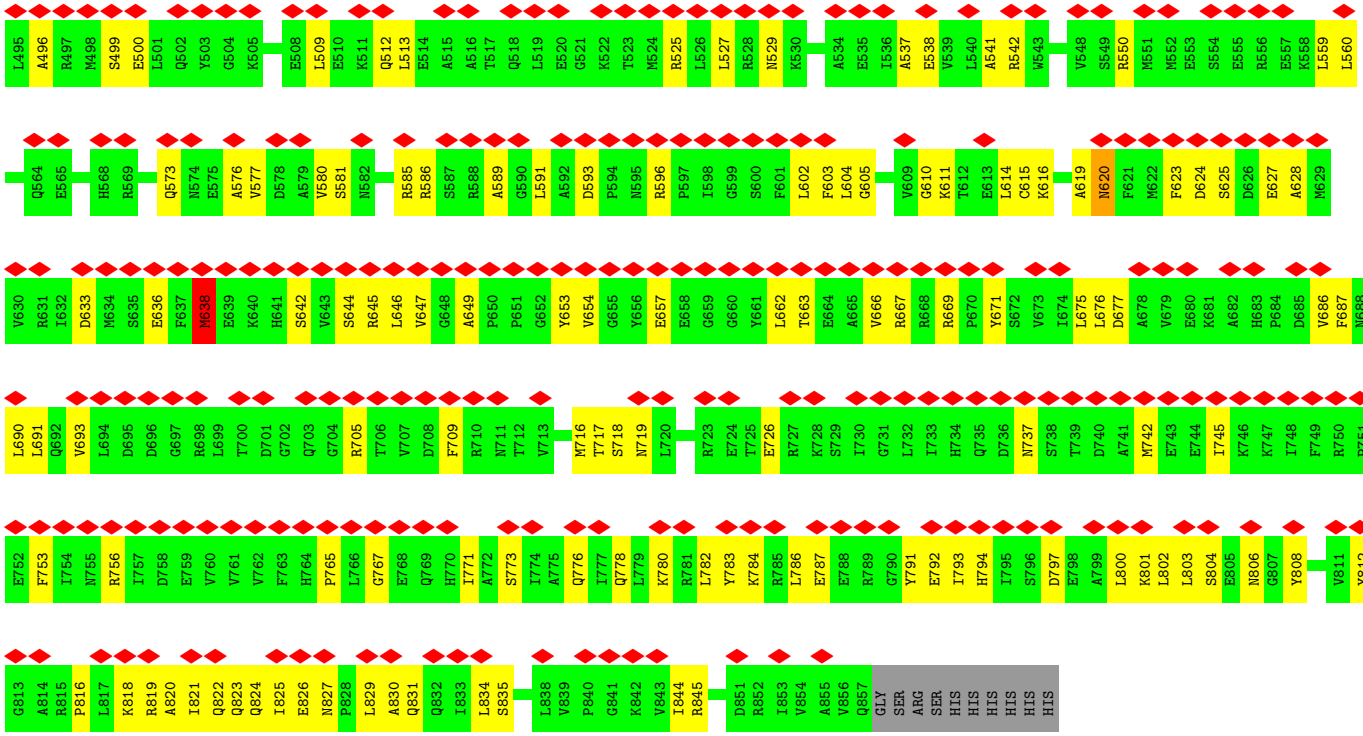
Chain C:





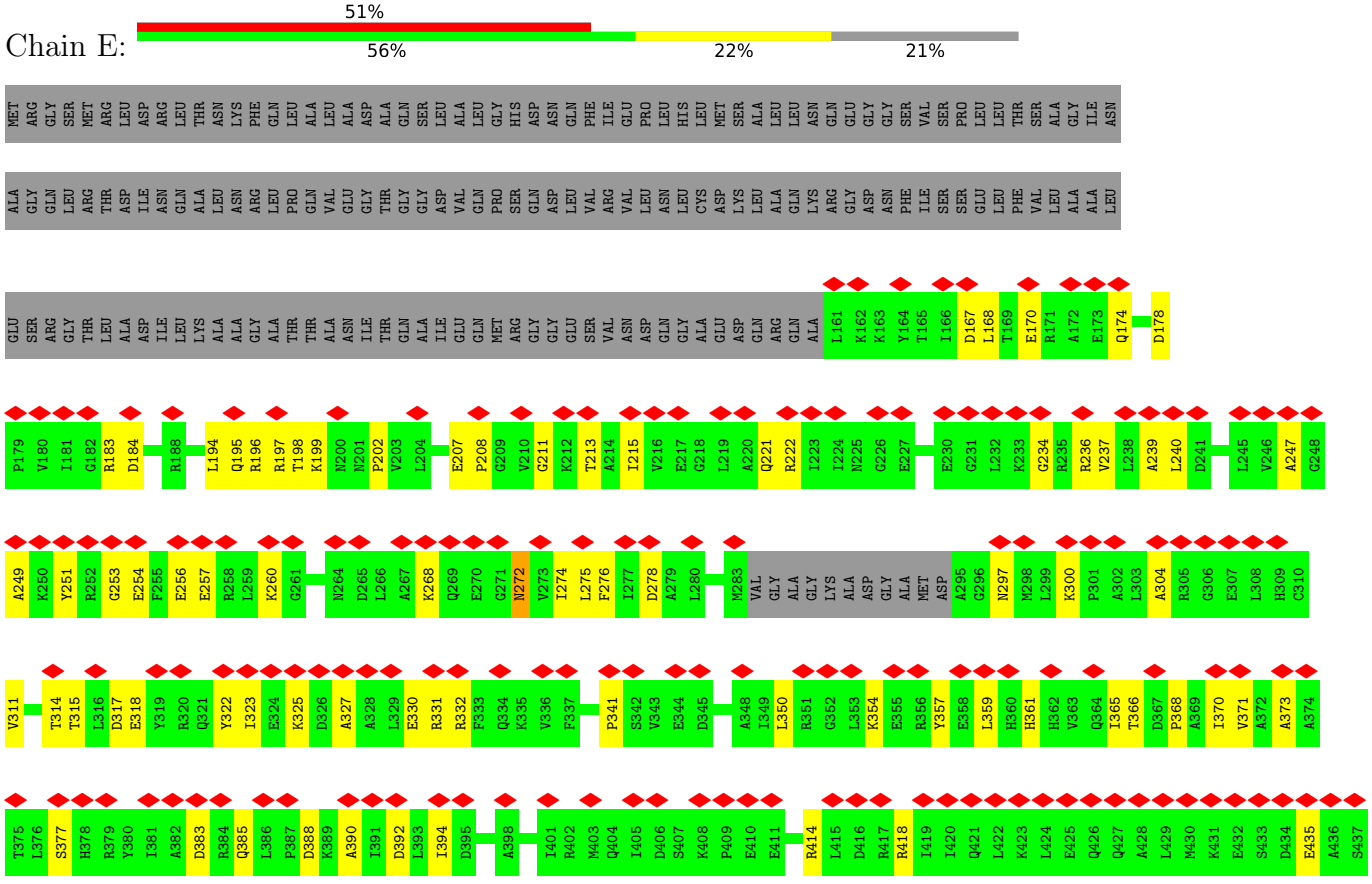
• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

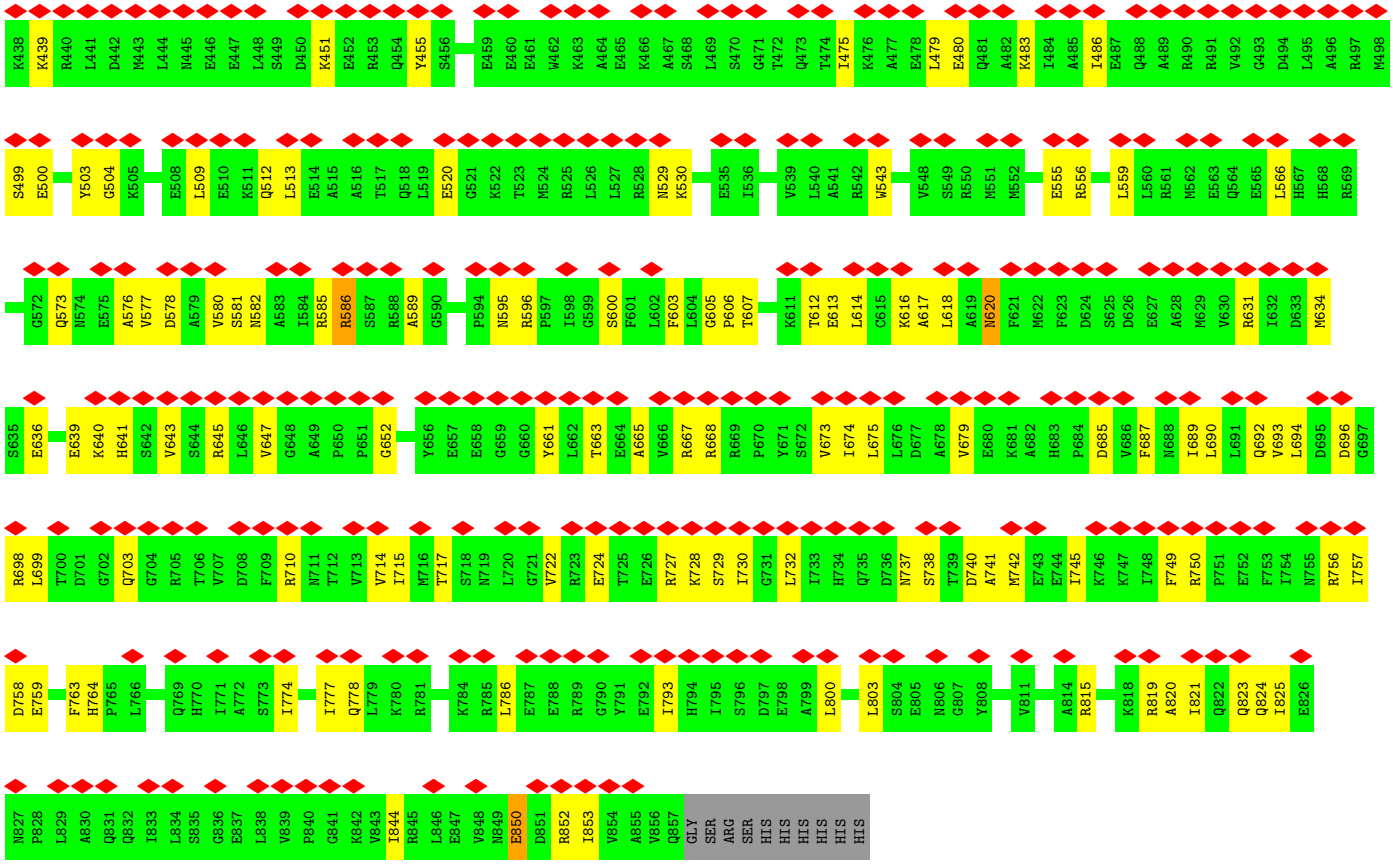




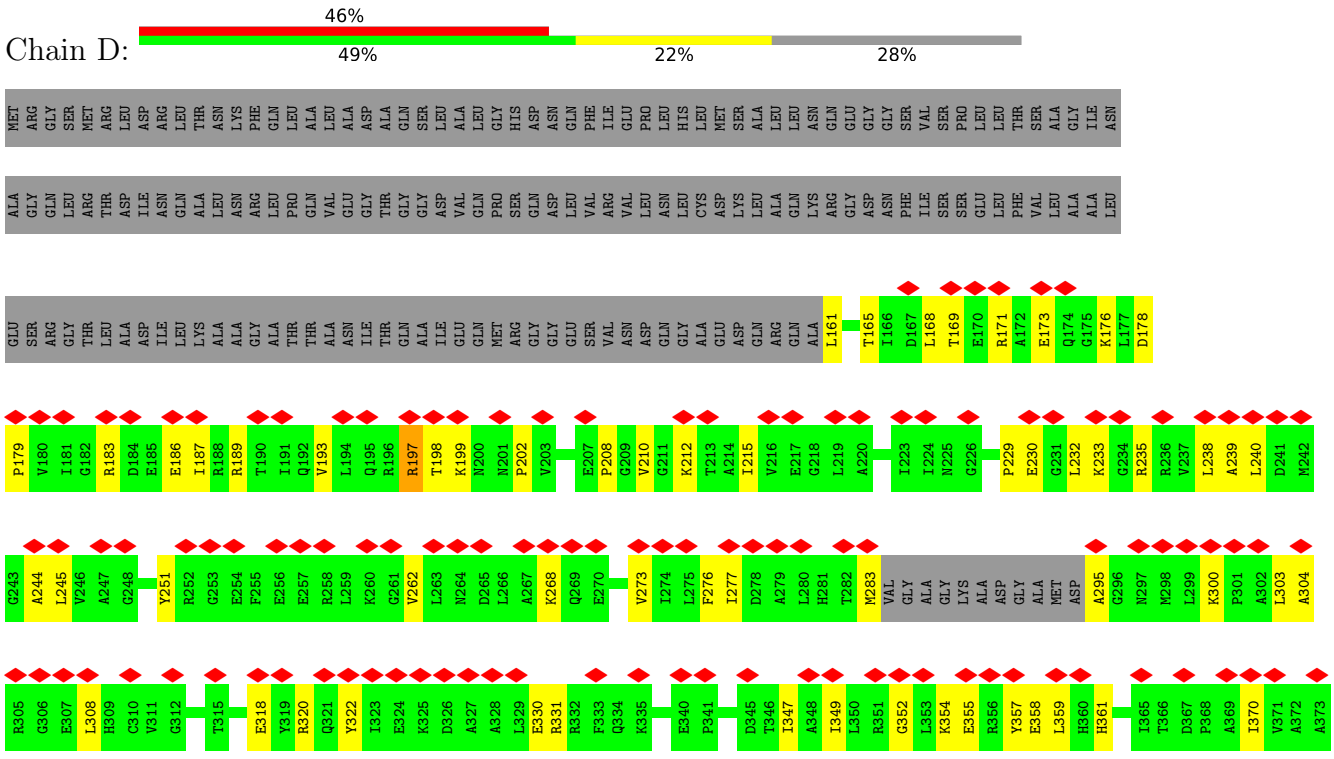
• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

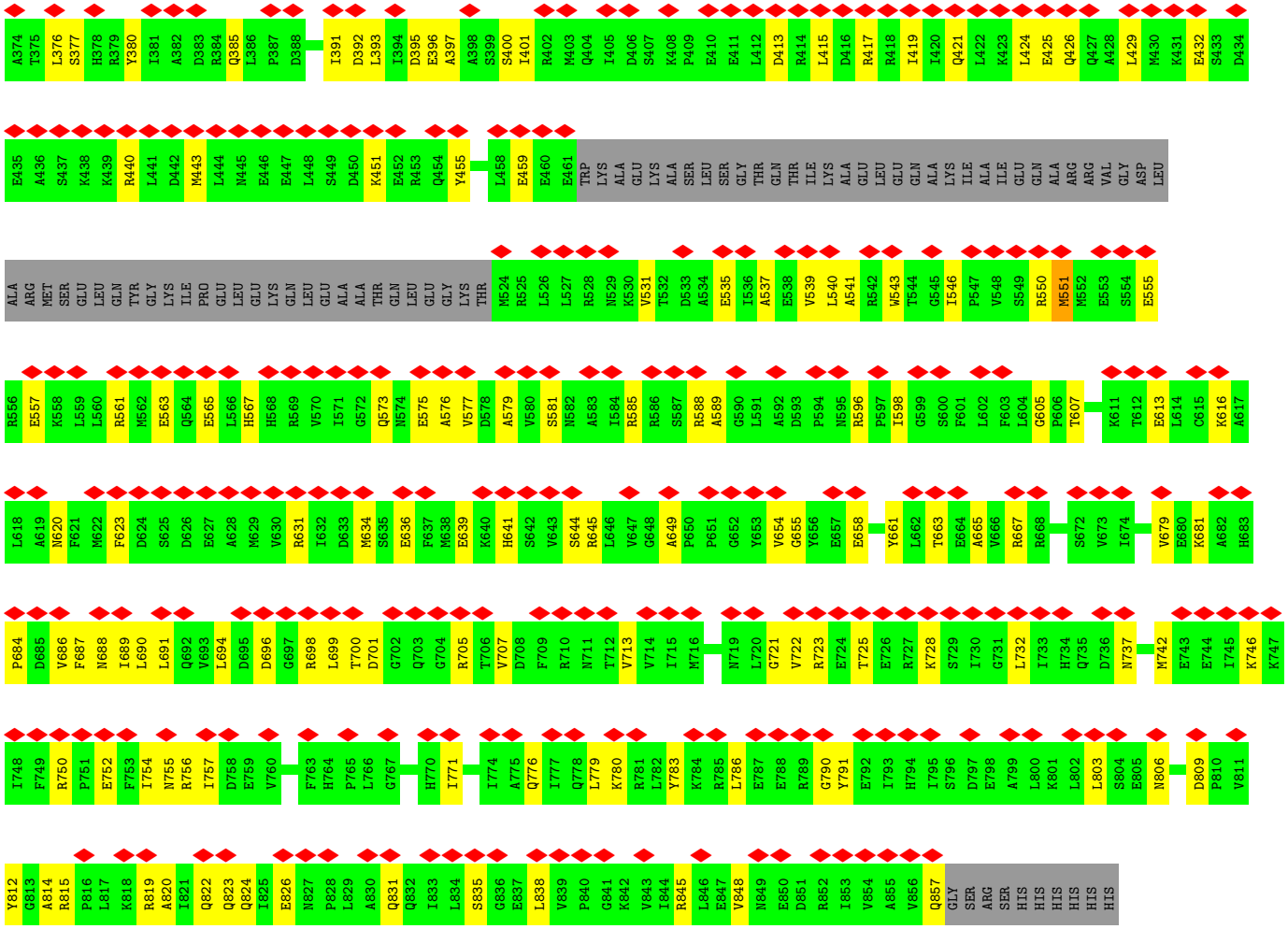
Chain E:





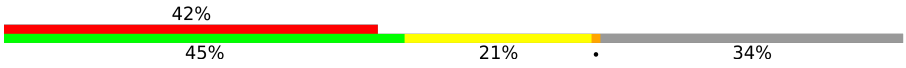
• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

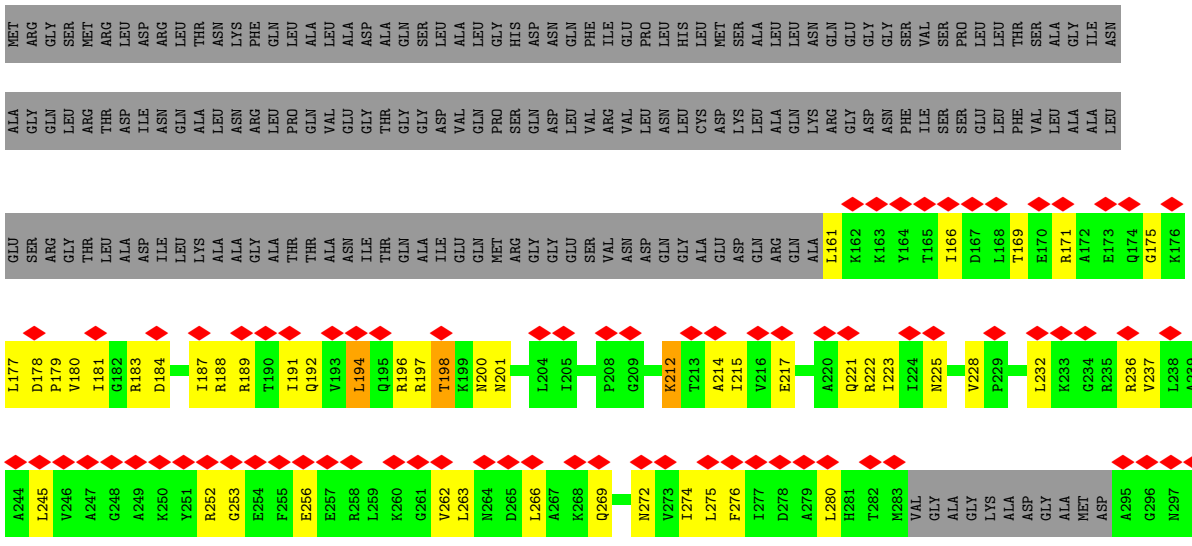


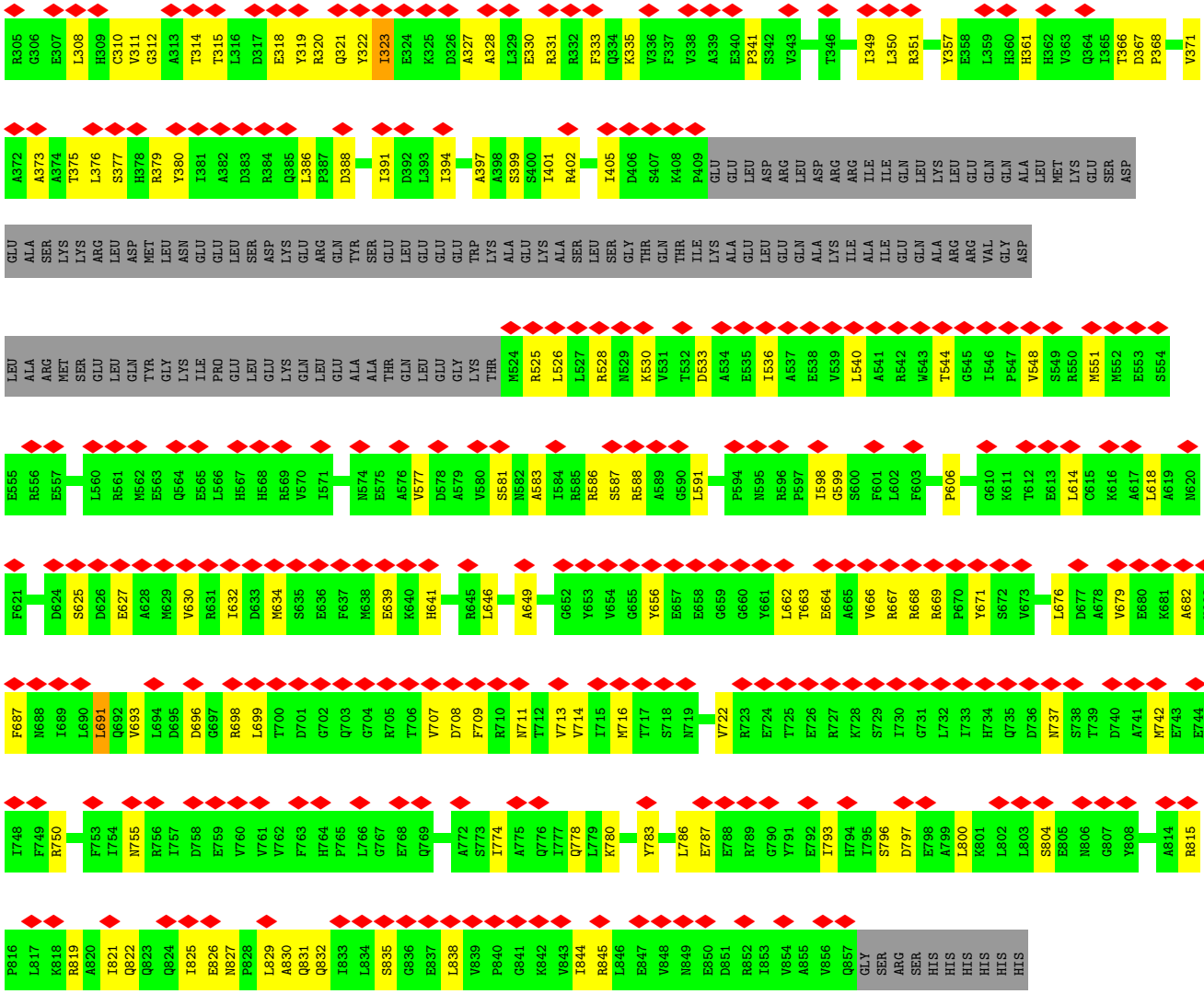


• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

Chain B:

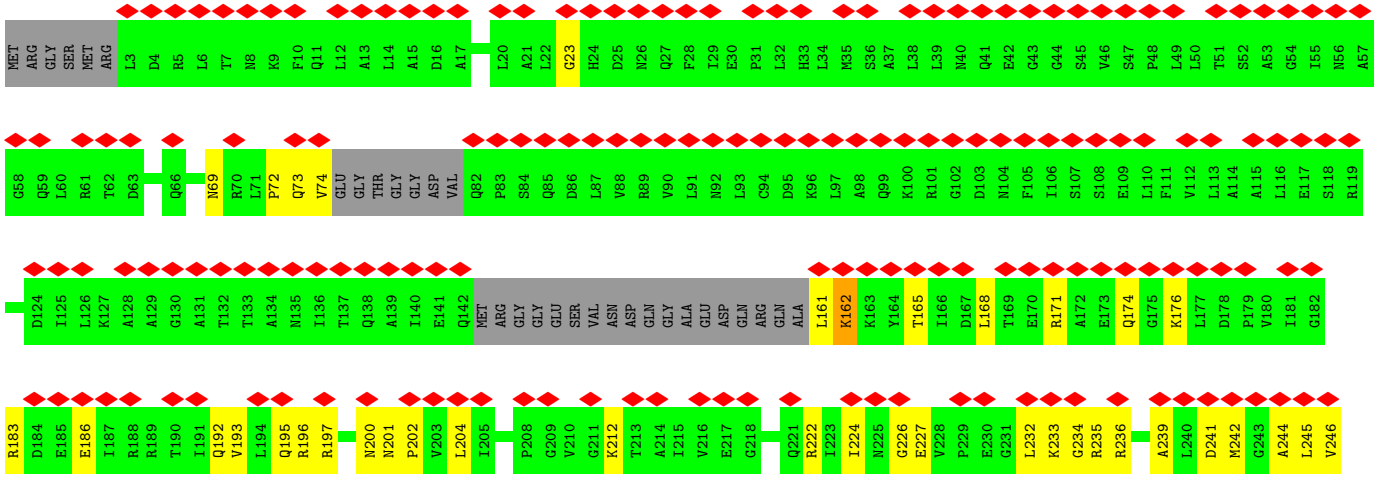


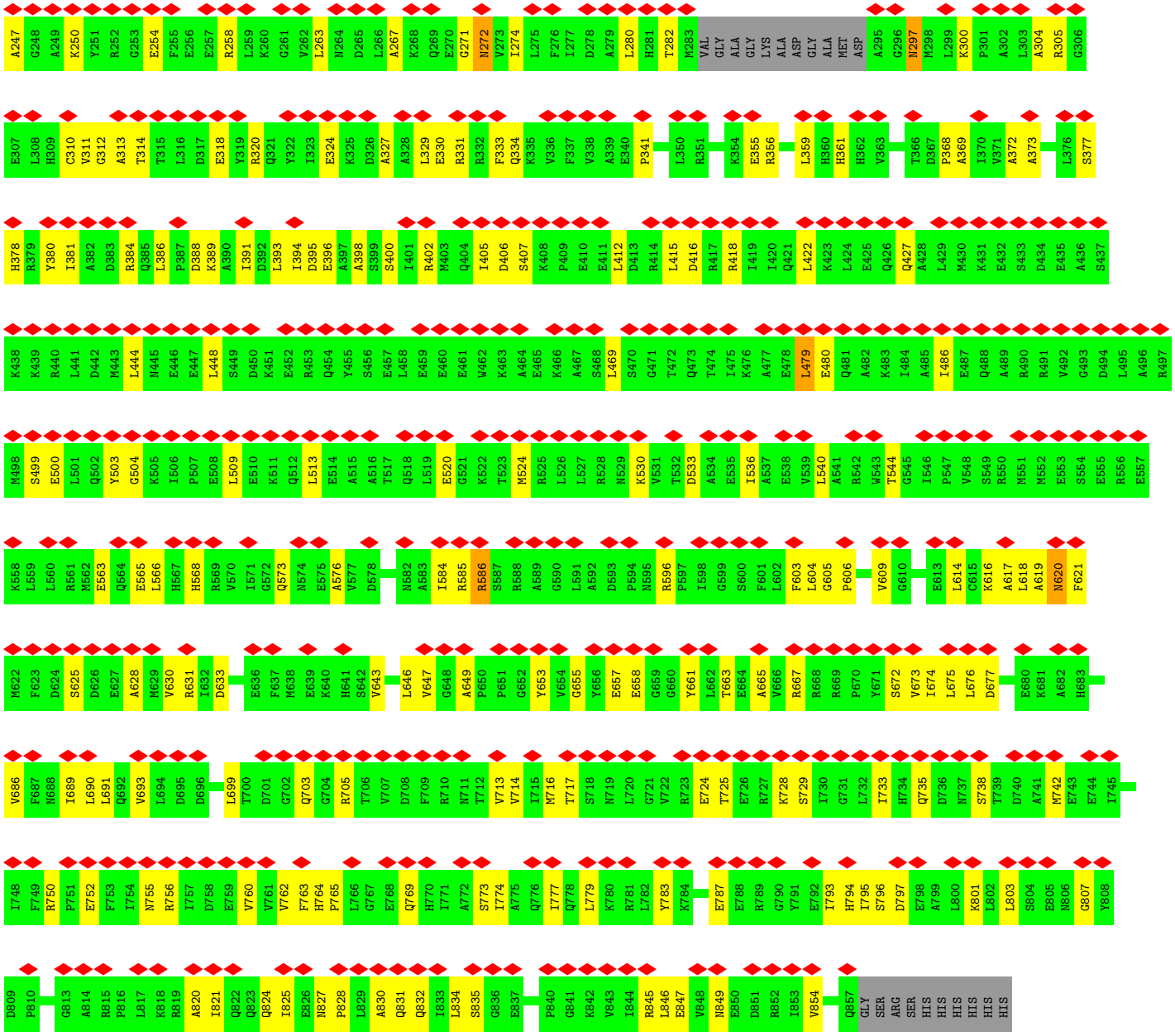




• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

Chain A:




A247 G248 A249 K250 Y251 R252 G253 E254 F255 E256 E257 R258 L259 K260 G261 V262 L263 N264 D265 L266 A267 K268 Q269 E270 G271 N272 V273 I274 L275 F276 I277 D278 A279 L280 H281 T282 M283 VAL GLY ALA GLY LYS ALA ASP GLY ALA MET ASP A295 G296 N297 M298 L299 K300 P301 A302 L303 A304 R305 G306
E307 L308 H309 C310 V311 G312 A313 T314 T315 L316 D317 E318 Y319 R320 Q321 Y322 I323 E324 K325 D326 A327 A328 L329 E330 R331 R332 F333 Q334 K335 V336 F337 V338 A339 E340 P341 L350 R351 K354 E355 R356 L359 H360 H361 H362 V363 T366 D367 P368 A369 I370 V371 A372 A373 L376 S377
H378 R379 Y380 I381 A382 D383 R384 Q385 L386 P387 D388 K389 A390 I391 D392 L393 I394 D395 E396 A397 A398 S399 S400 I401 R402 M403 Q404 I405 D406 S407 K408 P409 E410 E411 L412 D413 R414 L415 D416 R417 R418 I419 I420 Q421 L422 K423 L424 E425 Q426 Q427 A428 L429 M430 K431 E432 S433 D434 E435 A436 S437
K438 K439 R440 L441 D442 M443 L444 N445 E446 E447 L448 S449 D450 K451 E452 R453 Q454 Y455 S456 E457 L458 E459 E460 E461 W462 K463 A464 E465 K466 A467 S468 L469 S470 G471 T472 Q473 T474 I475 K476 A477 E478 L479 E480 Q481 A482 K483 I484 A485 I486 E487 Q488 A489 R490 R491 V492 G493 D494 L495 A496 R497
M498 S499 E500 L501 Q502 Y503 G504 K505 I506 P507 E508 L509 E510 K511 Q512 L513 E514 A515 A516 T517 Q518 L519 E520 G521 K522 T523 M524 R525 L526 L527 R528 N529 K530 V531 T532 D533 A534 E535 I536 A537 E538 V539 L540 A541 R542 W543 T544 G545 I546 P547 V548 S549 R550 M551 M552 E553 S554 E555 R556 E557
K558 L559 L560 R561 M562 E563 Q564 E565 L566 H567 H568 R569 V570 I571 G572 Q573 N574 E575 A576 V577 D578 N582 A583 I584 R585 R586 S587 R588 A589 G590 L591 A592 D593 P594 N595 R596 P597 I598 G599 S600 F601 L602 F603 L604 G605 P606 V609 G610 E613 L614 C615 K616 A617 L618 A619 N620 F621
M622 F623 D624 S625 D626 E627 A628 M629 V630 R631 I632 D633 E636 F637 M638 E639 K640 H641 S642 V643 L646 V647 G648 A649 P650 P651 G652 Y653 V654 G655 Y656 E657 E658 G659 G660 Y661 L662 T663 E664 A665 V666 R667 R668 R669 P670 Y671 S672 V673 I674 L675 L676 D677 E680 K681 A682 H683
V686 F687 N688 I689 L690 L691 Q692 V693 L694 D695 D696 L699 T700 D701 G702 Q703 G704 R705 T706 V707 D708 F709 R710 N711 T712 V713 V714 I715 M716 T717 S718 N719 L720 G721 V722 R723 E724 T725 E726 R727 K728 S729 I730 G731 L732 I733 H734 Q735 D736 N737 S738 T739 D740 A741 M742 E743 E744 I745
I748 F749 R750 P751 E752 F753 I754 N755 R756 I757 D758 E759 V760 V761 V762 F763 H764 P765 L766 G767 E768 Q769 H770 I771 A772 S773 I774 A775 Q776 I777 Q778 L779 K780 R781 L782 Y783 K784 E787 E788 R789 G790 Y791 E792 I793 H794 I795 S796 D797 E798 A799 L800 K801 L802 L803 S804 E805 N806 G807 Y808
D809 P810 G813 A814 R815 P816 L817 K818 R819 A820 I821 Q822 Q823 Q824 I825 E826 N827 P828 L829 A830 Q831 Q832 I833 L834 S835 G836 E837 P840 G841 K842 V843 I844 R845 L846 E847 V848 N849 E850 D851 R852 I853 V854 Q857 GLY SER ARG SER HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60000	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 ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.757	Depositor
Minimum map value	-1.595	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.225	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/5909	0.60	2/7815 (0.0%)
1	B	0.33	0/4582	0.64	3/6178 (0.0%)
1	C	0.34	0/5025	0.64	0/6766
1	D	0.32	0/5025	0.62	0/6766
1	E	0.31	0/5512	0.60	1/7420 (0.0%)
1	F	0.32	0/5512	0.61	1/7420 (0.0%)
All	All	0.32	0/31565	0.62	7/42365 (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
1	B	0	3
1	C	0	1
1	D	0	4
1	E	0	1
1	F	0	2
All	All	0	11

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	682	ALA	C-N-CA	6.61	138.21	121.70
1	E	194	LEU	CA-CB-CG	6.37	129.96	115.30
1	B	194	LEU	CA-CB-CG	6.37	129.95	115.30
1	B	691	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	A	271	GLY	N-CA-C	5.59	127.07	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	339	ALA	C-N-CA	5.27	134.87	121.70
1	A	271	GLY	C-N-CA	5.16	134.61	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	THR	Peptide
1	B	322	TYR	Peptide
1	B	405	ILE	Peptide
1	C	409	PRO	Peptide
1	D	550	ARG	Peptide
1	D	551	MET	Peptide
1	D	623	PHE	Peptide
1	D	848	VAL	Peptide
1	E	850	GLU	Peptide
1	F	636	GLU	Peptide
1	F	638	MET	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	A	5841	0	5696	169	0
1	B	4518	0	4613	121	0
1	C	4960	0	5051	177	0
1	D	4960	0	5051	140	0
1	E	5442	0	5552	144	0
1	F	5442	0	5551	176	0
2	B	31	0	12	4	0
2	C	62	0	24	4	0
2	D	62	0	24	5	0
2	E	62	0	24	10	0
All	All	31380	0	31598	858	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 14.

All (858) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:TYR:CE1	1:A:73:GLN:N	2.07	1.22
1:E:614:LEU:O	1:E:618:LEU:HB2	1.54	1.06
1:B:663:THR:O	1:B:667:ARG:HB2	1.59	1.03
1:F:663:THR:O	1:F:667:ARG:HB2	1.57	1.01
1:C:357:TYR:O	1:C:361:HIS:HB2	1.58	1.01
1:C:643:VAL:O	1:C:647:VAL:HB	1.61	1.00
1:E:318:GLU:O	1:E:322:TYR:HB2	1.62	1.00
1:C:743:GLU:O	1:C:747:LYS:HB2	1.63	0.99
1:D:820:ALA:O	1:D:824:GLN:HB2	1.63	0.98
1:D:251:TYR:CZ	1:A:74:VAL:CA	2.48	0.96
1:E:577:VAL:O	1:E:581:SER:HB2	1.66	0.95
1:C:617:ALA:O	1:C:621:PHE:HB2	1.66	0.95
1:C:663:THR:O	1:C:667:ARG:HB2	1.68	0.94
1:F:820:ALA:O	1:F:824:GLN:HB2	1.66	0.94
1:A:500:GLU:O	1:A:504:GLY:HA3	1.66	0.94
1:A:783:TYR:O	1:A:787:GLU:HB2	1.69	0.93
1:E:251:TYR:HE1	1:A:73:GLN:N	1.49	0.93
1:D:819:ARG:O	1:D:823:GLN:HB3	1.67	0.92
1:B:783:TYR:O	1:B:787:GLU:HB2	1.71	0.90
1:E:500:GLU:O	1:E:504:GLY:HA3	1.70	0.90
1:D:251:TYR:CE1	1:A:74:VAL:CA	2.55	0.90
1:D:251:TYR:CE1	1:A:74:VAL:C	2.46	0.88
1:E:251:TYR:HE1	1:A:73:GLN:CA	1.86	0.87
1:E:357:TYR:O	1:E:361:HIS:HB2	1.75	0.86
1:B:821:ILE:O	1:B:825:ILE:HB	1.75	0.86
1:A:355:GLU:O	1:A:359:LEU:HB2	1.76	0.86
1:E:251:TYR:CZ	1:A:73:GLN:N	2.43	0.85
1:D:391:ILE:O	1:D:395:ASP:HB2	1.77	0.84
1:B:373:ALA:O	1:B:377:SER:HB3	1.75	0.84
1:F:221:GLN:O	1:F:225:ASN:HB2	1.76	0.84
1:E:373:ALA:O	1:E:377:SER:HB3	1.78	0.84
1:F:576:ALA:O	1:F:580:VAL:HB	1.78	0.83
1:E:475:ILE:O	1:E:479:LEU:HB2	1.80	0.81
1:D:686:VAL:O	1:D:690:LEU:HB2	1.80	0.81
1:E:578:ASP:O	1:E:582:ASN:HB2	1.81	0.81
1:D:419:ILE:HG22	1:D:451:LYS:HB3	1.62	0.81
1:A:724:GLU:O	1:A:728:LYS:HB3	1.79	0.81
1:A:643:VAL:O	1:A:647:VAL:HB	1.82	0.80
1:A:821:ILE:O	1:A:825:ILE:HB	1.82	0.80
1:F:251:TYR:HE1	1:A:69:ASN:CA	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:TYR:O	1:D:361:HIS:HB2	1.82	0.79
1:F:469:LEU:O	1:F:473:GLN:HB2	1.85	0.77
1:F:169:THR:O	1:F:173:GLU:HB2	1.85	0.77
1:F:830:ALA:O	1:F:834:LEU:HB2	1.84	0.77
1:A:738:SER:O	1:A:742:MET:HB2	1.85	0.77
1:E:616:LYS:O	1:E:620:ASN:HB2	1.85	0.77
1:F:802:LEU:O	1:F:806:ASN:HB2	1.84	0.76
1:E:663:THR:O	1:E:667:ARG:HB2	1.85	0.76
1:F:686:VAL:O	1:F:690:LEU:HB3	1.85	0.76
1:D:819:ARG:HG2	1:D:822:GLN:HE21	1.52	0.75
1:C:576:ALA:O	1:C:580:VAL:HB	1.86	0.75
1:C:578:ASP:O	1:C:582:ASN:HB2	1.86	0.75
1:E:738:SER:O	1:E:742:MET:HB2	1.86	0.74
1:A:402:ARG:O	1:A:406:ASP:HB2	1.88	0.74
1:E:251:TYR:CE1	1:A:73:GLN:CA	2.67	0.73
1:F:509:LEU:O	1:F:513:LEU:HB2	1.89	0.73
1:E:323:ILE:HG13	1:E:325:LYS:H	1.54	0.72
1:A:752:GLU:HA	1:A:755:ASN:HB2	1.73	0.71
1:C:372:ALA:O	1:C:376:LEU:HB2	1.91	0.70
1:B:583:ALA:O	1:B:587:SER:HB3	1.91	0.70
1:F:687:PHE:O	1:F:691:LEU:HB2	1.92	0.70
1:B:221:GLN:O	1:B:225:ASN:HB2	1.91	0.69
1:C:783:TYR:O	1:C:787:GLU:HB2	1.91	0.69
1:D:663:THR:O	1:D:667:ARG:HB2	1.93	0.69
1:D:631:ARG:NH2	2:D:902:AGS:O2G	2.27	0.68
1:B:800:LEU:O	1:B:804:SER:HB3	1.94	0.68
1:F:797:ASP:O	1:F:801:LYS:HB2	1.94	0.68
1:C:619:ALA:O	1:C:623:PHE:HB2	1.93	0.67
1:D:585:ARG:O	1:D:589:ALA:HB2	1.94	0.67
1:A:412:LEU:O	1:A:416:ASP:HB2	1.95	0.67
1:C:821:ILE:O	1:C:825:ILE:HB	1.94	0.67
1:A:655:GLY:HA2	1:A:658:GLU:HB3	1.77	0.67
1:C:451:LYS:O	1:C:455:TYR:HB3	1.95	0.67
1:C:577:VAL:O	1:C:581:SER:HB2	1.94	0.67
1:F:277:ILE:HD13	1:F:283:MET:HG3	1.76	0.67
1:C:429:LEU:O	1:C:439:LYS:NZ	2.28	0.67
1:C:457:GLU:O	1:C:461:GLU:HB3	1.95	0.67
1:A:222:ARG:HG3	1:A:227:GLU:HB2	1.75	0.66
1:C:618:LEU:HD23	1:C:715:ILE:HD11	1.76	0.66
1:E:674:ILE:HB	1:E:714:VAL:HA	1.78	0.66
1:C:373:ALA:O	1:C:377:SER:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:821:ILE:O	1:E:825:ILE:HB	1.96	0.65
1:D:212:LYS:HA	1:D:215:ILE:HD12	1.78	0.65
1:A:444:LEU:O	1:A:448:LEU:HB2	1.96	0.65
1:E:435:GLU:O	1:E:439:LYS:HB2	1.96	0.65
1:D:318:GLU:O	1:D:322:TYR:HB2	1.97	0.65
1:B:380:TYR:OH	1:B:711:ASN:ND2	2.30	0.65
1:C:170:GLU:HG2	1:C:174:GLN:HE22	1.62	0.65
1:E:499:SER:O	1:E:503:TYR:HB2	1.96	0.65
1:B:375:THR:O	1:B:379:ARG:HB2	1.96	0.64
1:F:164:TYR:OH	1:F:258:ARG:NH1	2.30	0.64
1:E:603:PHE:HB2	1:E:717:THR:HA	1.78	0.64
1:C:577:VAL:O	1:C:581:SER:CB	2.46	0.64
1:C:674:ILE:HB	1:C:714:VAL:HG23	1.79	0.64
1:E:631:ARG:HD3	1:D:698:ARG:HD2	1.80	0.64
1:A:242:MET:SD	1:A:282:THR:OG1	2.55	0.64
1:C:318:GLU:O	1:C:322:TYR:HB2	1.98	0.64
1:E:509:LEU:O	1:E:513:LEU:HB2	1.98	0.64
1:F:475:ILE:O	1:F:479:LEU:HB2	1.98	0.63
1:B:350:LEU:HD22	1:B:394:ILE:HD12	1.80	0.63
1:A:204:LEU:HB3	1:A:212:LYS:HD2	1.81	0.63
1:C:750:ARG:HG2	1:D:722:VAL:HG21	1.81	0.63
1:E:197:ARG:O	1:E:332:ARG:NH1	2.32	0.63
1:F:196:ARG:HE	1:A:396:GLU:HB2	1.62	0.63
1:D:239:ALA:HA	1:D:276:PHE:HB3	1.80	0.63
1:F:605:GLY:O	1:F:719:ASN:ND2	2.32	0.63
1:E:170:GLU:HG2	1:E:174:GLN:HE22	1.62	0.63
1:F:161:LEU:N	1:F:265:ASP:OD2	2.32	0.63
1:E:184:ASP:OD1	1:E:222:ARG:NH2	2.31	0.63
1:E:774:ILE:O	1:E:778:GLN:HB2	1.98	0.62
1:D:169:THR:O	1:D:173:GLU:HB2	1.98	0.62
1:F:559:LEU:HB3	1:F:585:ARG:HG2	1.81	0.62
1:F:662:LEU:O	1:F:666:VAL:HB	2.00	0.62
1:E:737:ASN:O	1:E:741:ALA:HB3	1.97	0.62
1:D:742:MET:O	1:D:746:LYS:HB2	1.99	0.62
1:C:327:ALA:HA	1:C:330:GLU:HG2	1.82	0.62
1:C:690:LEU:O	1:C:694:LEU:HB2	1.99	0.62
1:F:391:ILE:O	1:F:395:ASP:HB2	2.00	0.62
1:D:831:GLN:O	1:D:835:SER:HB2	1.99	0.62
1:F:263:LEU:O	1:F:267:ALA:HB2	2.00	0.61
1:F:469:LEU:HD11	1:F:529:ASN:HD21	1.65	0.61
1:C:457:GLU:O	1:C:461:GLU:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:ARG:NE	1:B:671:TYR:O	2.34	0.61
1:E:696:ASP:O	1:E:698:ARG:NH1	2.34	0.61
1:D:531:VAL:HA	1:D:535:GLU:HG3	1.82	0.61
1:A:769:GLN:O	1:A:773:SER:HB2	1.99	0.61
1:D:691:LEU:HD22	1:D:750:ARG:HH21	1.65	0.61
1:B:240:LEU:H	1:B:275:LEU:HD11	1.66	0.61
1:B:831:GLN:O	1:B:835:SER:HB2	2.00	0.61
1:F:356:ARG:O	1:F:360:HIS:HB3	2.01	0.61
1:D:644:SER:HB3	1:D:649:ALA:HA	1.82	0.61
1:C:537:ALA:O	1:C:541:ALA:HB2	2.01	0.61
1:A:663:THR:O	1:A:667:ARG:HB2	2.00	0.61
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.83	0.61
1:A:617:ALA:O	1:A:621:PHE:HB2	2.01	0.61
1:A:794:HIS:HB2	1:A:845:ARG:HG2	1.82	0.61
1:F:297:ASN:HB3	1:A:246:VAL:HG21	1.82	0.60
1:C:781:ARG:HG2	1:C:785:ARG:HE	1.66	0.60
1:F:819:ARG:O	1:F:823:GLN:HB3	2.02	0.60
1:E:183:ARG:HH12	1:E:341:PRO:HB3	1.66	0.60
1:B:276:PHE:HA	1:B:311:VAL:HB	1.82	0.60
1:F:577:VAL:O	1:F:581:SER:HB2	2.01	0.60
1:B:315:THR:O	1:B:319:TYR:N	2.33	0.60
1:B:698:ARG:HA	1:B:709:PHE:H	1.66	0.60
1:A:674:ILE:HB	1:A:714:VAL:HA	1.83	0.60
1:C:831:GLN:O	1:C:835:SER:HB2	2.01	0.60
1:E:645:ARG:NH2	1:D:701:ASP:O	2.35	0.60
1:C:759:GLU:OE2	1:D:823:GLN:NE2	2.35	0.60
1:D:655:GLY:HA2	1:D:658:GLU:HB2	1.83	0.60
1:B:223:ILE:HG12	1:B:232:LEU:HB3	1.84	0.60
1:D:197:ARG:NH1	1:D:198:THR:OG1	2.35	0.60
1:C:208:PRO:HB2	1:B:327:ALA:HB3	1.83	0.59
1:F:202:PRO:HG2	1:F:311:VAL:HG13	1.84	0.59
1:E:605:GLY:HA3	1:E:763:PHE:HB2	1.84	0.59
1:A:280:LEU:HD22	1:A:312:GLY:HA3	1.84	0.59
1:A:703:GLN:HG2	1:A:705:ARG:HH21	1.68	0.59
1:E:698:ARG:HD2	1:E:710:ARG:HH11	1.67	0.59
1:D:421:GLN:O	1:D:425:GLU:HB2	2.02	0.59
1:A:661:TYR:O	1:A:665:ALA:HB2	2.03	0.59
1:B:399:SER:HA	1:B:402:ARG:HE	1.68	0.59
1:D:413:ASP:O	1:D:417:ARG:HB2	2.02	0.59
1:C:722:VAL:O	1:C:726:GLU:HB2	2.02	0.59
1:F:400:SER:OG	1:E:195:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:786:LEU:HB3	1:F:791:TYR:HB2	1.85	0.59
1:A:596:ARG:NH2	1:A:756:ARG:O	2.36	0.59
1:A:649:ALA:HB1	1:A:653:TYR:HB3	1.84	0.59
1:C:541:ALA:HB1	1:C:547:PRO:HA	1.84	0.59
1:D:551:MET:O	1:D:555:GLU:HB2	2.02	0.59
1:E:673:VAL:HG13	1:E:715:ILE:HD12	1.84	0.58
2:E:901:AGS:S1G	2:E:901:AGS:O1B	2.61	0.58
1:A:509:LEU:O	1:A:513:LEU:HB2	2.02	0.58
1:C:636:GLU:O	1:C:645:ARG:NH1	2.36	0.58
1:F:726:GLU:HG2	1:F:765:PRO:HG2	1.85	0.58
1:D:183:ARG:NH1	1:D:186:GLU:OE2	2.30	0.58
1:E:727:ARG:NH2	1:E:740:ASP:OD2	2.36	0.58
1:D:809:ASP:HB3	1:D:812:TYR:HB2	1.84	0.58
1:F:318:GLU:O	1:F:322:TYR:HB2	2.03	0.58
1:A:631:ARG:HG2	1:A:675:LEU:HD23	1.84	0.58
1:C:181:ILE:HG23	1:D:424:LEU:HB3	1.85	0.58
1:C:426:GLN:HA	1:C:429:LEU:HB2	1.86	0.58
1:F:377:SER:HB2	1:F:389:LYS:HD2	1.84	0.58
1:F:573:GLN:HB3	1:F:576:ALA:HB3	1.85	0.58
1:F:169:THR:O	1:F:173:GLU:CB	2.51	0.58
1:F:469:LEU:HA	1:F:472:THR:HG22	1.85	0.58
1:C:357:TYR:HA	1:C:360:HIS:HB3	1.85	0.58
1:E:573:GLN:NE2	1:E:764:HIS:O	2.35	0.58
1:E:639:GLU:OE2	1:E:645:ARG:NH1	2.34	0.58
1:E:820:ALA:HA	1:E:823:GLN:HG2	1.86	0.58
1:B:242:MET:HA	1:B:245:LEU:HD12	1.86	0.58
1:A:314:THR:OG1	1:A:318:GLU:OE1	2.22	0.58
1:D:187:ILE:HG12	1:D:215:ILE:HG23	1.84	0.57
1:A:242:MET:HA	1:A:245:LEU:HB2	1.86	0.57
1:A:329:LEU:O	1:A:333:PHE:N	2.37	0.57
1:A:676:LEU:HB2	1:A:716:MET:HA	1.86	0.57
1:C:826:GLU:HB3	1:B:591:LEU:HD23	1.86	0.57
1:E:314:THR:OG1	1:E:318:GLU:OE1	2.22	0.57
1:D:561:ARG:NH1	1:D:565:GLU:OE2	2.37	0.57
1:F:196:ARG:NH2	1:A:396:GLU:OE1	2.38	0.57
1:E:631:ARG:NH2	2:E:902:AGS:O3G	2.38	0.57
1:F:509:LEU:HD23	1:F:512:GLN:HE21	1.69	0.57
1:F:537:ALA:O	1:F:541:ALA:CB	2.53	0.57
1:E:211:GLY:O	1:E:215:ILE:N	2.37	0.57
1:A:359:LEU:HD21	1:A:479:LEU:HD12	1.87	0.57
1:F:577:VAL:O	1:F:581:SER:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:596:ARG:HH22	1:F:756:ARG:HB3	1.70	0.57
1:A:657:GLU:HA	1:A:703:GLN:HE22	1.70	0.57
1:F:388:ASP:OD2	1:E:331:ARG:NH1	2.38	0.57
1:F:344:GLU:HA	1:F:347:ILE:HD12	1.86	0.56
1:F:803:LEU:HD22	1:F:821:ILE:HA	1.86	0.56
1:D:168:LEU:HD23	1:D:171:ARG:HD3	1.87	0.56
1:D:393:LEU:O	1:D:397:ALA:CB	2.54	0.56
1:C:745:ILE:O	1:C:749:PHE:N	2.37	0.56
1:F:374:ALA:O	1:F:378:HIS:HB2	2.06	0.56
1:E:237:VAL:HG22	1:E:274:ILE:HB	1.87	0.56
1:F:405:ILE:HA	1:F:527:LEU:HD22	1.88	0.56
1:E:354:LYS:HB2	1:E:365:ILE:HG13	1.87	0.56
1:D:684:PRO:O	1:D:688:ASN:ND2	2.38	0.56
1:B:222:ARG:HG2	1:B:228:VAL:HB	1.87	0.56
1:C:579:ALA:HB1	1:C:759:GLU:HG3	1.87	0.56
1:F:222:ARG:O	1:F:227:GLU:N	2.39	0.56
1:A:174:GLN:HG2	1:A:176:LYS:HE2	1.87	0.56
1:F:778:GLN:HE21	1:F:818:LYS:HD3	1.71	0.56
1:C:678:ALA:H	1:C:718:SER:HA	1.71	0.56
1:F:686:VAL:O	1:F:690:LEU:CB	2.53	0.56
1:F:596:ARG:HH12	1:F:756:ARG:HD3	1.71	0.56
1:E:640:LYS:NZ	1:E:685:ASP:OD2	2.39	0.56
1:B:240:LEU:HD22	1:B:262:VAL:HG11	1.87	0.56
1:B:663:THR:HA	1:B:666:VAL:HG22	1.88	0.56
1:C:222:ARG:HG3	1:C:227:GLU:HB2	1.88	0.56
1:A:803:LEU:HD11	1:A:825:ILE:HD11	1.86	0.56
1:C:724:GLU:O	1:C:728:LYS:HB3	2.07	0.55
1:E:643:VAL:O	1:E:647:VAL:HB	2.06	0.55
1:A:573:GLN:HB3	1:A:576:ALA:HB3	1.86	0.55
1:F:394:ILE:O	1:F:398:ALA:CB	2.53	0.55
1:F:396:GLU:HB2	1:E:196:ARG:HE	1.71	0.55
1:F:550:ARG:NE	1:F:624:ASP:OD1	2.34	0.55
1:A:827:ASN:O	1:A:831:GLN:HB2	2.06	0.55
1:D:819:ARG:O	1:D:823:GLN:CB	2.50	0.55
1:A:247:ALA:O	1:A:258:ARG:NH1	2.40	0.55
1:A:630:VAL:HB	1:A:674:ILE:HA	1.89	0.55
1:C:616:LYS:O	1:C:620:ASN:HB2	2.06	0.55
1:F:170:GLU:HA	1:F:173:GLU:HB3	1.88	0.55
1:F:326:ASP:HB3	1:F:329:LEU:HB2	1.88	0.55
1:F:780:LYS:HA	1:F:783:TYR:HD2	1.72	0.55
1:A:250:LYS:HB2	1:A:254:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:619:ALA:O	1:F:623:PHE:HB2	2.07	0.55
1:C:758:ASP:HA	1:D:819:ARG:HH21	1.71	0.55
1:C:410:GLU:H	1:C:526:LEU:HD22	1.71	0.55
1:A:369:ALA:O	1:A:373:ALA:HB2	2.07	0.55
2:C:901:AGS:O3B	2:C:901:AGS:O2A	2.25	0.55
1:C:267:ALA:HA	1:C:307:GLU:HB3	1.89	0.55
1:F:825:ILE:O	1:F:829:LEU:N	2.37	0.55
1:D:303:LEU:HD23	1:D:308:LEU:HD21	1.88	0.55
1:D:699:LEU:HB3	1:D:707:VAL:HB	1.87	0.55
1:C:373:ALA:O	1:C:377:SER:CB	2.55	0.55
1:B:376:LEU:HA	1:B:379:ARG:HB3	1.89	0.55
1:F:189:ARG:NH1	1:A:396:GLU:OE2	2.39	0.54
1:E:634:MET:HG3	1:E:679:VAL:HG23	1.88	0.54
1:B:166:ILE:HG21	1:A:305:ARG:HD2	1.89	0.54
1:C:199:LYS:HB3	1:C:334:GLN:HB2	1.90	0.54
1:C:409:PRO:HB2	1:C:412:LEU:HD13	1.88	0.54
1:C:458:LEU:HA	1:C:461:GLU:HB3	1.88	0.54
1:C:583:ALA:O	1:C:587:SER:HB3	2.08	0.54
1:F:496:ALA:O	1:F:500:GLU:HB2	2.07	0.54
1:B:269:GLN:HG2	1:B:272:ASN:HB2	1.87	0.54
1:C:632:ILE:HD11	1:C:665:ALA:HB3	1.88	0.54
1:F:602:LEU:HD22	1:F:753:PHE:HE2	1.72	0.54
1:E:595:ASN:OD1	1:E:698:ARG:NH1	2.40	0.54
1:E:692:GLN:O	1:E:696:ASP:HB2	2.06	0.54
1:D:393:LEU:O	1:D:397:ALA:HB2	2.06	0.54
1:A:300:LYS:O	1:A:304:ALA:HB2	2.07	0.54
1:A:520:GLU:HG2	1:A:524:MET:HG3	1.89	0.54
1:C:350:LEU:HB3	1:C:370:ILE:HB	1.89	0.54
1:E:786:LEU:HD13	1:E:793:ILE:HD12	1.88	0.54
1:A:393:LEU:HD11	1:A:540:LEU:HD13	1.87	0.54
1:F:183:ARG:HD3	1:F:215:ILE:HG12	1.90	0.54
1:D:455:TYR:O	1:D:459:GLU:HB2	2.08	0.54
1:B:181:ILE:HD13	1:B:349:ILE:HA	1.89	0.54
1:B:361:HIS:HA	1:B:402:ARG:HD3	1.90	0.54
1:F:831:GLN:O	1:F:835:SER:CB	2.55	0.54
1:F:591:LEU:HD21	1:A:830:ALA:HB3	1.89	0.54
1:A:796:SER:OG	1:A:845:ARG:NH2	2.41	0.54
1:F:638:MET:SD	1:F:638:MET:N	2.79	0.54
1:B:536:ILE:O	1:B:540:LEU:HB3	2.08	0.54
1:F:373:ALA:O	1:F:377:SER:OG	2.22	0.53
1:E:728:LYS:HD3	1:E:737:ASN:HD22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ALA:O	1:B:331:ARG:N	2.40	0.53
1:A:604:LEU:HB2	1:A:762:VAL:HG22	1.89	0.53
1:C:349:ILE:HG13	1:C:387:PRO:HG3	1.89	0.53
1:B:588:ARG:HA	1:B:598:ILE:HD13	1.89	0.53
1:C:663:THR:O	1:C:667:ARG:CB	2.51	0.53
1:F:394:ILE:O	1:F:398:ALA:HB3	2.08	0.53
1:E:170:GLU:O	1:E:174:GLN:NE2	2.41	0.53
1:D:240:LEU:HD22	1:D:277:ILE:HG12	1.90	0.53
1:D:819:ARG:HA	1:D:822:GLN:HG2	1.91	0.53
1:B:540:LEU:O	1:B:544:THR:HB	2.07	0.53
1:B:684:PRO:HA	1:B:687:PHE:HD2	1.73	0.53
1:C:597:PRO:HG3	1:C:694:LEU:HA	1.90	0.53
1:E:350:LEU:HD11	1:E:390:ALA:HB1	1.90	0.53
1:A:783:TYR:HE1	1:A:793:ILE:H	1.55	0.53
1:B:366:THR:OG1	1:B:367:ASP:N	2.34	0.53
1:A:183:ARG:NH2	1:A:186:GLU:OE2	2.41	0.53
1:F:591:LEU:HD13	1:A:827:ASN:HA	1.90	0.53
1:D:688:ASN:OD1	1:D:750:ARG:NH2	2.39	0.53
1:B:632:ILE:HD11	1:B:662:LEU:HD13	1.90	0.53
1:A:368:PRO:O	1:A:372:ALA:HB3	2.09	0.53
1:C:212:LYS:NZ	2:C:901:AGS:S1G	2.82	0.53
1:C:738:SER:O	1:C:742:MET:CB	2.56	0.53
1:F:581:SER:OG	1:F:585:ARG:NH1	2.42	0.53
1:D:636:GLU:O	1:D:645:ARG:NH2	2.41	0.53
1:A:628:ALA:HB1	1:A:672:SER:HA	1.91	0.53
1:A:674:ILE:N	1:A:713:VAL:O	2.40	0.53
1:E:383:ASP:O	1:E:385:GLN:NE2	2.42	0.53
1:D:397:ALA:HA	1:D:539:VAL:HG21	1.91	0.53
1:A:738:SER:O	1:A:742:MET:CB	2.56	0.53
1:A:797:ASP:O	1:A:801:LYS:HB2	2.08	0.53
1:C:161:LEU:O	1:C:165:THR:OG1	2.27	0.53
1:B:774:ILE:O	1:B:778:GLN:HB2	2.09	0.53
1:B:819:ARG:HA	1:B:822:GLN:HG2	1.91	0.53
1:C:774:ILE:O	1:C:778:GLN:HB2	2.09	0.52
1:F:783:TYR:O	1:F:787:GLU:HB3	2.09	0.52
1:D:754:ILE:HA	1:D:757:ILE:HG12	1.91	0.52
1:A:373:ALA:O	1:A:377:SER:CB	2.57	0.52
1:C:199:LYS:NZ	1:D:392:ASP:OD2	2.33	0.52
1:D:318:GLU:O	1:D:322:TYR:CB	2.57	0.52
1:A:384:ARG:HE	1:A:389:LYS:HB3	1.74	0.52
1:F:619:ALA:O	1:F:624:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:784:LYS:HA	1:F:787:GLU:HG2	1.90	0.52
1:E:586:ARG:NH2	1:E:759:GLU:OE2	2.42	0.52
1:B:676:LEU:HB2	1:B:716:MET:HG2	1.90	0.52
1:C:327:ALA:HB3	1:D:208:PRO:HD2	1.90	0.52
1:E:631:ARG:HG2	1:E:675:LEU:HD23	1.91	0.52
1:E:738:SER:O	1:E:742:MET:CB	2.55	0.52
1:C:652:GLY:H	1:D:654:VAL:HB	1.75	0.52
1:F:356:ARG:O	1:F:360:HIS:CB	2.57	0.52
1:D:240:LEU:HD21	1:D:245:LEU:HD11	1.90	0.52
1:D:575:GLU:O	1:D:579:ALA:HB2	2.09	0.52
1:B:318:GLU:HA	1:B:321:GLN:HB2	1.91	0.52
1:D:377:SER:HB3	1:D:393:LEU:HD12	1.91	0.52
1:D:426:GLN:HA	1:D:429:LEU:HB2	1.90	0.52
1:B:826:GLU:O	1:B:830:ALA:N	2.41	0.52
1:F:208:PRO:O	1:E:331:ARG:NH2	2.43	0.52
1:E:385:GLN:OE1	1:D:331:ARG:NH2	2.43	0.52
1:B:536:ILE:O	1:B:540:LEU:CB	2.58	0.52
1:C:631:ARG:NH1	1:B:696:ASP:OD2	2.42	0.52
1:F:463:LYS:HD3	1:F:466:LYS:HD3	1.90	0.52
1:F:619:ALA:HA	1:F:623:PHE:HD2	1.74	0.52
1:E:483:LYS:HA	1:E:486:ILE:HG22	1.92	0.52
1:E:724:GLU:OE1	1:E:727:ARG:NH2	2.43	0.52
2:E:901:AGS:O3B	2:E:901:AGS:O2A	2.26	0.52
1:B:540:LEU:O	1:B:544:THR:CB	2.57	0.52
1:B:691:LEU:HD21	1:B:750:ARG:HD2	1.92	0.52
1:E:612:THR:OG1	2:E:902:AGS:O1B	2.28	0.52
1:C:342:SER:OG	1:C:343:VAL:N	2.41	0.51
1:C:583:ALA:HA	1:C:586:ARG:HE	1.74	0.51
1:F:347:ILE:HG12	1:F:371:VAL:HA	1.92	0.51
1:F:593:ASP:HB3	1:F:596:ARG:HG3	1.93	0.51
1:E:392:ASP:OD2	1:D:199:LYS:NZ	2.42	0.51
1:E:745:ILE:HG23	1:E:749:PHE:HB2	1.91	0.51
1:D:721:GLY:O	1:D:725:THR:HB	2.10	0.51
1:E:239:ALA:HA	1:E:276:PHE:HB3	1.93	0.51
1:E:612:THR:N	2:E:902:AGS:O1A	2.39	0.51
1:A:235:ARG:HG2	1:A:274:ILE:HG13	1.92	0.51
1:A:380:TYR:HB3	1:A:544:THR:HG21	1.92	0.51
1:B:699:LEU:N	1:B:707:VAL:O	2.43	0.51
1:A:165:THR:OG1	1:A:239:ALA:O	2.21	0.51
1:F:251:TYR:CE1	1:A:69:ASN:CA	2.86	0.51
1:C:812:TYR:HB3	1:B:755:ASN:HD21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:399:SER:OG	1:F:402:ARG:NH2	2.44	0.51
1:F:509:LEU:O	1:F:513:LEU:CB	2.58	0.51
1:D:639:GLU:OE1	1:D:645:ARG:NH2	2.43	0.51
1:B:180:VAL:HB	1:B:183:ARG:HD2	1.91	0.51
1:A:263:LEU:O	1:A:267:ALA:CB	2.58	0.51
1:E:661:TYR:O	1:E:665:ALA:CB	2.58	0.51
1:D:376:LEU:HB3	1:D:540:LEU:HD22	1.92	0.51
1:A:422:LEU:HD22	1:A:444:LEU:HD11	1.93	0.51
1:C:666:VAL:HG11	1:C:674:ILE:HG12	1.92	0.51
1:D:786:LEU:HA	1:D:791:TYR:HD2	1.76	0.51
1:B:391:ILE:HG21	2:B:901:AGS:H1'	1.92	0.51
1:A:596:ARG:HH12	1:A:756:ARG:HB3	1.76	0.51
1:C:617:ALA:O	1:C:621:PHE:CB	2.51	0.51
1:C:636:GLU:OE1	1:C:645:ARG:NH2	2.43	0.51
1:C:780:LYS:HA	1:C:783:TYR:HD2	1.76	0.51
1:E:256:GLU:O	1:E:260:LYS:HB2	2.11	0.51
1:D:771:ILE:HG12	1:D:814:ALA:HB2	1.92	0.51
1:B:253:GLY:HA2	1:B:256:GLU:HB2	1.93	0.51
1:C:318:GLU:O	1:C:322:TYR:CB	2.58	0.51
1:D:605:GLY:HA2	1:D:725:THR:HG21	1.92	0.51
1:B:214:ALA:HA	1:B:217:GLU:HG2	1.92	0.51
1:A:499:SER:O	1:A:503:TYR:HB2	2.11	0.51
1:C:752:GLU:OE2	2:D:902:AGS:H8	2.11	0.51
1:E:300:LYS:O	1:E:304:ALA:HB2	2.10	0.51
1:A:183:ARG:HD3	1:A:341:PRO:HB3	1.94	0.51
1:A:373:ALA:O	1:A:377:SER:HB3	2.10	0.51
1:C:384:ARG:HB2	1:C:389:LYS:HB3	1.93	0.50
1:E:318:GLU:O	1:E:322:TYR:CB	2.48	0.50
1:B:577:VAL:O	1:B:581:SER:CB	2.59	0.50
1:B:625:SER:OG	1:B:627:GLU:OE1	2.28	0.50
1:B:649:ALA:HB3	1:B:656:TYR:HB2	1.93	0.50
1:B:664:GLU:OE1	1:B:667:ARG:NH2	2.44	0.50
1:A:369:ALA:HB1	1:A:536:ILE:HG13	1.93	0.50
1:C:451:LYS:O	1:C:455:TYR:CB	2.59	0.50
1:C:738:SER:O	1:C:742:MET:HB2	2.10	0.50
1:F:831:GLN:O	1:F:835:SER:HB2	2.10	0.50
1:E:256:GLU:O	1:E:260:LYS:CB	2.60	0.50
1:D:822:GLN:O	1:D:826:GLU:HB2	2.10	0.50
1:B:177:LEU:HD13	1:B:217:GLU:HB2	1.93	0.50
1:A:234:GLY:O	1:A:272:ASN:ND2	2.44	0.50
1:A:673:VAL:HG22	1:A:713:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:HB2	1:B:200:ASN:HA	1.94	0.50
1:C:616:LYS:O	1:C:620:ASN:CB	2.59	0.50
1:F:242:MET:HA	1:F:245:LEU:HB2	1.92	0.50
1:D:783:TYR:HA	1:D:786:LEU:HD12	1.94	0.50
1:C:750:ARG:HD2	1:D:607:THR:HG21	1.92	0.50
1:F:472:THR:HA	1:F:475:ILE:HG22	1.94	0.50
1:A:168:LEU:HA	1:A:171:ARG:HB2	1.94	0.50
1:C:195:GLN:NE2	1:D:400:SER:OG	2.45	0.50
1:E:509:LEU:HA	1:E:512:GLN:HG2	1.94	0.50
1:E:820:ALA:O	1:E:824:GLN:HB2	2.11	0.50
1:F:354:LYS:HA	1:F:357:TYR:HB2	1.92	0.50
1:B:201:ASN:HB2	1:B:333:PHE:CD1	2.46	0.50
1:F:819:ARG:O	1:F:823:GLN:CB	2.60	0.50
1:D:283:MET:O	1:D:295:ALA:N	2.45	0.50
1:A:690:LEU:HA	1:A:693:VAL:HG22	1.94	0.50
1:C:747:LYS:O	1:D:723:ARG:NH1	2.44	0.50
1:F:823:GLN:HA	1:F:827:ASN:HD22	1.77	0.50
1:D:721:GLY:O	1:D:725:THR:CB	2.60	0.50
1:F:586:ARG:HA	1:F:591:LEU:HD12	1.93	0.49
1:C:194:LEU:HD22	1:C:309:HIS:HE1	1.76	0.49
1:C:351:ARG:NH2	1:C:367:ASP:OD2	2.41	0.49
1:C:745:ILE:HA	1:C:749:PHE:HD2	1.77	0.49
1:E:668:ARG:HH21	1:D:320:ARG:HH21	1.60	0.49
1:B:614:LEU:O	1:B:618:LEU:CB	2.60	0.49
1:B:780:LYS:HA	1:B:783:TYR:HD2	1.76	0.49
1:F:822:GLN:HA	1:F:826:GLU:HB2	1.94	0.49
1:D:679:VAL:HG22	1:D:687:PHE:HE1	1.76	0.49
1:A:584:ILE:HD11	1:A:618:LEU:HD21	1.93	0.49
1:C:687:PHE:HD2	1:C:748:ILE:HG12	1.76	0.49
1:E:234:GLY:O	1:E:272:ASN:ND2	2.45	0.49
1:E:368:PRO:HA	1:E:371:VAL:HG12	1.93	0.49
1:C:783:TYR:O	1:C:787:GLU:CB	2.61	0.49
1:F:373:ALA:O	1:F:377:SER:CB	2.60	0.49
1:F:409:PRO:HB2	1:F:412:LEU:HD23	1.95	0.49
1:C:600:SER:N	1:C:758:ASP:OD2	2.45	0.49
1:C:631:ARG:HG2	1:C:675:LEU:HD23	1.94	0.49
1:B:341:PRO:HG2	1:B:386:LEU:HB2	1.94	0.49
1:C:830:ALA:HA	1:C:833:ILE:HG22	1.95	0.49
1:D:557:GLU:HG3	1:D:561:ARG:HH21	1.78	0.49
1:A:565:GLU:HA	1:A:568:HIS:HD1	1.78	0.49
1:C:561:ARG:HB2	1:C:564:GLN:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:THR:O	1:B:379:ARG:CB	2.60	0.49
1:A:832:GLN:HA	1:A:835:SER:HB3	1.95	0.49
1:C:202:PRO:HG2	1:C:311:VAL:HG13	1.95	0.49
1:C:599:GLY:HA3	1:C:713:VAL:HG13	1.95	0.49
1:C:831:GLN:O	1:C:835:SER:CB	2.60	0.49
1:D:165:THR:HG22	1:D:238:LEU:HB3	1.95	0.49
1:D:396:GLU:OE1	1:D:543:TRP:NE1	2.40	0.49
1:D:537:ALA:O	1:D:541:ALA:CB	2.61	0.49
1:B:832:GLN:HB3	1:B:838:LEU:HD13	1.94	0.49
1:A:263:LEU:O	1:A:267:ALA:HB2	2.12	0.49
1:A:620:ASN:HA	1:A:625:SER:H	1.77	0.49
1:E:317:ASP:N	1:E:317:ASP:OD1	2.45	0.48
1:D:354:LYS:O	1:D:358:GLU:HB2	2.13	0.48
1:D:585:ARG:O	1:D:589:ALA:CB	2.60	0.48
1:B:171:ARG:O	1:B:175:GLY:N	2.46	0.48
1:F:235:ARG:HH11	1:F:274:ILE:HD11	1.77	0.48
1:F:252:ARG:HH12	1:A:250:LYS:HD2	1.78	0.48
1:D:634:MET:HG3	1:D:679:VAL:HA	1.95	0.48
1:A:774:ILE:HA	1:A:777:ILE:HG12	1.94	0.48
1:F:826:GLU:O	1:F:830:ALA:N	2.43	0.48
1:D:193:VAL:HG11	1:D:202:PRO:HB3	1.95	0.48
1:A:405:ILE:HG23	1:A:469:LEU:HD21	1.94	0.48
1:A:661:TYR:O	1:A:665:ALA:CB	2.61	0.48
1:A:738:SER:HB2	1:A:760:VAL:HG11	1.94	0.48
1:C:276:PHE:HD1	1:C:311:VAL:HB	1.78	0.48
1:C:542:ARG:HH12	1:B:189:ARG:HD3	1.78	0.48
1:F:388:ASP:OD1	1:E:199:LYS:NZ	2.47	0.48
1:D:780:LYS:HA	1:D:783:TYR:HD2	1.78	0.48
1:A:691:LEU:HD21	1:A:750:ARG:HH21	1.78	0.48
1:C:632:ILE:HD12	1:C:662:LEU:HD12	1.96	0.48
1:C:723:ARG:O	1:C:727:ARG:CB	2.61	0.48
1:E:607:THR:HB	1:E:815:ARG:HD2	1.96	0.48
1:C:742:MET:O	1:C:746:LYS:HB2	2.13	0.48
2:D:902:AGS:O1A	2:D:902:AGS:O1B	2.31	0.48
1:B:588:ARG:HD2	1:B:598:ILE:HD13	1.96	0.48
1:A:769:GLN:O	1:A:773:SER:CB	2.62	0.48
1:C:189:ARG:HG2	1:C:336:VAL:HG13	1.96	0.48
1:C:537:ALA:O	1:C:541:ALA:CB	2.61	0.48
1:C:346:THR:HG21	1:C:386:LEU:HD13	1.96	0.48
1:C:723:ARG:O	1:C:727:ARG:HB2	2.13	0.48
1:F:620:ASN:HA	1:F:625:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:782:LEU:O	1:F:786:LEU:HB2	2.14	0.48
1:E:253:GLY:O	1:E:257:GLU:N	2.47	0.48
1:D:838:LEU:HG	1:D:857:GLN:HB2	1.95	0.48
1:B:228:VAL:HG21	1:B:232:LEU:HB2	1.95	0.48
1:E:213:THR:OG1	1:E:278:ASP:OD1	2.32	0.48
1:D:563:GLU:O	1:D:567:HIS:ND1	2.35	0.48
1:D:786:LEU:HB3	1:D:791:TYR:HB2	1.94	0.48
1:B:634:MET:HG3	1:B:679:VAL:HA	1.95	0.48
1:C:280:LEU:H	1:C:314:THR:HB	1.79	0.47
1:C:300:LYS:O	1:C:304:ALA:HB2	2.14	0.47
1:C:585:ARG:O	1:C:589:ALA:CB	2.63	0.47
1:C:678:ALA:HA	1:C:719:ASN:H	1.80	0.47
1:F:263:LEU:O	1:F:267:ALA:CB	2.62	0.47
1:E:509:LEU:O	1:E:513:LEU:CB	2.62	0.47
1:E:647:VAL:HA	1:E:689:ILE:HD13	1.96	0.47
1:E:774:ILE:HA	1:E:777:ILE:HG12	1.96	0.47
1:B:169:THR:HG21	1:B:236:ARG:HB2	1.95	0.47
1:B:280:LEU:HD22	1:B:312:GLY:HA3	1.96	0.47
1:C:743:GLU:O	1:C:747:LYS:CB	2.48	0.47
1:F:208:PRO:HG2	1:E:327:ALA:HB2	1.95	0.47
1:F:806:ASN:HB3	1:F:824:GLN:HE22	1.79	0.47
1:F:826:GLU:HA	1:F:829:LEU:HB3	1.95	0.47
1:E:520:GLU:OE1	1:E:529:ASN:ND2	2.45	0.47
1:E:690:LEU:HA	1:E:693:VAL:HG22	1.96	0.47
1:E:850:GLU:O	1:E:852:ARG:N	2.46	0.47
1:D:598:ILE:HB	1:D:713:VAL:HG22	1.95	0.47
1:B:614:LEU:O	1:B:618:LEU:HB3	2.14	0.47
1:C:671:TYR:HA	1:C:712:THR:HB	1.96	0.47
1:F:238:LEU:H	1:F:273:VAL:HG13	1.79	0.47
1:B:201:ASN:ND2	1:B:310:CYS:SG	2.87	0.47
1:B:368:PRO:HA	1:B:371:VAL:HG12	1.95	0.47
1:B:198:THR:OG1	1:B:331:ARG:O	2.30	0.47
1:B:815:ARG:HB3	1:A:756:ARG:HH22	1.79	0.47
1:B:525:ARG:HG3	1:B:526:LEU:HD12	1.96	0.47
1:C:234:GLY:O	1:C:272:ASN:ND2	2.47	0.47
1:C:742:MET:SD	1:D:812:TYR:OH	2.69	0.47
1:F:391:ILE:O	1:F:395:ASP:CB	2.63	0.47
1:F:465:GLU:OE2	1:F:525:ARG:N	2.45	0.47
1:F:644:SER:HA	1:F:647:VAL:HG22	1.96	0.47
1:F:693:VAL:HG22	1:F:709:PHE:HE2	1.80	0.47
1:E:690:LEU:O	1:E:694:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:694:LEU:HD23	1:E:756:ARG:HB2	1.97	0.47
1:D:347:ILE:HG12	1:D:370:ILE:HG22	1.97	0.47
1:D:689:ILE:HG23	1:D:699:LEU:HD13	1.96	0.47
1:B:302:ALA:O	1:B:308:LEU:N	2.48	0.47
1:B:577:VAL:O	1:B:581:SER:HB2	2.15	0.47
1:A:606:PRO:HD3	1:A:725:THR:HG21	1.97	0.47
1:C:677:ASP:OD1	1:C:717:THR:OG1	2.27	0.47
1:F:619:ALA:HB1	1:F:628:ALA:HB3	1.96	0.47
1:E:600:SER:HB2	1:E:757:ILE:HA	1.97	0.47
1:B:827:ASN:HD22	1:A:586:ARG:HH12	1.63	0.47
1:E:689:ILE:HD12	1:E:699:LEU:HD11	1.97	0.47
1:A:388:ASP:HA	1:A:391:ILE:HD12	1.96	0.47
1:F:603:PHE:HB2	1:F:717:THR:HG22	1.97	0.47
1:E:573:GLN:HB3	1:E:576:ALA:HB3	1.97	0.47
1:A:573:GLN:HE22	1:A:764:HIS:H	1.62	0.47
1:E:202:PRO:HG2	1:E:311:VAL:HG13	1.97	0.46
1:B:698:ARG:HG2	1:B:708:ASP:HA	1.96	0.46
1:C:555:GLU:HG2	1:C:559:LEU:HD23	1.96	0.46
1:F:611:LYS:HD2	1:F:717:THR:HG21	1.98	0.46
1:F:633:ASP:HA	1:F:677:ASP:HB2	1.97	0.46
1:E:168:LEU:N	1:E:237:VAL:O	2.40	0.46
1:B:184:ASP:HA	1:B:187:ILE:HG12	1.96	0.46
1:B:831:GLN:O	1:B:835:SER:CB	2.64	0.46
1:A:236:ARG:O	1:A:274:ILE:N	2.48	0.46
1:F:252:ARG:HE	1:A:23:GLY:C	2.18	0.46
1:E:370:ILE:HG22	1:E:394:ILE:HG13	1.97	0.46
1:E:543:TRP:HE1	1:D:189:ARG:HH12	1.64	0.46
1:B:829:LEU:HD11	1:B:844:ILE:HD13	1.96	0.46
1:C:613:GLU:HG3	2:C:902:AGS:C4	2.46	0.46
1:F:800:LEU:HA	1:F:803:LEU:HD12	1.97	0.46
1:E:819:ARG:HH21	1:D:596:ARG:HD2	1.80	0.46
1:D:165:THR:HA	1:D:240:LEU:HA	1.98	0.46
1:D:605:GLY:H	1:D:721:GLY:HA3	1.80	0.46
1:A:192:GLN:O	1:A:196:ARG:NH2	2.45	0.46
1:A:300:LYS:O	1:A:304:ALA:CB	2.64	0.46
1:C:368:PRO:HA	1:C:371:VAL:HG12	1.97	0.46
1:C:672:SER:O	1:C:712:THR:OG1	2.33	0.46
1:F:393:LEU:O	1:F:397:ALA:HB3	2.15	0.46
1:D:238:LEU:HD13	1:D:273:VAL:HG13	1.97	0.46
1:D:355:GLU:O	1:D:359:LEU:HB2	2.15	0.46
1:F:585:ARG:O	1:F:589:ALA:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:ASP:O	1:E:221:GLN:NE2	2.40	0.46
1:A:201:ASN:O	1:A:334:GLN:N	2.48	0.46
1:A:274:ILE:HG23	1:A:311:VAL:HG21	1.97	0.46
1:C:533:ASP:O	1:C:537:ALA:HB2	2.15	0.46
1:C:729:SER:HA	1:C:730:ILE:HA	1.63	0.46
1:E:576:ALA:O	1:E:580:VAL:HB	2.15	0.46
1:E:728:LYS:HA	1:E:732:LEU:HB3	1.98	0.46
1:C:211:GLY:O	1:C:215:ILE:N	2.49	0.46
1:F:341:PRO:HB2	1:F:345:ASP:HB3	1.98	0.46
1:F:499:SER:HB2	1:A:427:GLN:HG3	1.98	0.46
1:E:414:ARG:HB3	1:E:418:ARG:HH21	1.81	0.46
1:D:415:LEU:HD13	1:D:455:TYR:HA	1.97	0.46
1:D:696:ASP:O	1:D:698:ARG:NH1	2.49	0.46
1:D:786:LEU:O	1:D:790:GLY:N	2.45	0.46
1:B:188:ARG:O	1:B:192:GLN:HB2	2.16	0.46
1:F:280:LEU:HD22	1:F:312:GLY:HA3	1.98	0.46
1:F:767:GLY:O	1:F:771:ILE:N	2.41	0.46
1:D:776:GLN:HA	1:D:779:LEU:HD12	1.96	0.46
1:C:573:GLN:HB3	1:C:576:ALA:HB3	1.98	0.45
1:C:575:GLU:O	1:C:579:ALA:HB3	2.15	0.45
1:F:221:GLN:HA	1:F:224:ILE:HG22	1.97	0.45
1:E:585:ARG:O	1:E:589:ALA:CB	2.64	0.45
1:D:178:ASP:HA	1:D:179:PRO:HD3	1.80	0.45
1:D:661:TYR:O	1:D:665:ALA:CB	2.64	0.45
1:B:639:GLU:HG2	1:B:641:HIS:H	1.80	0.45
1:B:819:ARG:NE	1:A:755:ASN:O	2.50	0.45
1:A:356:ARG:NH1	1:A:480:GLU:OE2	2.48	0.45
1:A:369:ALA:O	1:A:373:ALA:CB	2.63	0.45
1:E:451:LYS:O	1:E:455:TYR:HB2	2.16	0.45
1:E:596:ARG:NH2	1:E:758:ASP:OD1	2.49	0.45
1:D:330:GLU:OE2	1:D:331:ARG:NH1	2.48	0.45
1:D:613:GLU:HA	1:D:616:LYS:HE3	1.99	0.45
1:B:191:ILE:HA	1:B:194:LEU:HD12	1.99	0.45
1:A:201:ASN:ND2	1:A:310:CYS:O	2.50	0.45
1:A:204:LEU:HB2	1:A:313:ALA:HB1	1.98	0.45
1:A:378:HIS:HB2	1:A:386:LEU:HD21	1.99	0.45
1:F:357:TYR:HA	1:F:361:HIS:HD2	1.82	0.45
1:F:537:ALA:O	1:F:541:ALA:HB2	2.16	0.45
1:F:616:LYS:O	1:F:620:ASN:HB2	2.16	0.45
1:E:247:ALA:O	1:E:249:ALA:N	2.47	0.45
1:D:251:TYR:CD1	1:A:74:VAL:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:ILE:O	1:D:352:GLY:N	2.49	0.45
1:D:575:GLU:O	1:D:579:ALA:CB	2.64	0.45
1:A:729:SER:HB2	1:A:765:PRO:HD2	1.99	0.45
2:C:902:AGS:O2G	2:C:902:AGS:O1B	2.35	0.45
1:B:800:LEU:O	1:B:804:SER:CB	2.63	0.45
1:C:533:ASP:O	1:C:537:ALA:CB	2.64	0.45
1:E:825:ILE:HG23	1:E:853:ILE:HG21	1.98	0.45
1:B:303:LEU:HG	1:B:308:LEU:HD23	1.99	0.45
1:A:444:LEU:O	1:A:448:LEU:CB	2.65	0.45
1:C:269:GLN:HG3	1:C:273:VAL:HB	1.98	0.45
1:C:299:LEU:O	1:C:303:LEU:N	2.48	0.45
1:C:575:GLU:O	1:C:579:ALA:CB	2.65	0.45
1:C:585:ARG:O	1:C:589:ALA:HB2	2.15	0.45
1:F:649:ALA:HB1	1:F:653:TYR:HB2	1.98	0.45
1:F:812:TYR:HB2	1:F:816:PRO:HD3	1.97	0.45
1:E:606:PRO:HA	1:E:722:VAL:HG13	1.99	0.45
1:B:161:LEU:HG	1:B:262:VAL:HA	1.99	0.45
1:B:586:ARG:HA	1:B:591:LEU:HD22	1.98	0.45
1:A:616:LYS:O	1:A:620:ASN:HB2	2.16	0.45
1:A:820:ALA:O	1:A:824:GLN:HB2	2.16	0.45
1:C:326:ASP:HB3	1:C:329:LEU:HB2	1.98	0.45
1:F:623:PHE:HB3	1:F:671:TYR:CZ	2.52	0.45
1:F:677:ASP:OD1	1:F:717:THR:OG1	2.34	0.45
1:B:166:ILE:HD13	1:A:305:ARG:HH11	1.82	0.45
1:B:240:LEU:HD13	1:B:262:VAL:HG21	1.98	0.45
1:B:599:GLY:HA3	1:B:713:VAL:HA	1.97	0.45
1:A:603:PHE:HB2	1:A:717:THR:HA	1.98	0.45
1:F:487:GLU:OE2	1:F:490:ARG:NH1	2.49	0.45
1:E:687:PHE:HD1	1:E:690:LEU:HD12	1.81	0.45
1:E:687:PHE:O	1:E:750:ARG:NH2	2.50	0.45
1:B:263:LEU:HA	1:B:266:LEU:HD12	1.98	0.45
1:E:636:GLU:OE1	1:D:700:THR:OG1	2.35	0.44
1:D:376:LEU:O	1:D:380:TYR:HB2	2.17	0.44
1:B:237:VAL:HA	1:B:274:ILE:HB	1.99	0.44
1:B:323:ILE:HD13	1:B:323:ILE:HA	1.93	0.44
1:B:630:VAL:HG21	1:B:666:VAL:HG12	1.99	0.44
1:F:496:ALA:O	1:F:500:GLU:CB	2.64	0.44
1:E:249:ALA:HB1	1:E:254:GLU:HB3	1.98	0.44
1:B:796:SER:OG	1:B:797:ASP:N	2.51	0.44
1:A:193:VAL:HG11	1:A:202:PRO:HB3	1.98	0.44
1:A:195:GLN:HE21	1:A:196:ARG:HH21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:NH1	1:A:324:GLU:OE1	2.49	0.44
1:C:691:LEU:O	1:C:695:ASP:HB2	2.17	0.44
1:E:213:THR:OG1	2:E:901:AGS:O1B	2.35	0.44
1:D:567:HIS:CE1	1:D:577:VAL:HG11	2.53	0.44
1:C:698:ARG:HH11	1:C:710:ARG:HH11	1.66	0.44
1:B:786:LEU:HD22	1:B:793:ILE:HD11	1.98	0.44
1:A:686:VAL:HA	1:A:689:ILE:HG12	2.00	0.44
1:C:668:ARG:HE	1:B:320:ARG:NH1	2.15	0.44
1:E:613:GLU:O	1:E:617:ALA:CB	2.66	0.44
1:B:388:ASP:OD2	1:A:331:ARG:NH2	2.51	0.44
1:A:633:ASP:HA	1:A:677:ASP:HB2	2.00	0.44
1:C:196:ARG:HG3	1:D:396:GLU:HB2	1.99	0.44
1:C:260:LYS:HE3	1:D:244:ALA:HA	2.00	0.44
1:A:394:ILE:O	1:A:398:ALA:HB3	2.18	0.44
1:A:509:LEU:O	1:A:513:LEU:CB	2.66	0.44
1:A:821:ILE:HG23	1:A:825:ILE:HD12	2.00	0.44
1:C:263:LEU:O	1:C:267:ALA:HB2	2.18	0.44
1:C:555:GLU:HG3	1:C:558:LYS:HE2	2.00	0.44
1:C:650:PRO:HG2	1:D:641:HIS:HB3	1.99	0.44
1:B:693:VAL:HG13	1:B:709:PHE:HD2	1.82	0.44
1:A:845:ARG:NH1	1:A:847:GLU:OE2	2.51	0.44
1:C:641:HIS:O	1:C:644:SER:OG	2.30	0.44
1:F:167:ASP:HA	1:F:238:LEU:HA	1.99	0.44
1:A:241:ASP:O	1:A:245:LEU:N	2.50	0.44
1:A:619:ALA:HB1	1:A:628:ALA:HB3	2.00	0.44
1:C:384:ARG:NH1	1:B:330:GLU:OE2	2.45	0.44
1:F:537:ALA:O	1:F:541:ALA:HB3	2.17	0.44
1:A:327:ALA:HA	1:A:330:GLU:HG2	1.98	0.44
1:A:803:LEU:O	1:A:807:GLY:HA3	2.17	0.44
1:C:377:SER:HB2	1:C:389:LYS:HG3	2.00	0.43
1:C:418:ARG:O	1:C:422:LEU:HB2	2.18	0.43
1:C:439:LYS:HA	1:C:439:LYS:HD3	1.79	0.43
1:F:792:GLU:OE2	1:F:794:HIS:NE2	2.47	0.43
1:C:168:LEU:HD22	1:C:217:GLU:HG2	2.00	0.43
1:C:317:ASP:O	1:C:321:GLN:HB2	2.19	0.43
1:D:694:LEU:HD13	1:D:756:ARG:HB2	2.00	0.43
1:D:752:GLU:HA	1:D:755:ASN:HB2	2.00	0.43
1:A:197:ARG:O	1:A:200:ASN:ND2	2.45	0.43
1:C:183:ARG:NH2	1:C:341:PRO:HD2	2.33	0.43
1:E:737:ASN:O	1:E:741:ALA:CB	2.63	0.43
1:E:793:ILE:HG12	1:E:844:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:OD1	1:B:222:ARG:NH2	2.37	0.43
1:A:795:ILE:HG12	1:A:846:LEU:HD12	2.00	0.43
1:C:183:ARG:HH22	1:C:341:PRO:HD2	1.83	0.43
1:F:791:TYR:HD1	1:F:844:ILE:HD11	1.83	0.43
1:A:195:GLN:HE21	1:A:196:ARG:NH2	2.16	0.43
1:C:279:ALA:HB1	1:C:281:HIS:CE1	2.53	0.43
1:C:608:GLY:HA2	1:C:815:ARG:HD2	1.98	0.43
1:D:393:LEU:HD21	1:D:540:LEU:HD13	2.01	0.43
1:B:639:GLU:HG3	1:B:641:HIS:HD2	1.83	0.43
1:A:631:ARG:HA	1:A:675:LEU:HB3	2.00	0.43
1:A:693:VAL:HG11	1:A:699:LEU:HD12	2.01	0.43
1:F:654:VAL:HG22	1:E:652:GLY:HA3	2.01	0.43
1:D:232:LEU:HA	1:D:235:ARG:HD2	2.01	0.43
1:D:722:VAL:HG13	1:D:723:ARG:HG3	2.01	0.43
1:B:192:GLN:O	1:B:196:ARG:NE	2.51	0.43
1:A:563:GLU:OE1	1:A:585:ARG:NH2	2.51	0.43
1:C:429:LEU:HD23	1:B:351:ARG:HH12	1.83	0.43
1:C:619:ALA:HA	1:C:623:PHE:HD2	1.82	0.43
1:F:483:LYS:HA	1:F:486:ILE:HG22	2.01	0.43
1:F:627:GLU:HB2	1:F:669:ARG:NH2	2.33	0.43
1:D:208:PRO:O	1:D:385:GLN:NE2	2.47	0.43
1:A:361:HIS:NE2	1:A:395:ASP:OD1	2.43	0.43
1:C:619:ALA:O	1:C:624:ASP:N	2.52	0.43
1:F:179:PRO:HA	1:F:221:GLN:HE22	1.83	0.43
1:D:161:LEU:HD21	1:D:262:VAL:HG13	2.01	0.43
1:D:230:GLU:HA	1:D:233:LYS:HG2	2.00	0.43
1:C:679:VAL:HG21	1:C:690:LEU:HD11	2.01	0.43
1:C:820:ALA:HA	1:C:823:GLN:HG2	2.01	0.43
1:A:161:LEU:HD22	1:A:162:LYS:HZ2	1.84	0.43
1:C:751:PRO:HB3	1:D:812:TYR:CD1	2.54	0.42
1:F:742:MET:HA	1:F:745:ILE:HB	2.00	0.42
1:E:167:ASP:HB2	1:E:236:ARG:HH21	1.84	0.42
1:E:803:LEU:HD13	1:E:821:ILE:HG12	2.00	0.42
1:C:532:THR:H	1:C:535:GLU:HB2	1.83	0.42
1:C:686:VAL:HA	1:C:689:ILE:HG12	2.01	0.42
1:E:359:LEU:HD23	1:E:480:GLU:HB2	2.01	0.42
2:B:901:AGS:O2G	2:B:901:AGS:O1B	2.36	0.42
1:F:827:ASN:HD21	1:E:586:ARG:HD2	1.83	0.42
1:D:330:GLU:HG3	1:D:331:ARG:HG3	2.00	0.42
1:A:605:GLY:HA3	1:A:606:PRO:HD3	1.84	0.42
1:E:207:GLU:HA	1:E:208:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:566:LEU:HD13	1:E:614:LEU:HD11	1.99	0.42
1:D:573:GLN:HB3	1:D:576:ALA:HB3	2.01	0.42
1:D:728:LYS:HD3	1:D:732:LEU:HD22	2.01	0.42
1:D:803:LEU:HD23	1:D:806:ASN:HD22	1.84	0.42
1:B:827:ASN:HA	1:B:830:ALA:HB3	2.00	0.42
1:F:269:GLN:HG3	1:F:272:ASN:HB3	2.00	0.42
1:F:625:SER:OG	1:F:669:ARG:NH2	2.42	0.42
1:C:299:LEU:HD22	1:C:308:LEU:HD22	2.00	0.42
1:F:560:LEU:HD11	1:A:834:LEU:HB3	2.02	0.42
1:E:612:THR:OG1	2:E:902:AGS:O3G	2.27	0.42
1:E:661:TYR:O	1:E:665:ALA:HB3	2.20	0.42
1:F:585:ARG:O	1:F:589:ALA:HB2	2.19	0.42
1:F:615:CYS:O	1:F:619:ALA:CB	2.68	0.42
1:C:447:GLU:O	1:C:451:LYS:HG2	2.19	0.42
1:F:238:LEU:HD13	1:F:273:VAL:HG22	2.01	0.42
1:F:408:LYS:HE3	1:F:412:LEU:HB3	2.01	0.42
1:F:619:ALA:HA	1:F:623:PHE:HB2	2.01	0.42
1:F:657:GLU:OE2	1:E:703:GLN:NE2	2.53	0.42
2:E:902:AGS:O1B	2:E:902:AGS:O2G	2.37	0.42
1:D:183:ARG:NH2	1:D:210:VAL:O	2.53	0.42
1:C:222:ARG:HG2	1:C:228:VAL:HB	2.01	0.42
1:C:240:LEU:HD21	1:C:245:LEU:HD11	2.01	0.42
1:F:221:GLN:O	1:F:225:ASN:CB	2.59	0.42
1:A:232:LEU:HD13	1:A:232:LEU:HA	1.94	0.42
1:A:373:ALA:O	1:A:377:SER:OG	2.34	0.42
1:C:629:MET:HG2	1:C:631:ARG:HG3	2.02	0.42
1:C:632:ILE:HD13	1:C:662:LEU:HA	2.02	0.42
1:E:240:LEU:HD22	1:E:275:LEU:HD11	2.01	0.42
1:A:609:VAL:HG23	1:A:763:PHE:HD2	1.85	0.42
1:A:849:ASN:H	1:A:854:VAL:HG12	1.85	0.42
1:C:752:GLU:O	1:C:756:ARG:HB2	2.19	0.41
1:F:395:ASP:OD2	1:E:198:THR:N	2.47	0.41
1:E:555:GLU:O	1:E:559:LEU:HB2	2.20	0.41
1:E:729:SER:HA	1:E:730:ILE:HA	1.63	0.41
1:B:197:ARG:HG3	1:B:198:THR:HG22	2.02	0.41
1:B:742:MET:HA	1:B:745:ILE:HG22	2.01	0.41
1:A:728:LYS:HZ2	1:A:762:VAL:HG11	1.85	0.41
1:A:779:LEU:HD21	1:A:795:ILE:HD12	2.01	0.41
1:C:203:VAL:N	1:C:334:GLN:O	2.54	0.41
1:C:698:ARG:HD2	1:C:706:THR:HB	2.02	0.41
1:F:611:LYS:HB3	1:F:675:LEU:HD11	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:ASP:HB2	2:E:901:AGS:H8	2.00	0.41
1:B:212:LYS:HA	1:B:215:ILE:HD12	2.02	0.41
2:B:901:AGS:H5'1	1:A:331:ARG:CZ	2.50	0.41
1:F:804:SER:O	1:F:808:TYR:N	2.51	0.41
1:B:599:GLY:HA3	1:B:714:VAL:H	1.85	0.41
1:A:415:LEU:HD13	1:A:418:ARG:HD2	2.02	0.41
1:F:422:LEU:HD22	1:F:448:LEU:HD23	2.03	0.41
1:F:628:ALA:HB2	1:F:669:ARG:HE	1.86	0.41
1:D:537:ALA:O	1:D:541:ALA:HB3	2.21	0.41
1:B:533:ASP:N	1:B:533:ASP:OD1	2.53	0.41
1:A:733:ILE:HG22	1:A:735:GLN:H	1.86	0.41
1:A:828:PRO:HA	1:A:831:GLN:HB3	2.02	0.41
1:F:538:GLU:HB3	1:F:542:ARG:HH21	1.85	0.41
1:D:171:ARG:HA	1:D:176:LYS:HE3	2.02	0.41
1:C:356:ARG:O	1:C:360:HIS:HB2	2.20	0.41
1:C:524:MET:HB2	1:C:527:LEU:HG	2.03	0.41
1:F:164:TYR:CZ	1:F:258:ARG:HD3	2.55	0.41
1:F:204:LEU:H	1:F:313:ALA:HA	1.85	0.41
1:E:251:TYR:CE1	1:A:72:PRO:C	2.87	0.41
1:E:327:ALA:HA	1:E:330:GLU:HG2	2.02	0.41
1:D:212:LYS:NZ	2:D:901:AGS:O1B	2.50	0.41
1:D:577:VAL:O	1:D:581:SER:CB	2.69	0.41
1:B:178:ASP:HA	1:B:179:PRO:HD3	1.90	0.41
1:A:224:ILE:O	1:A:233:LYS:NZ	2.53	0.41
1:F:166:ILE:O	1:F:239:ALA:N	2.39	0.41
1:C:702:GLY:HA2	1:D:645:ARG:HH11	1.85	0.41
1:F:405:ILE:HD11	1:F:529:ASN:HA	2.03	0.41
1:F:794:HIS:N	1:F:844:ILE:O	2.38	0.41
1:B:314:THR:HG23	1:B:319:TYR:HB2	2.03	0.41
1:A:226:GLY:HA2	1:A:233:LYS:HD2	2.03	0.41
1:C:194:LEU:HD11	1:C:219:LEU:HD21	2.03	0.41
1:C:280:LEU:HD13	1:C:312:GLY:HA2	2.03	0.41
1:F:305:ARG:HH21	1:A:244:ALA:HB2	1.86	0.41
1:F:350:LEU:HB2	1:F:370:ILE:HG23	2.03	0.41
1:F:355:GLU:O	1:F:359:LEU:HB2	2.20	0.41
1:F:604:LEU:HD23	1:F:718:SER:HB3	2.03	0.41
1:F:610:GLY:O	1:F:614:LEU:N	2.52	0.41
1:F:676:LEU:HB2	1:F:716:MET:HA	2.02	0.41
1:F:793:ILE:HA	1:F:844:ILE:HB	2.02	0.41
1:E:800:LEU:HA	1:E:803:LEU:HD12	2.03	0.41
1:D:546:ILE:HG21	1:D:588:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:THR:HG22	1:D:815:ARG:HH22	1.86	0.41
1:B:357:TYR:OH	2:B:901:AGS:O2'	2.39	0.41
1:A:174:GLN:HB3	1:A:176:LYS:HG3	2.02	0.41
1:A:297:ASN:HA	1:A:300:LYS:HE3	2.03	0.41
1:A:381:ILE:HG22	1:A:384:ARG:H	1.86	0.41
1:A:566:LEU:HD13	1:A:614:LEU:HD11	2.03	0.41
1:C:399:SER:HA	1:C:402:ARG:HH21	1.86	0.41
1:F:319:TYR:CE2	1:F:335:LYS:HG2	2.56	0.41
1:F:834:LEU:HB3	1:E:556:ARG:NH1	2.36	0.41
1:F:835:SER:HA	1:E:556:ARG:HG3	2.03	0.41
1:B:397:ALA:O	1:B:401:ILE:HG12	2.21	0.41
1:A:533:ASP:N	1:A:533:ASP:OD1	2.53	0.41
1:C:183:ARG:NH2	1:C:339:ALA:O	2.53	0.40
1:C:388:ASP:HA	1:C:391:ILE:HD12	2.02	0.40
1:C:655:GLY:O	1:C:659:GLY:N	2.55	0.40
1:D:663:THR:O	1:D:667:ARG:CB	2.66	0.40
1:B:548:VAL:HG11	1:B:551:MET:HG2	2.03	0.40
1:C:530:LYS:HB3	1:C:532:THR:HG23	2.03	0.40
1:C:695:ASP:OD2	2:D:902:AGS:O3G	2.38	0.40
1:C:758:ASP:HA	1:D:819:ARG:NH2	2.36	0.40
1:C:839:VAL:HB	1:C:842:LYS:HD3	2.03	0.40
1:E:314:THR:OG1	1:E:315:THR:N	2.50	0.40
1:E:815:ARG:HH22	2:E:902:AGS:H5'1	1.86	0.40
1:F:642:SER:HA	1:F:645:ARG:HE	1.87	0.40
1:D:229:PRO:O	1:D:233:LYS:N	2.50	0.40
1:C:411:GLU:HA	1:C:414:ARG:HD3	2.04	0.40
1:C:607:THR:OG1	1:C:726:GLU:OE2	2.29	0.40
1:F:192:GLN:HG3	1:A:400:SER:HB2	2.03	0.40
1:F:202:PRO:HD2	1:F:311:VAL:HA	2.02	0.40
1:E:639:GLU:HG3	1:E:641:HIS:HB2	2.04	0.40
1:B:606:PRO:HA	1:B:722:VAL:HG13	2.03	0.40
1:A:486:ILE:HD12	1:A:486:ILE:HA	1.98	0.40
1:C:821:ILE:HG23	1:C:825:ILE:HD12	2.02	0.40
1:F:230:GLU:HG3	1:A:407:SER:HA	2.03	0.40
1:F:483:LYS:HA	1:F:483:LYS:HD3	1.98	0.40
1:F:773:SER:HA	1:F:776:GLN:HG2	2.02	0.40
1:E:332:ARG:HD3	1:E:332:ARG:HA	1.95	0.40
1:D:300:LYS:O	1:D:304:ALA:CB	2.70	0.40
1:B:698:ARG:HB3	1:B:699:LEU:H	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	811/871 (93%)	764 (94%)	47 (6%)	0	100 100
1	B	566/871 (65%)	520 (92%)	45 (8%)	1 (0%)	47 81
1	C	618/871 (71%)	560 (91%)	58 (9%)	0	100 100
1	D	618/871 (71%)	572 (93%)	46 (7%)	0	100 100
1	E	682/871 (78%)	637 (93%)	45 (7%)	0	100 100
1	F	682/871 (78%)	630 (92%)	52 (8%)	0	100 100
All	All	3977/5226 (76%)	3683 (93%)	293 (7%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	582/726 (80%)	574 (99%)	8 (1%)	67 81
1	B	483/726 (66%)	474 (98%)	9 (2%)	57 75
1	C	533/726 (73%)	527 (99%)	6 (1%)	73 85
1	D	533/726 (73%)	522 (98%)	11 (2%)	53 72
1	E	582/726 (80%)	576 (99%)	6 (1%)	76 86
1	F	582/726 (80%)	572 (98%)	10 (2%)	60 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3295/4356 (76%)	3245 (98%)	50 (2%)	66 80

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	268	LYS
1	C	272	ASN
1	C	297	ASN
1	C	441	LEU
1	C	620	ASN
1	C	643	VAL
1	F	268	LYS
1	F	401	ILE
1	F	440	ARG
1	F	443	MET
1	F	620	ASN
1	F	638	MET
1	F	646	LEU
1	F	705	ARG
1	F	737	ASN
1	F	845	ARG
1	E	268	LYS
1	E	272	ASN
1	E	297	ASN
1	E	530	LYS
1	E	586	ARG
1	E	620	ASN
1	D	197	ARG
1	D	268	LYS
1	D	401	ILE
1	D	432	GLU
1	D	440	ARG
1	D	443	MET
1	D	620	ASN
1	D	681	LYS
1	D	705	ARG
1	D	737	ASN
1	D	845	ARG
1	B	212	LYS
1	B	252	ARG
1	B	335	LYS
1	B	528	ARG

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Mol	Chain	Res	Type
1	B	530	LYS
1	B	646	LEU
1	B	668	ARG
1	B	737	ASN
1	B	845	ARG
1	A	162	LYS
1	A	272	ASN
1	A	297	ASN
1	A	479	LEU
1	A	530	LYS
1	A	586	ARG
1	A	620	ASN
1	A	646	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
1	C	195	GLN
1	C	269	GLN
1	C	272	ASN
1	C	421	GLN
1	C	688	ASN
1	C	755	ASN
1	C	778	GLN
1	F	361	HIS
1	F	385	GLN
1	F	512	GLN
1	F	529	ASN
1	F	703	GLN
1	F	778	GLN
1	E	174	GLN
1	E	195	GLN
1	E	272	ASN
1	E	620	ASN
1	E	703	GLN
1	E	711	ASN
1	E	770	HIS
1	D	703	GLN
1	D	719	ASN
1	D	737	ASN
1	D	778	GLN

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Mol	Chain	Res	Type
1	D	806	ASN
1	D	822	GLN
1	B	192	GLN
1	B	201	ASN
1	B	641	HIS
1	B	683	HIS
1	B	711	ASN
1	B	737	ASN
1	B	755	ASN
1	B	778	GLN
1	B	849	ASN
1	A	195	GLN
1	A	272	ASN
1	A	620	ASN
1	A	703	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	AGS	E	902	-	26,33,33	0.76	0	26,52,52	1.26	2 (7%)
2	AGS	B	901	-	26,33,33	0.81	1 (3%)	26,52,52	1.07	2 (7%)
2	AGS	D	901	-	26,33,33	0.82	1 (3%)	26,52,52	1.03	2 (7%)
2	AGS	C	901	-	26,33,33	0.75	0	26,52,52	1.29	4 (15%)
2	AGS	E	901	-	26,33,33	0.77	1 (3%)	26,52,52	1.25	3 (11%)
2	AGS	C	902	-	26,33,33	0.84	1 (3%)	26,52,52	1.14	2 (7%)
2	AGS	D	902	-	26,33,33	0.82	1 (3%)	26,52,52	1.09	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	E	902	-	-	5/17/38/38	0/3/3/3
2	AGS	B	901	-	-	8/17/38/38	0/3/3/3
2	AGS	D	901	-	-	5/17/38/38	0/3/3/3
2	AGS	C	901	-	-	7/17/38/38	0/3/3/3
2	AGS	E	901	-	-	11/17/38/38	0/3/3/3
2	AGS	C	902	-	-	0/17/38/38	0/3/3/3
2	AGS	D	902	-	-	4/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	AGS	PG-S1G	2.36	1.95	1.90
2	D	902	AGS	PG-S1G	2.16	1.95	1.90
2	E	901	AGS	PG-S1G	2.15	1.95	1.90
2	D	901	AGS	PG-S1G	2.11	1.95	1.90
2	C	902	AGS	PG-S1G	2.11	1.95	1.90

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	902	AGS	PA-O3A-PB	-4.99	115.70	132.83
2	C	902	AGS	PA-O3A-PB	-4.53	117.28	132.83
2	E	901	AGS	C1'-N9-C4	3.73	133.20	126.64
2	D	902	AGS	PA-O3A-PB	-3.68	120.18	132.83
2	E	901	AGS	PA-O3A-PB	-3.49	120.83	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	AGS	PA-O3A-PB	-3.46	120.96	132.83
2	B	901	AGS	PA-O3A-PB	-3.45	120.98	132.83
2	C	901	AGS	PA-O3A-PB	-3.40	121.17	132.83
2	C	901	AGS	C1'-N9-C4	3.36	132.54	126.64
2	B	901	AGS	C5-C6-N6	2.58	124.27	120.35
2	E	901	AGS	C5-C6-N6	2.43	124.04	120.35
2	E	902	AGS	C5-C6-N6	2.31	123.87	120.35
2	D	902	AGS	C5-C6-N6	2.27	123.80	120.35
2	C	902	AGS	C5-C6-N6	2.25	123.77	120.35
2	D	901	AGS	C5-C6-N6	2.23	123.74	120.35
2	C	901	AGS	C5-C6-N6	2.20	123.69	120.35
2	C	901	AGS	C3'-C2'-C1'	2.02	104.02	100.98

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	AGS	C5'-O5'-PA-O1A
2	C	901	AGS	C5'-O5'-PA-O2A
2	E	901	AGS	C5'-O5'-PA-O1A
2	E	901	AGS	C5'-O5'-PA-O2A
2	E	902	AGS	C5'-O5'-PA-O2A
2	D	901	AGS	C5'-O5'-PA-O2A
2	D	901	AGS	C5'-O5'-PA-O3A
2	D	902	AGS	C5'-O5'-PA-O1A
2	B	901	AGS	PB-O3B-PG-O2G
2	B	901	AGS	PB-O3B-PG-O3G
2	B	901	AGS	C5'-O5'-PA-O1A
2	B	901	AGS	C5'-O5'-PA-O2A
2	B	901	AGS	O4'-C4'-C5'-O5'
2	B	901	AGS	C3'-C4'-C5'-O5'
2	E	901	AGS	O4'-C4'-C5'-O5'
2	E	901	AGS	C3'-C4'-C5'-O5'
2	E	902	AGS	O4'-C4'-C5'-O5'
2	E	902	AGS	C3'-C4'-C5'-O5'
2	E	901	AGS	PB-O3A-PA-O1A
2	D	901	AGS	C4'-C5'-O5'-PA
2	D	902	AGS	C4'-C5'-O5'-PA
2	D	901	AGS	PB-O3A-PA-O5'
2	C	901	AGS	C5'-O5'-PA-O3A
2	E	901	AGS	C5'-O5'-PA-O3A
2	E	902	AGS	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	902	AGS	C5'-O5'-PA-O3A
2	C	901	AGS	PB-O3A-PA-O2A
2	D	901	AGS	PB-O3A-PA-O1A
2	E	902	AGS	C5'-O5'-PA-O1A
2	D	902	AGS	C5'-O5'-PA-O2A
2	E	901	AGS	C4'-C5'-O5'-PA
2	C	901	AGS	PA-O3A-PB-O3B
2	E	901	AGS	PA-O3A-PB-O3B
2	E	901	AGS	PG-O3B-PB-O2B
2	B	901	AGS	C5'-O5'-PA-O3A
2	C	901	AGS	PA-O3A-PB-O1B
2	C	901	AGS	PB-O3A-PA-O1A
2	E	901	AGS	PA-O3A-PB-O1B
2	E	901	AGS	PB-O3A-PA-O2A
2	B	901	AGS	PA-O3A-PB-O2B

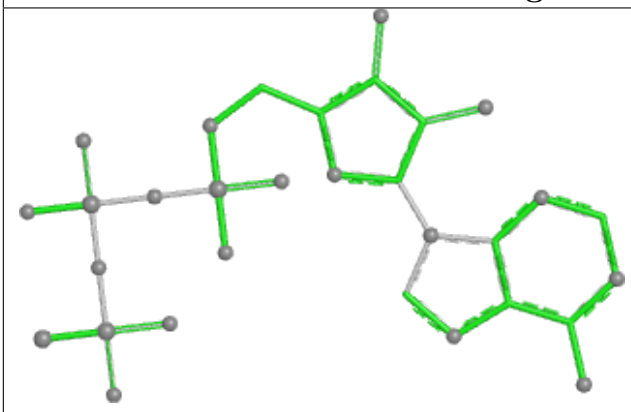
There are no ring outliers.

7 monomers are involved in 23 short contacts:

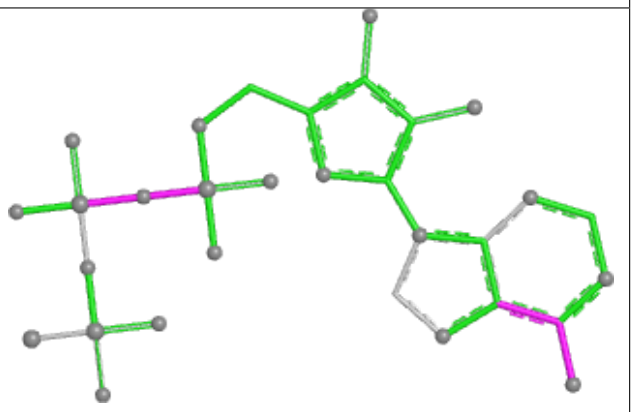
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	902	AGS	6	0
2	B	901	AGS	4	0
2	D	901	AGS	1	0
2	C	901	AGS	2	0
2	E	901	AGS	4	0
2	C	902	AGS	2	0
2	D	902	AGS	4	0

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.

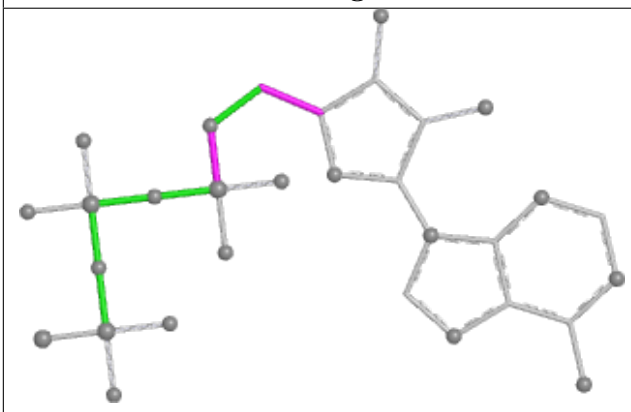
Ligand AGS E 902



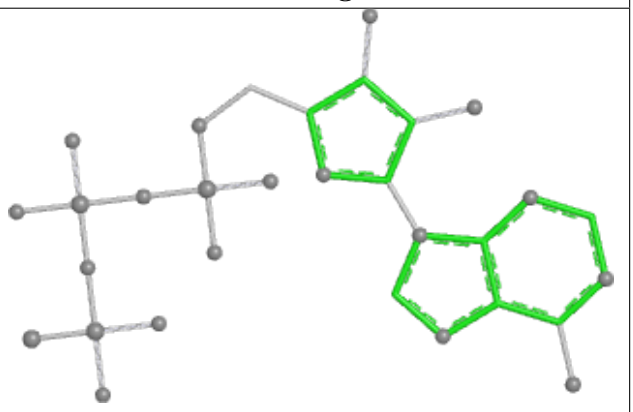
Bond lengths



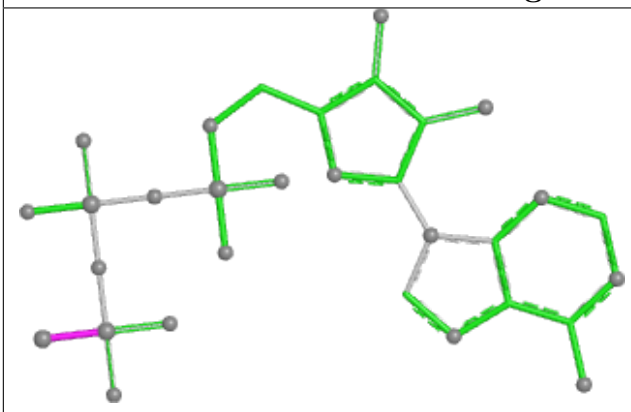
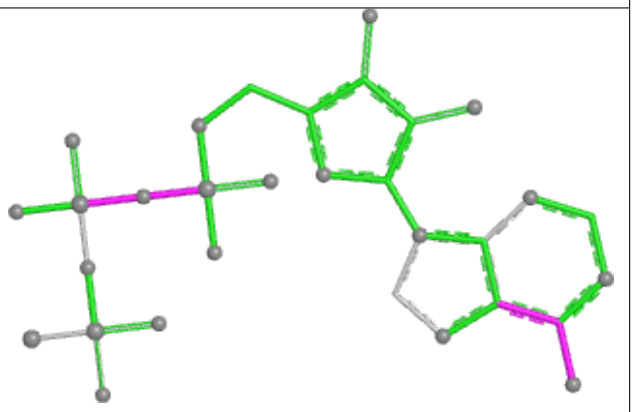
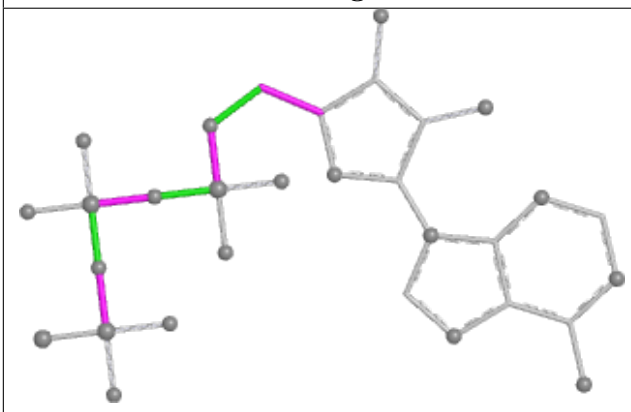
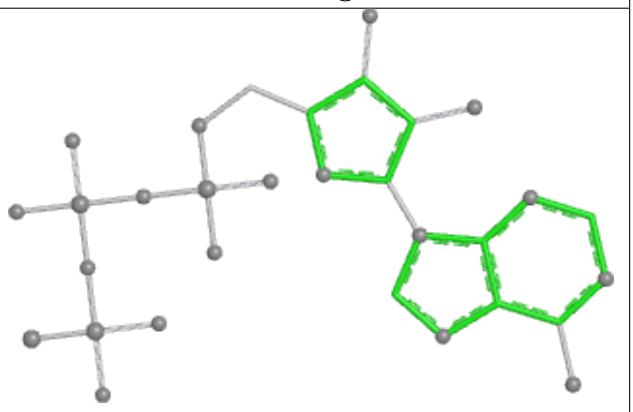
Bond angles

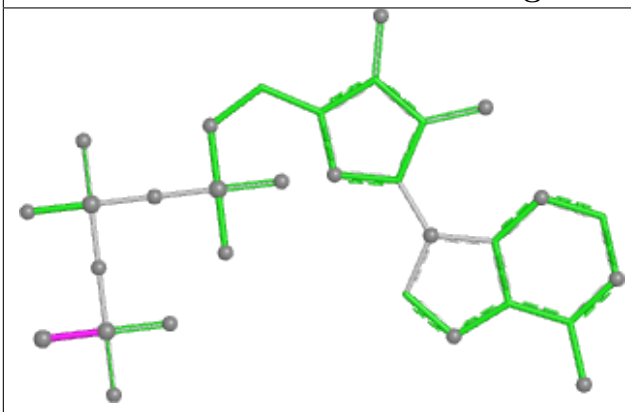
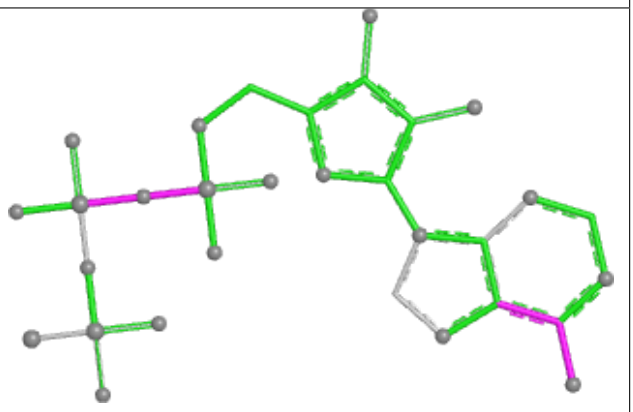
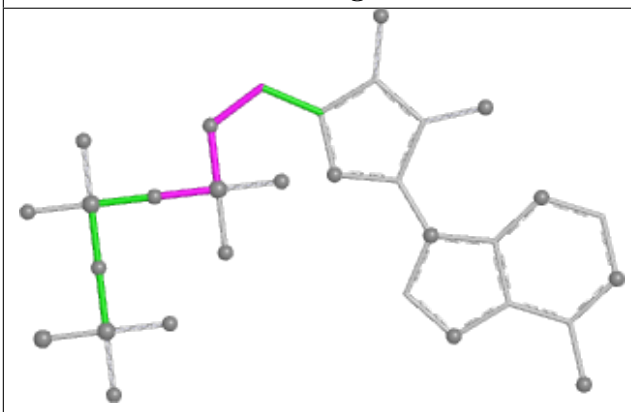
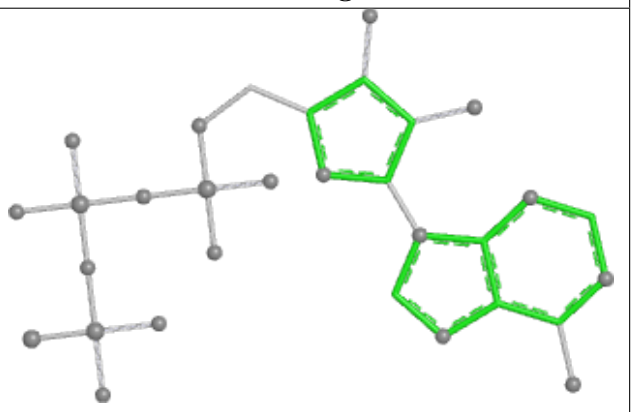


Torsions

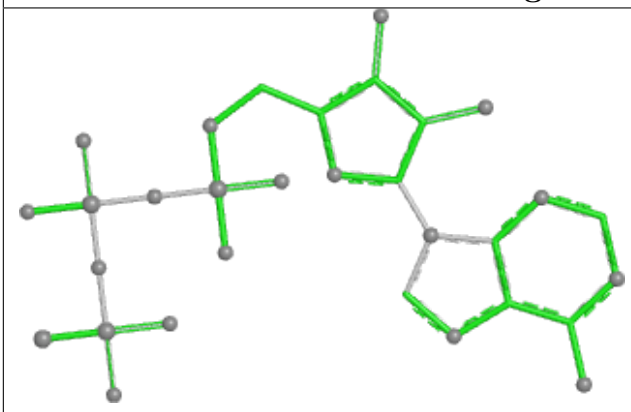


Rings

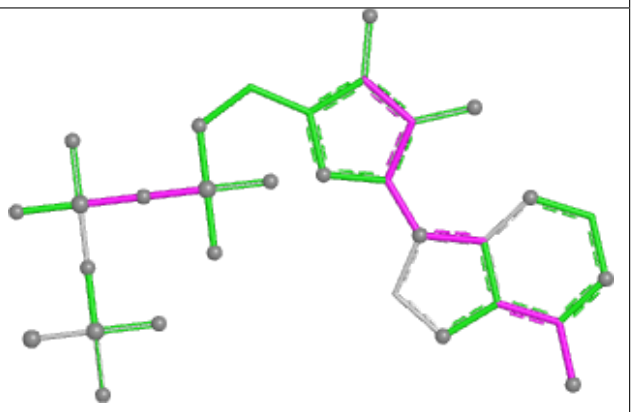
Ligand AGS B 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AGS D 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

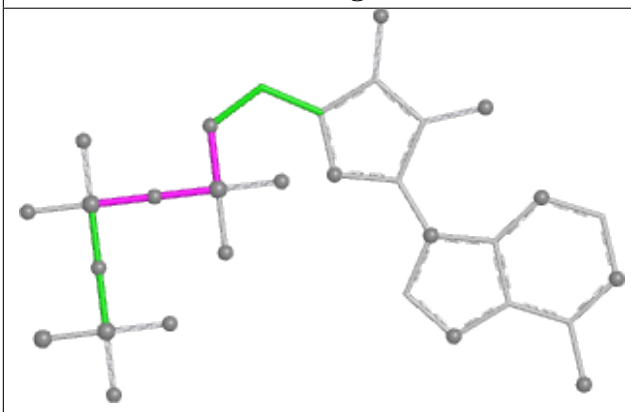
Ligand AGS C 901



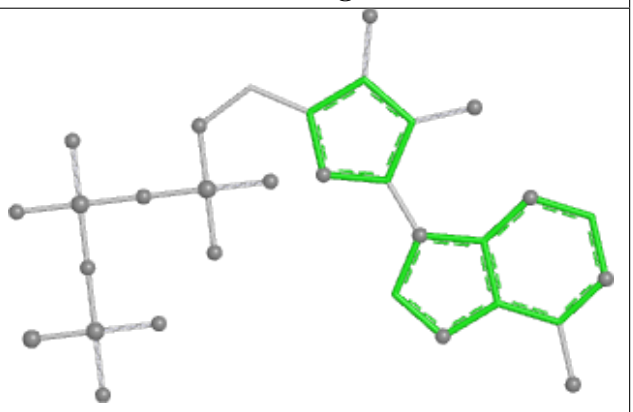
Bond lengths



Bond angles

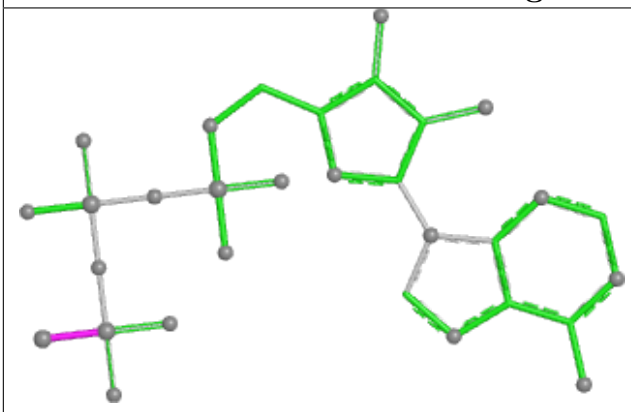


Torsions

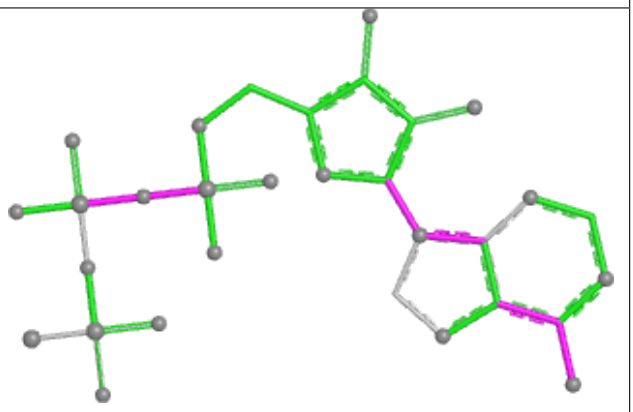


Rings

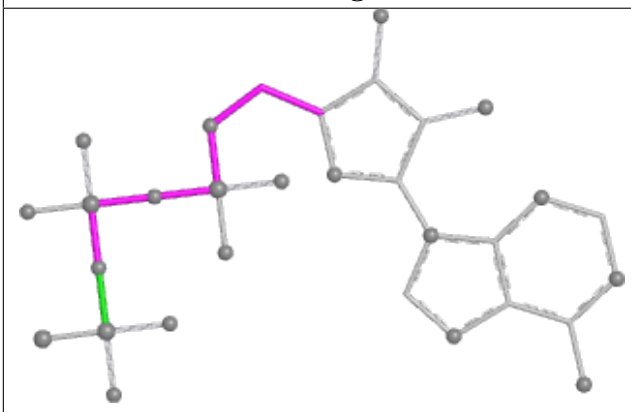
Ligand AGS E 901



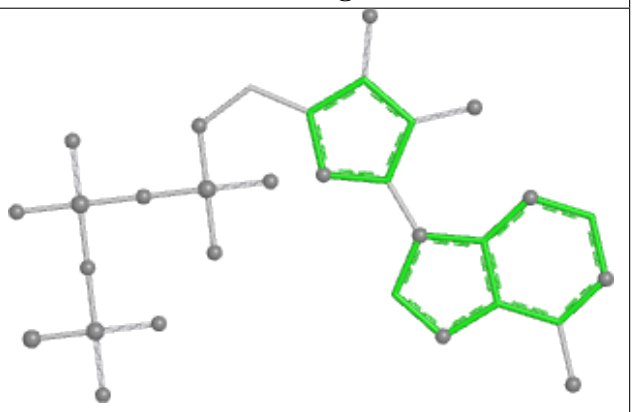
Bond lengths



Bond angles

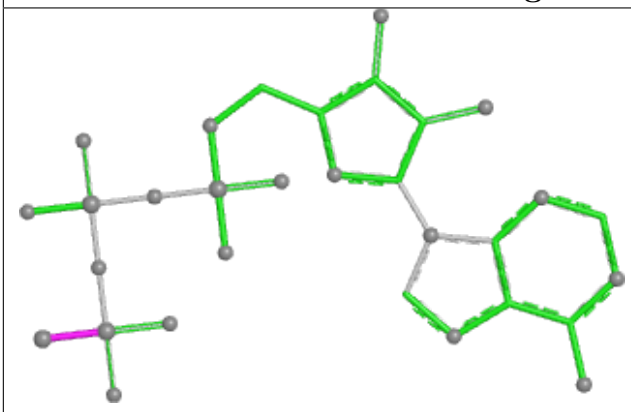


Torsions



Rings

Ligand AGS C 902



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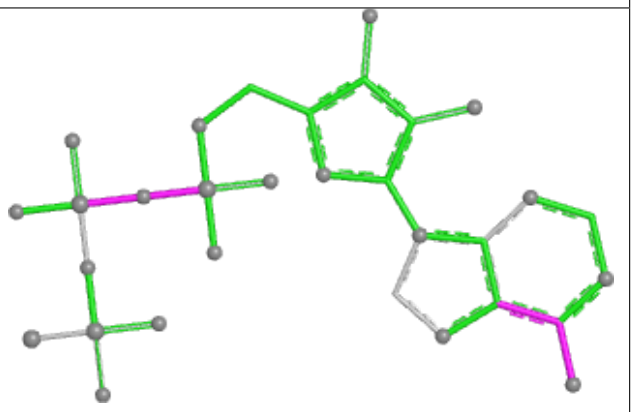
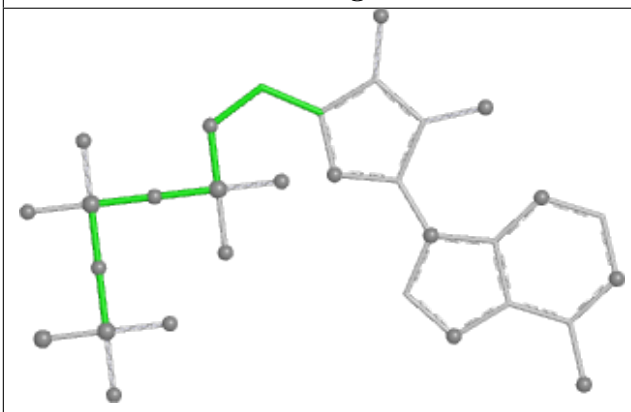
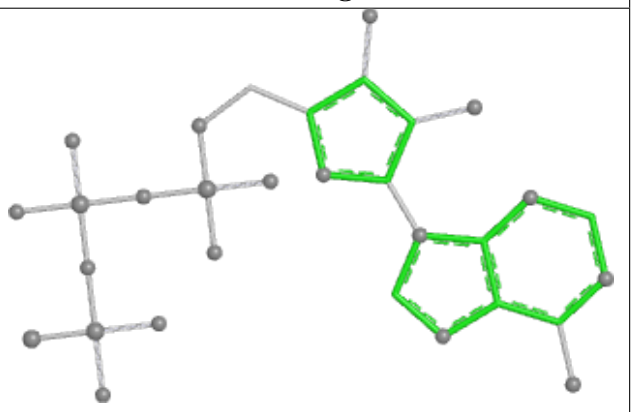


Bond angles

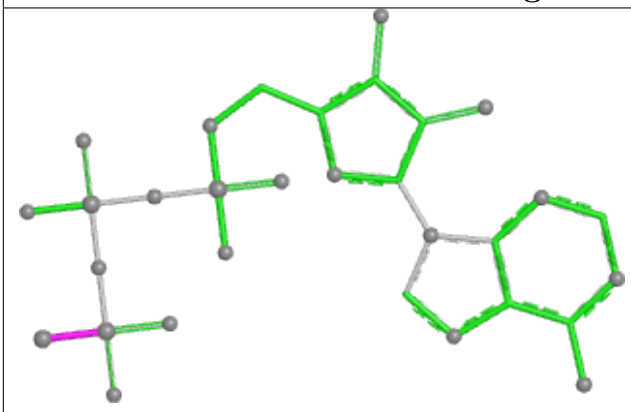


Torsions

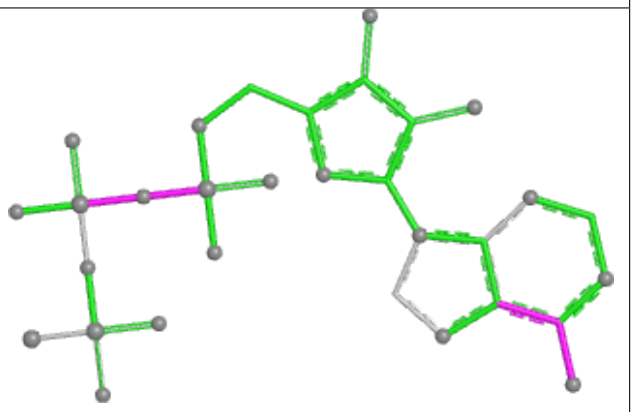


Rings

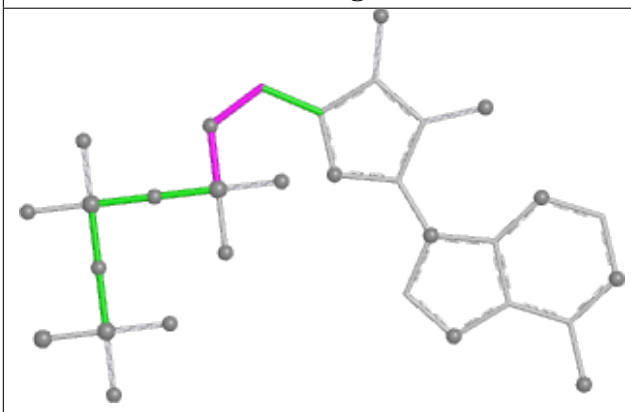
Ligand AGS D 902



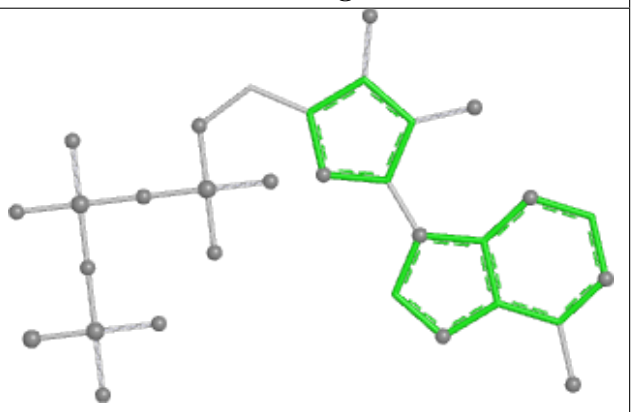
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

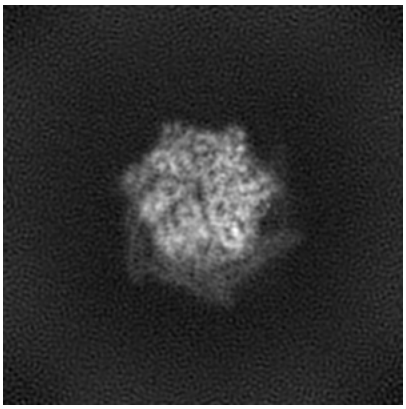
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3777. These allow visual inspection of the internal detail of the map and identification of artifacts.

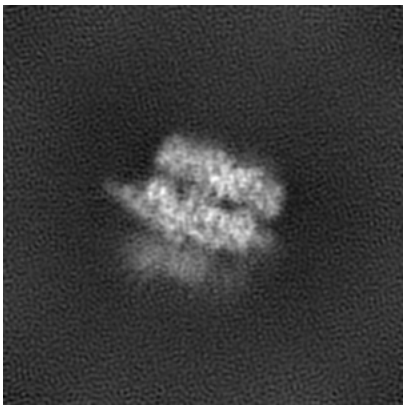
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

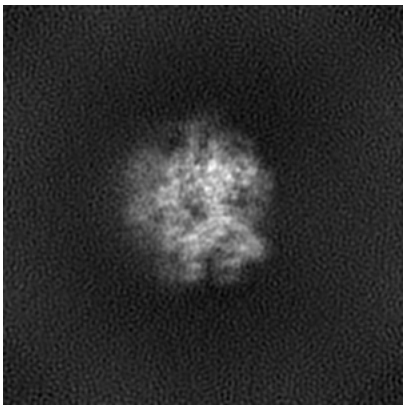
6.1.1 Primary map



X

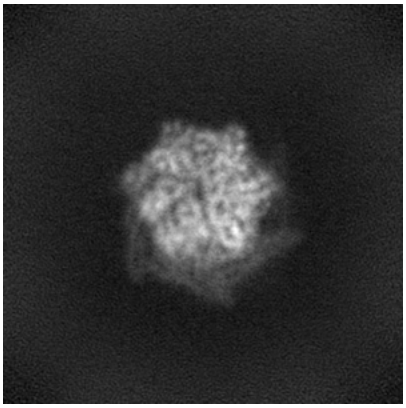


Y

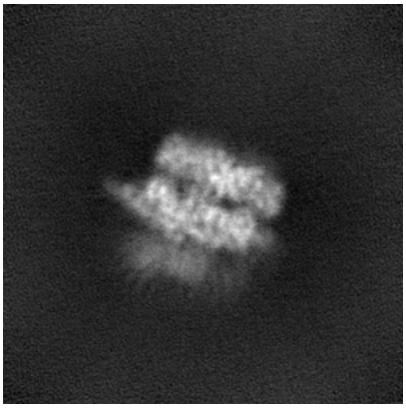


Z

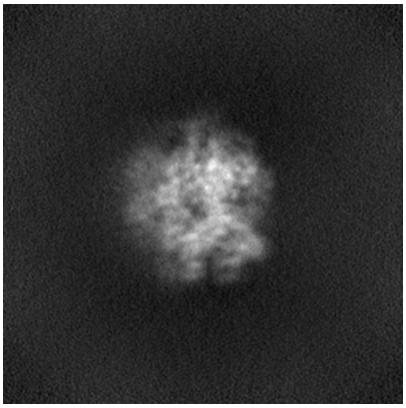
6.1.2 Raw map



X



Y

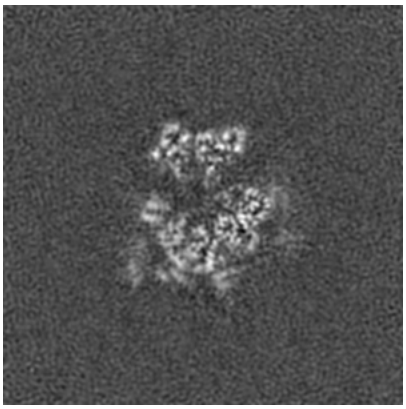


Z

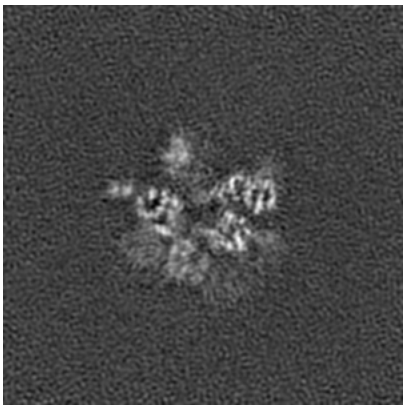
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

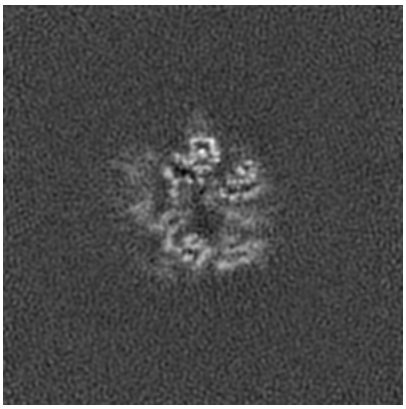
6.2.1 Primary map



X Index: 128

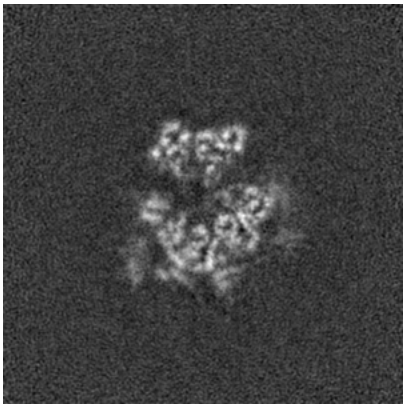


Y Index: 128

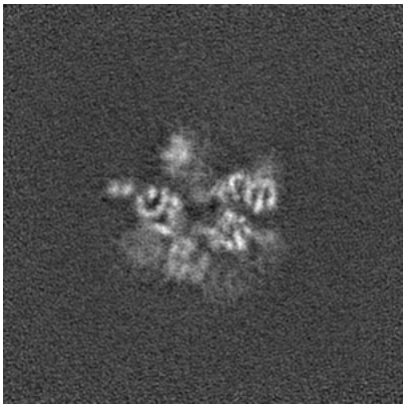


Z Index: 128

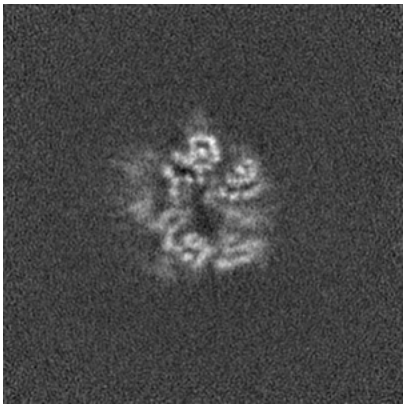
6.2.2 Raw map



X Index: 128



Y Index: 128

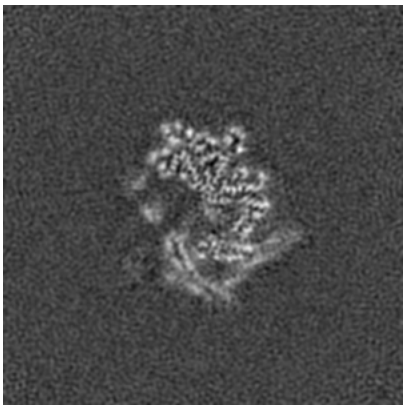


Z Index: 128

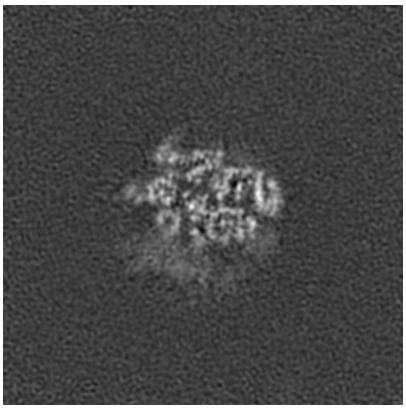
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

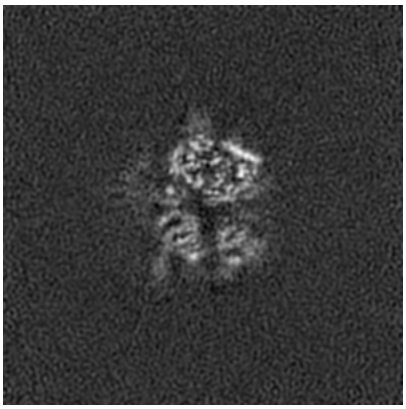
6.3.1 Primary map



X Index: 134

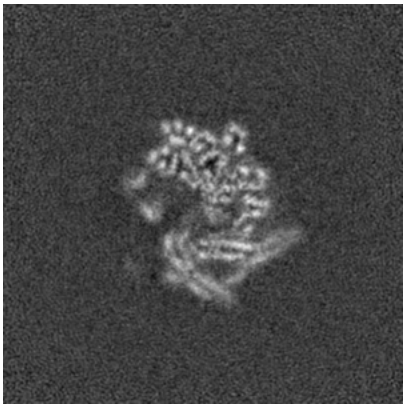


Y Index: 151

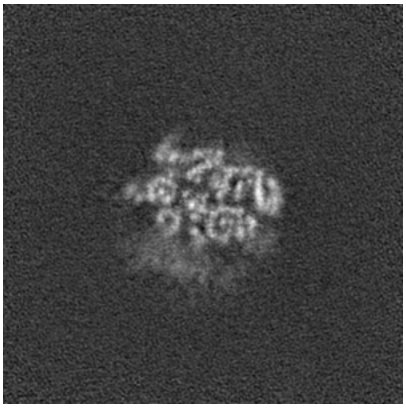


Z Index: 132

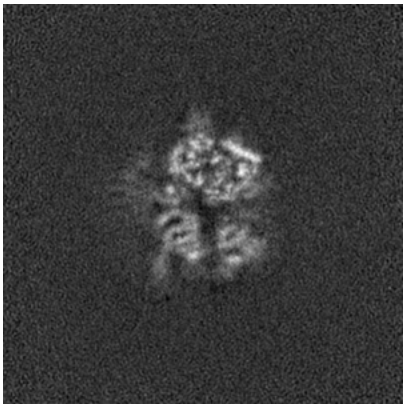
6.3.2 Raw map



X Index: 135



Y Index: 151



Z Index: 132

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

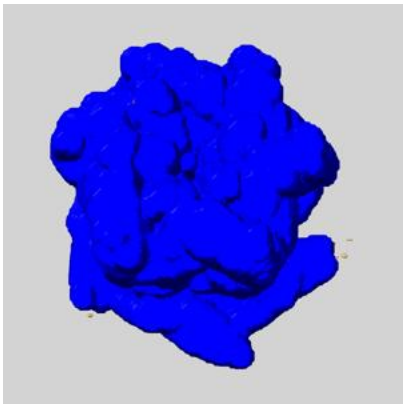
6.5 Mask visualisation

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

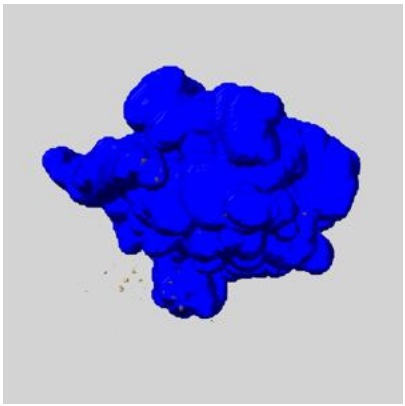
A mask typically either:

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

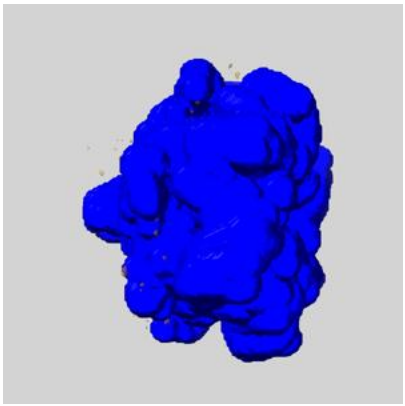
6.5.1 emd_3777_msk_1.map



X



Y

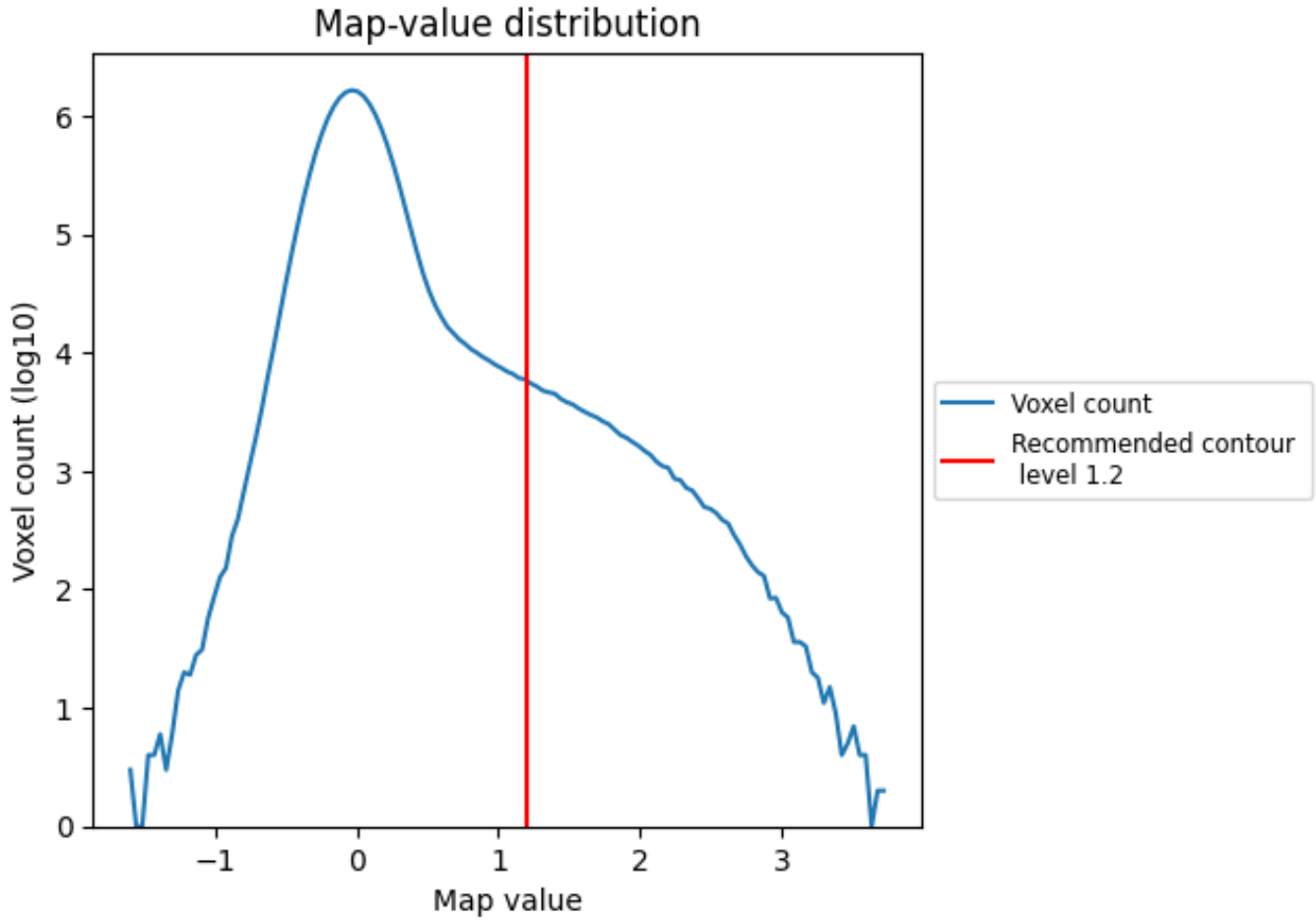


Z

7 Map analysis

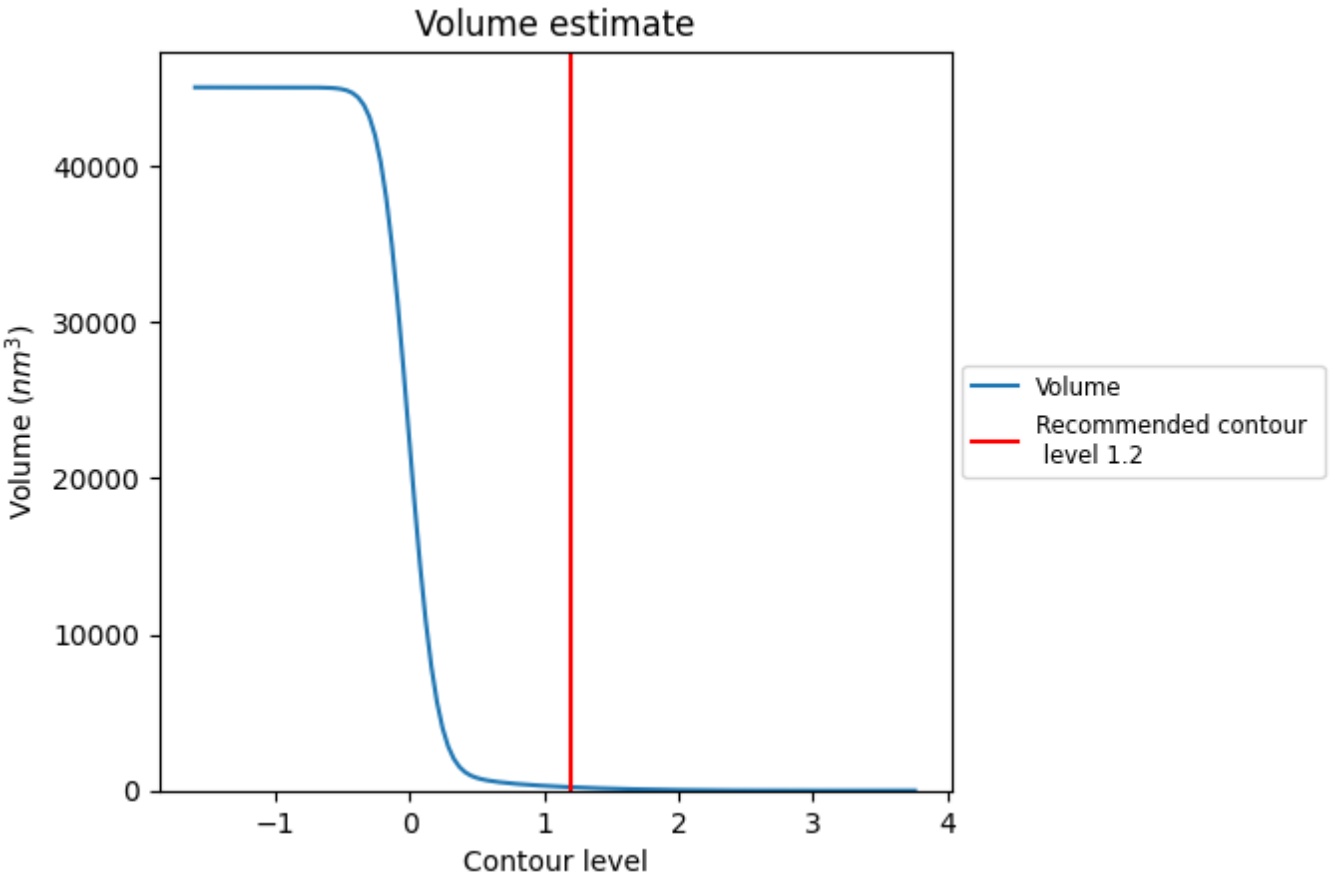
This section contains the results of statistical analysis of the map.

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.

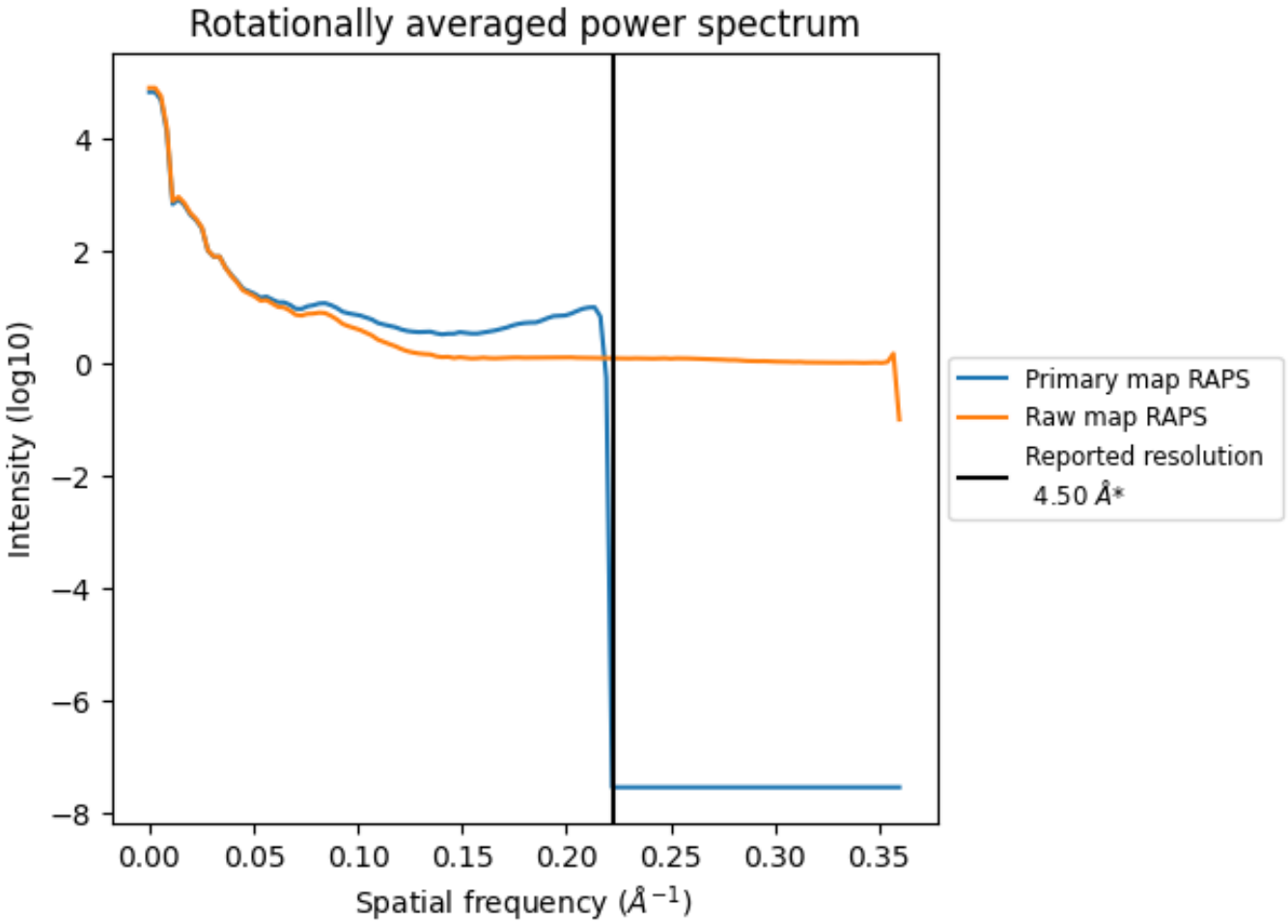
7.2 Volume estimate



The volume at the recommended contour level is 217 nm^3; this corresponds to an approximate mass of 196 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)

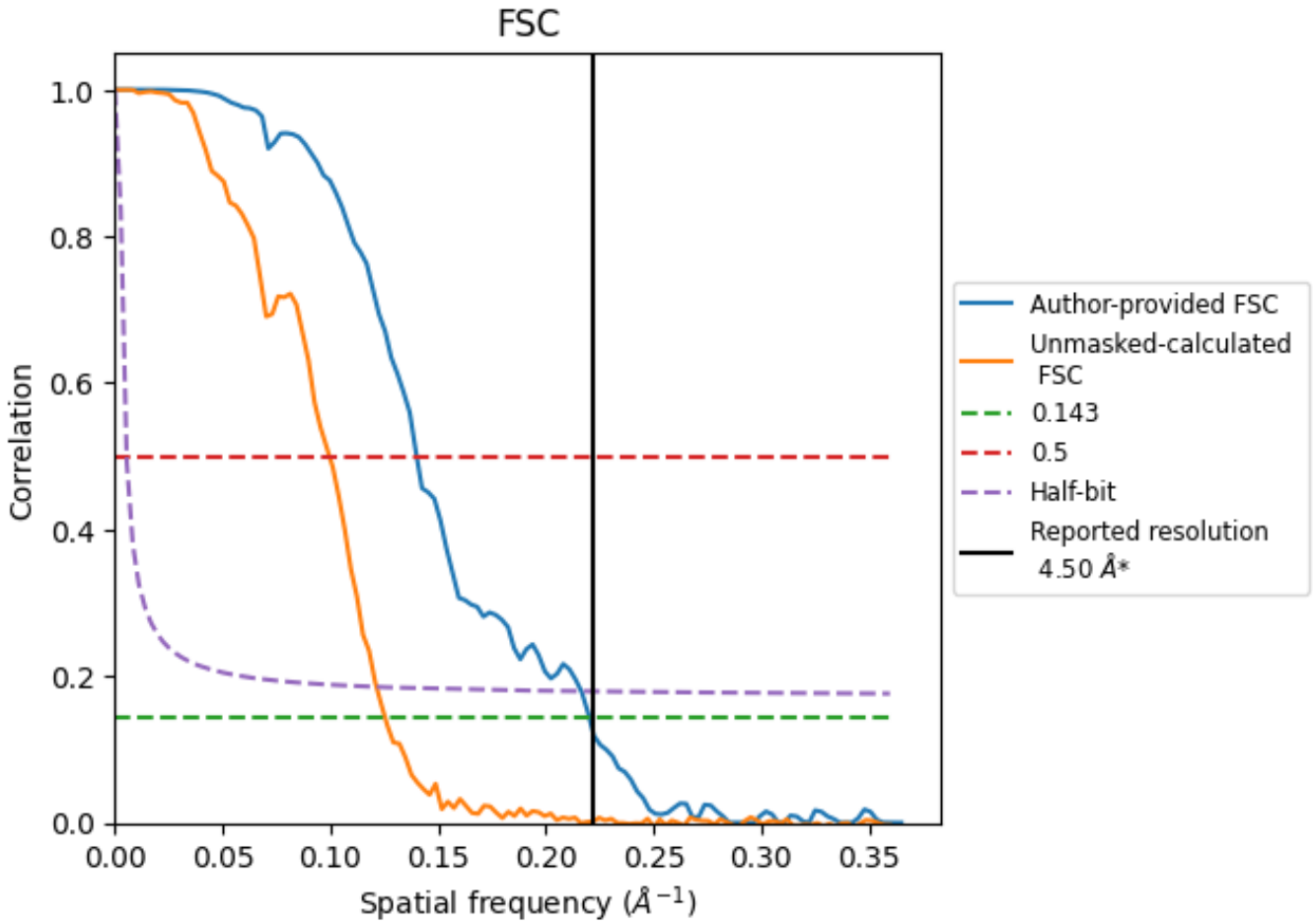


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

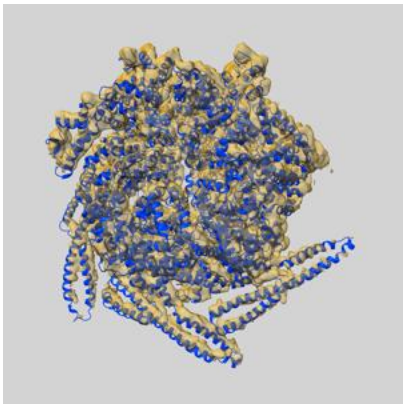
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.54	7.14	4.62
Unmasked-calculated*	7.97	10.04	8.23

*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 7.97 differs from the reported value 4.5 by more than 10 %

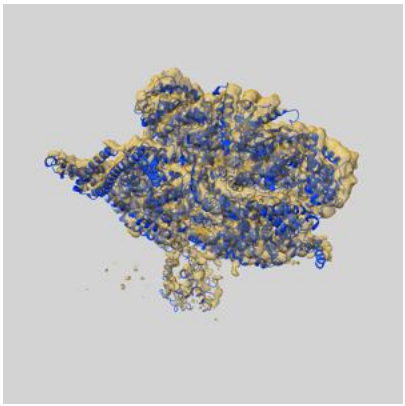
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3777 and PDB model 5OG1. Per-residue inclusion information can be found in section 3 on page 8.

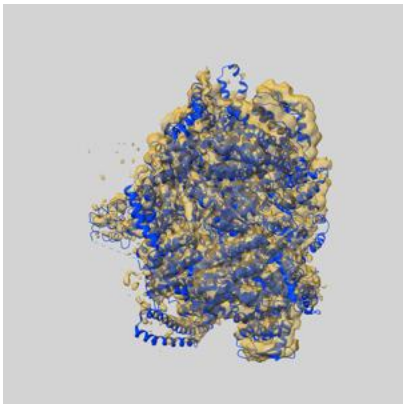
9.1 Map-model overlay



X



Y



Z

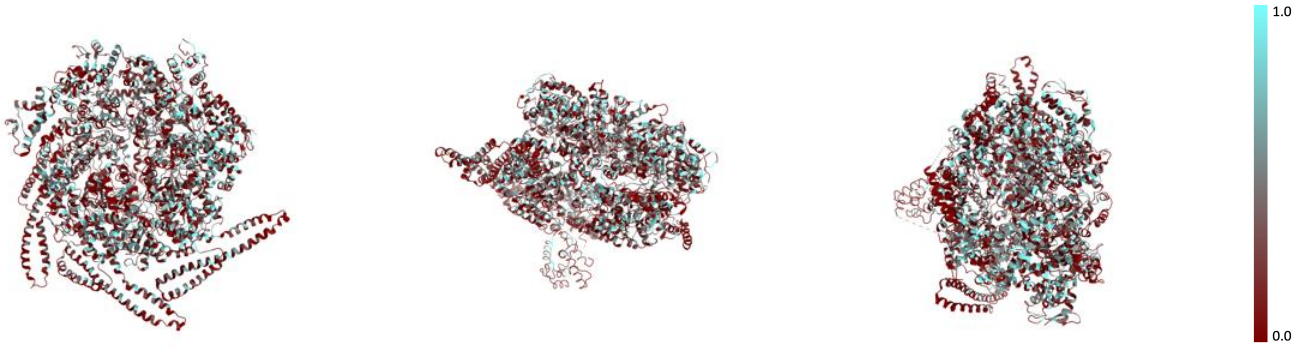
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

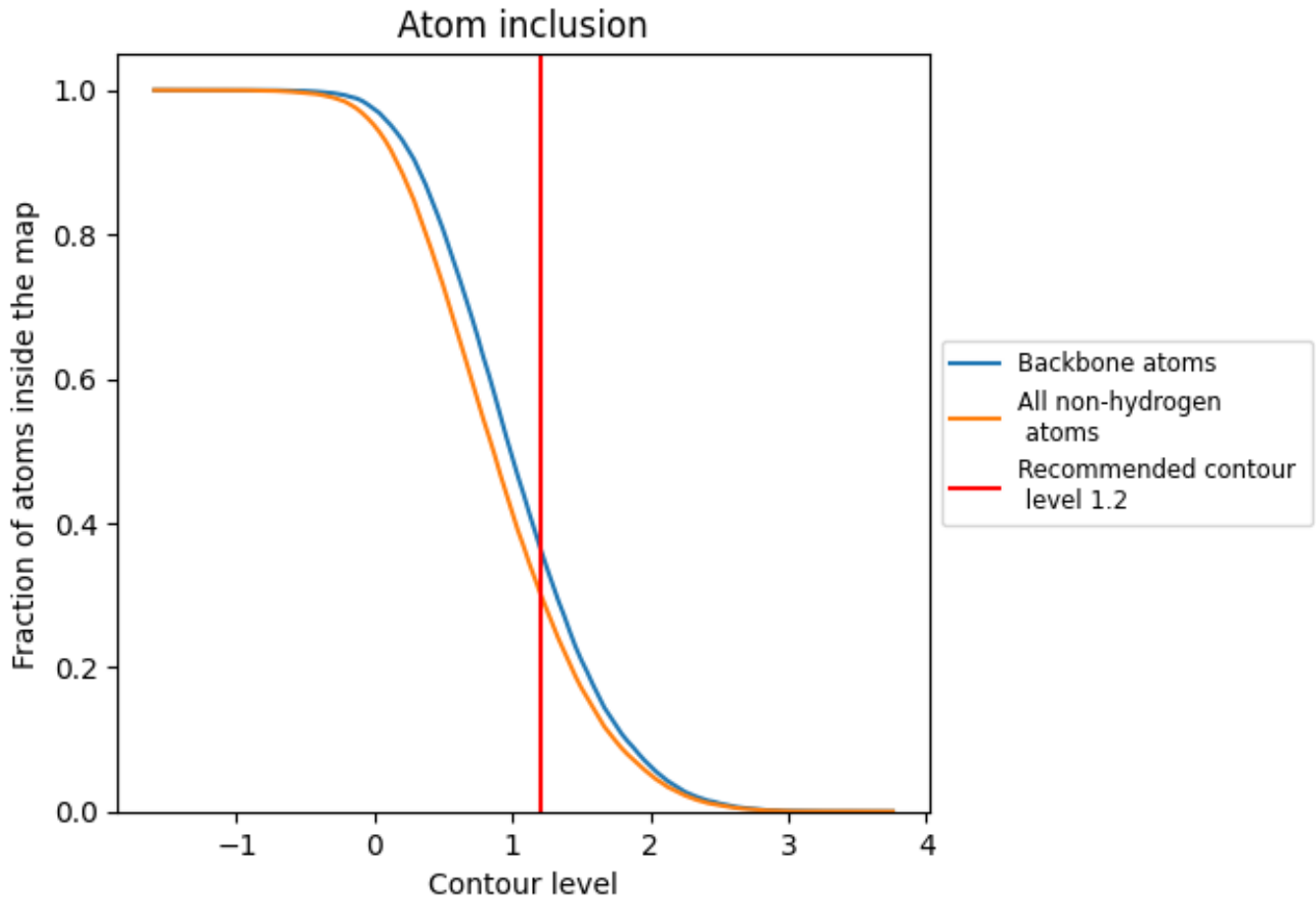
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.2).

9.4 Atom inclusion (i)



At the recommended contour level, 37% of all backbone atoms, 30% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3030	0.0230
A	0.2709	0.0440
B	0.3236	0.0230
C	0.3201	0.0170
D	0.3156	-0.0010
E	0.3160	0.0170
F	0.2796	0.0330