Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:47 PM UTC

PDB ID	:	3J95 / pdb_00003j95
EMDB ID	:	EMD-6205
Title	:	Structure of ADP-bound N-ethylmaleimide sensitive factor determined by single particle cryoelectron microscopy
Authors	:	Zhao, M.; Wu, S.; Cheng, Y.; Brunger, A.T.
Deposited on	:	2014-12-05
Resolution	:	7.60 Å(reported)
Based on initial model	:	1NSF

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:

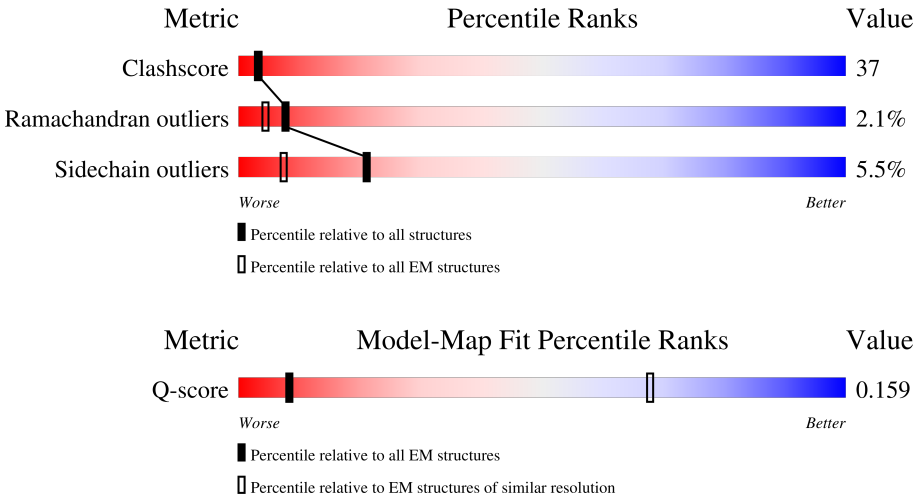
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 7.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	389 (7.10 - 8.10)

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	747	15% 27% 31% 7% 35%
1	B	747	10% 27% 33% • • 36%
1	C	747	7% 28% 32% 5% 35%
1	D	747	7% 29% 31% • 36%

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Mol	Chain	Length	Quality of chain
1	E	747	13% 24% 34% 6% 35%
1	F	747	36% 26% 33% 37%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	801	-	-	X	-
2	ADP	D	801	-	-	X	-
2	ADP	E	801	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21123 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.

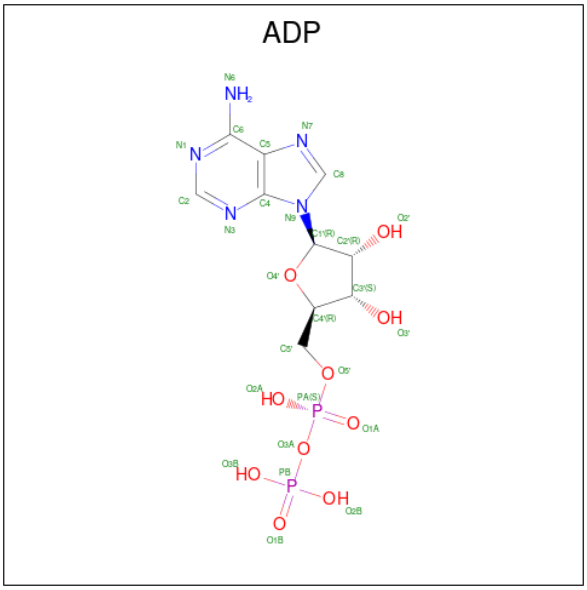
- Molecule 1 is a protein called Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	483	Total	C	N	O	S	0	0
			3513	2221	617	660	15		
1	B	481	Total	C	N	O	S	0	0
			3517	2230	611	660	16		
1	C	485	Total	C	N	O	S	0	0
			3535	2236	618	666	15		
1	D	479	Total	C	N	O	S	0	0
			3467	2203	594	654	16		
1	E	482	Total	C	N	O	S	0	0
			3516	2233	611	656	16		
1	F	473	Total	C	N	O	S	0	0
			3467	2197	609	645	16		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P18708
A	-1	ALA	-	expression tag	UNP P18708
A	0	HIS	-	expression tag	UNP P18708
B	-2	GLY	-	expression tag	UNP P18708
B	-1	ALA	-	expression tag	UNP P18708
B	0	HIS	-	expression tag	UNP P18708
C	-2	GLY	-	expression tag	UNP P18708
C	-1	ALA	-	expression tag	UNP P18708
C	0	HIS	-	expression tag	UNP P18708
D	-2	GLY	-	expression tag	UNP P18708
D	-1	ALA	-	expression tag	UNP P18708
D	0	HIS	-	expression tag	UNP P18708
E	-2	GLY	-	expression tag	UNP P18708
E	-1	ALA	-	expression tag	UNP P18708
E	0	HIS	-	expression tag	UNP P18708
F	-2	GLY	-	expression tag	UNP P18708
F	-1	ALA	-	expression tag	UNP P18708
F	0	HIS	-	expression tag	UNP P18708

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

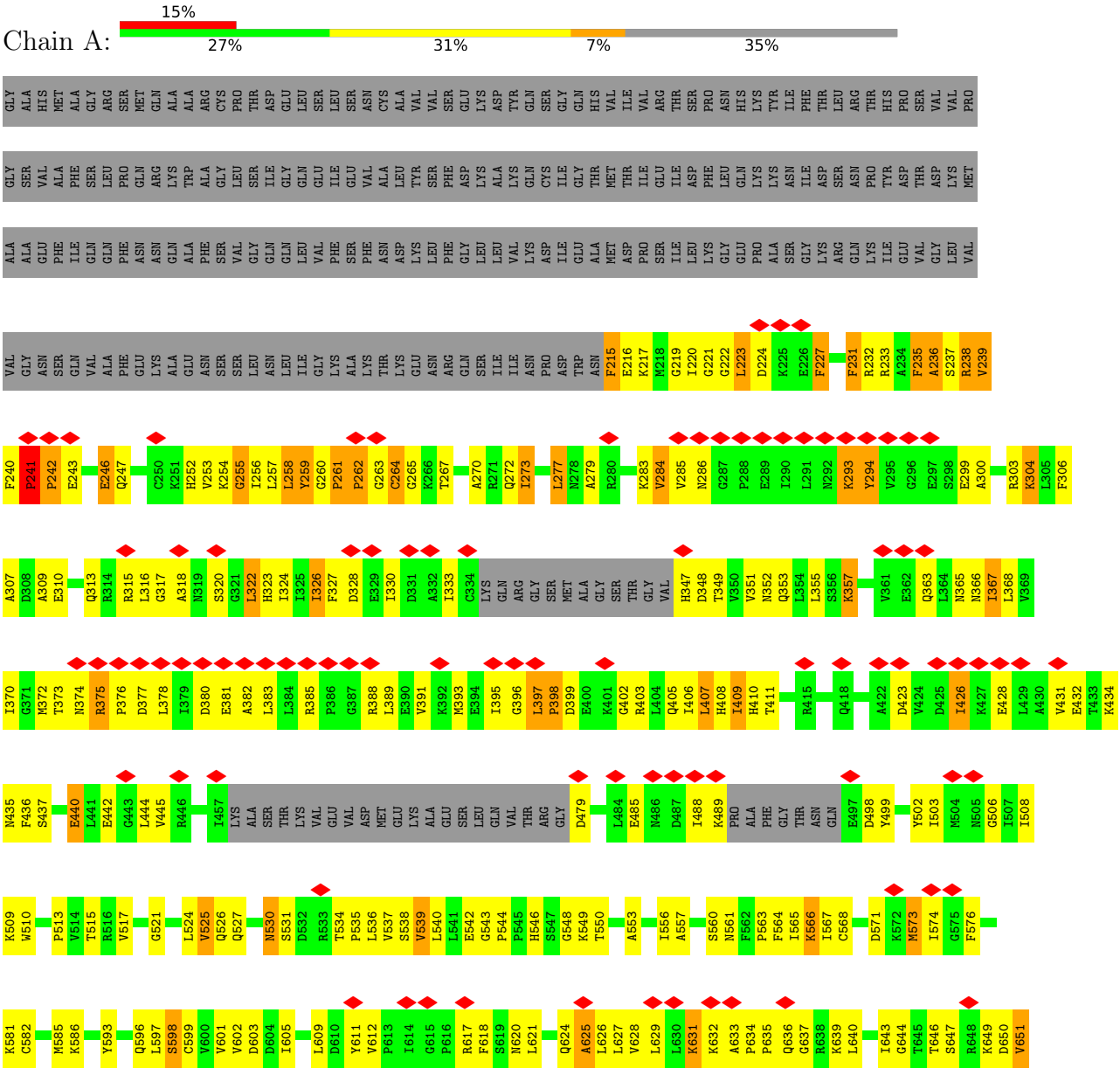


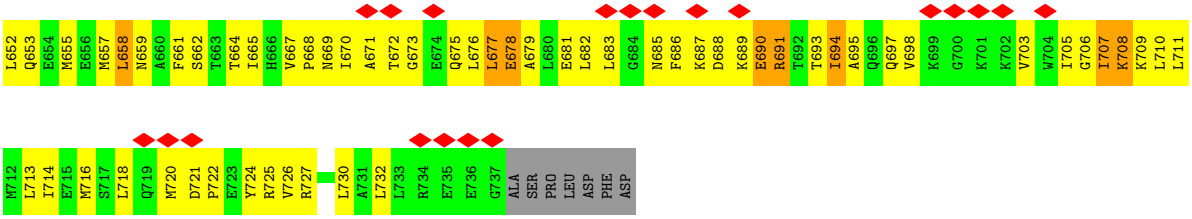
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

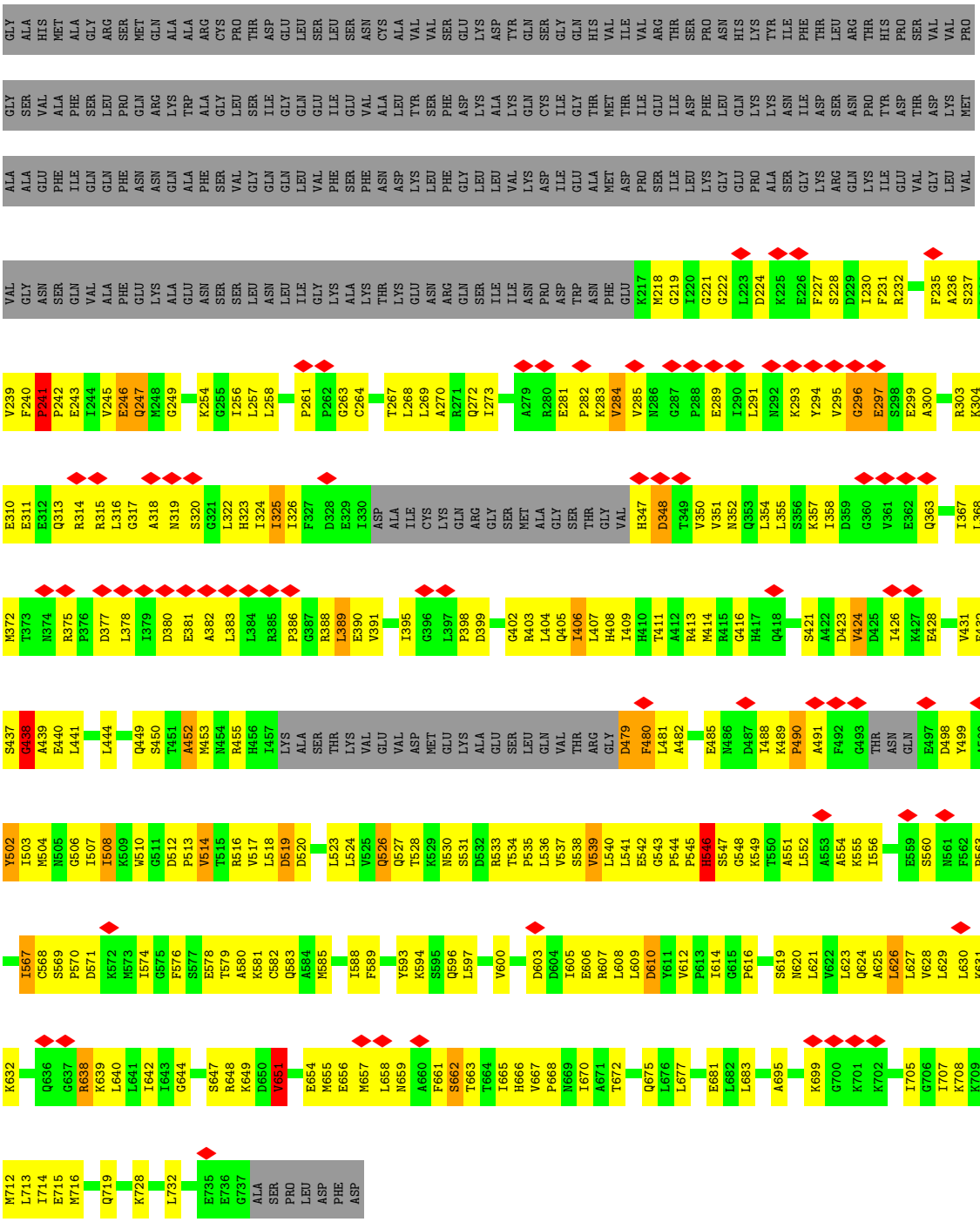
- Molecule 1: Vesicle-fusing ATPase





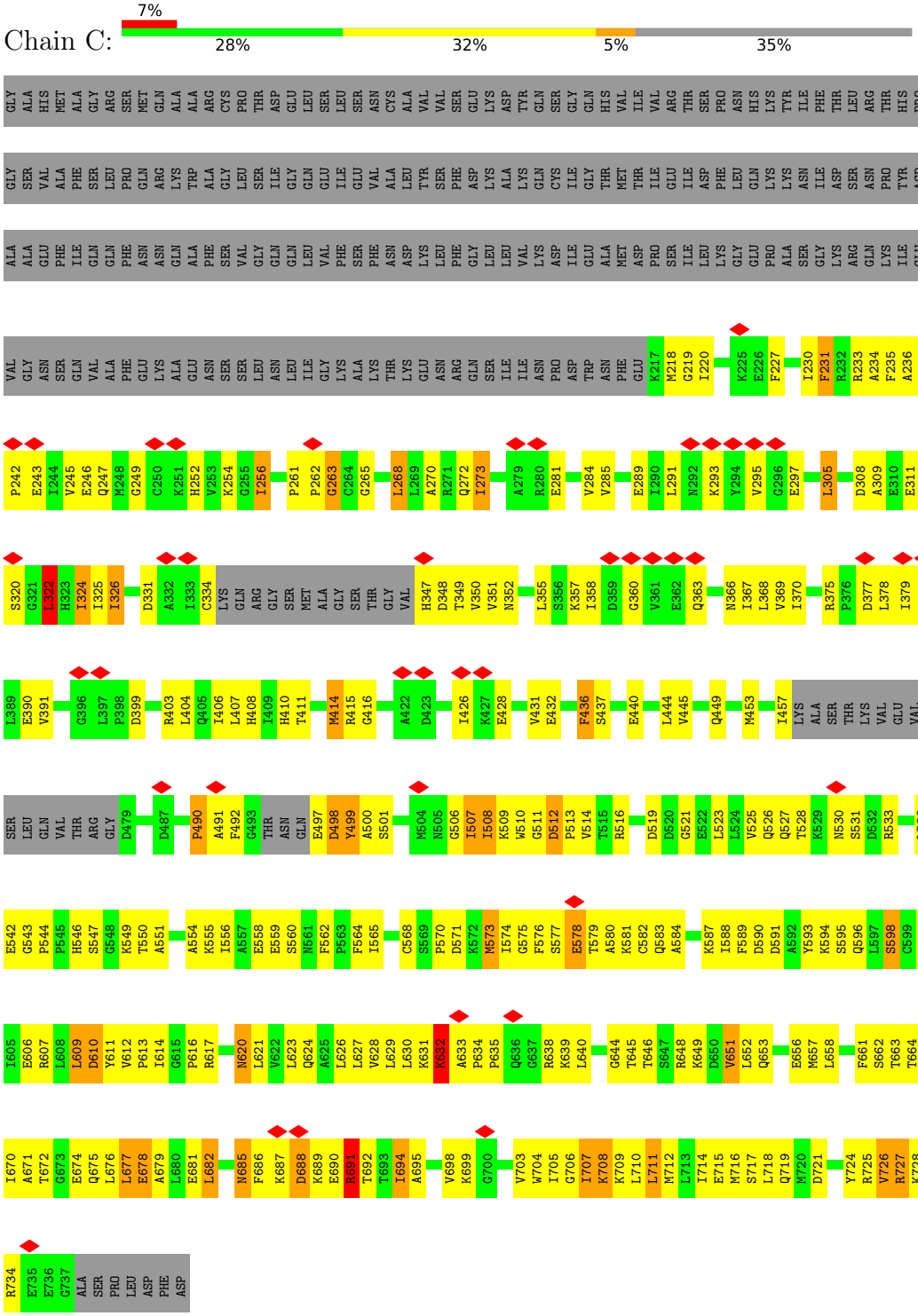
• Molecule 1: Vesicle-fusing ATPase

Chain B:



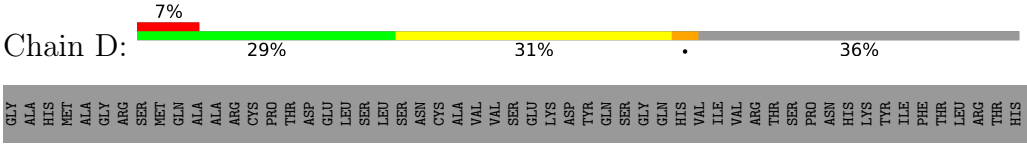
• Molecule 1: Vesicle-fusing ATPase

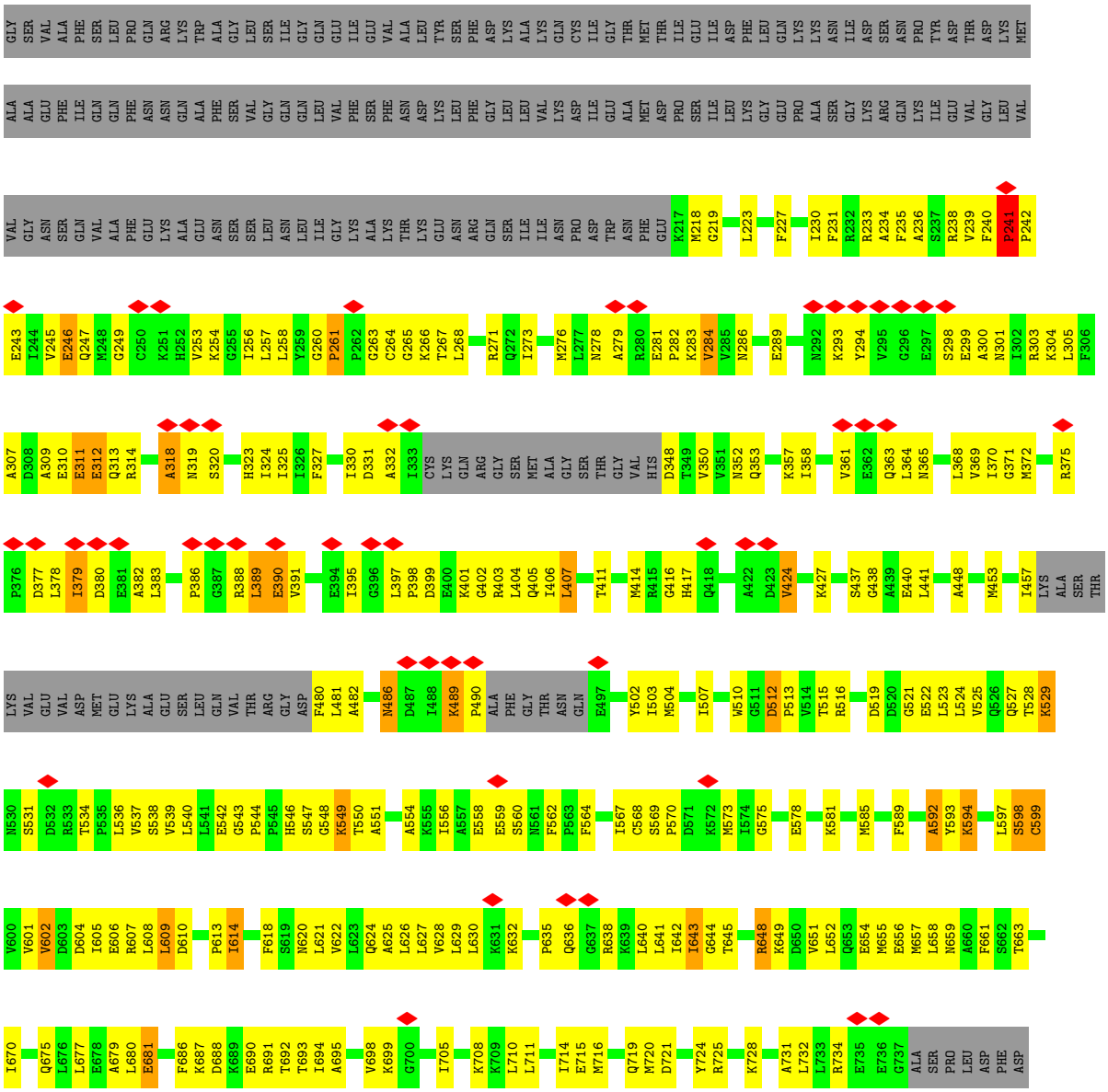
Chain C:



• Molecule 1: Vesicle-fusing ATPase

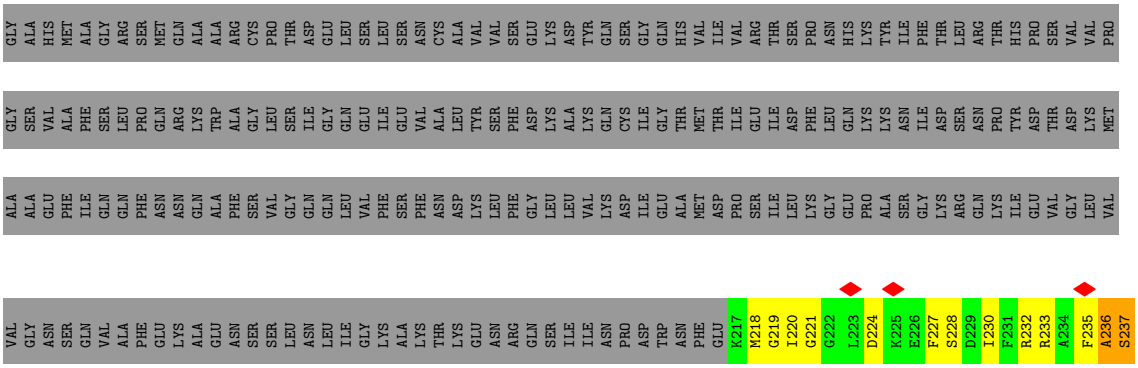
Chain D:

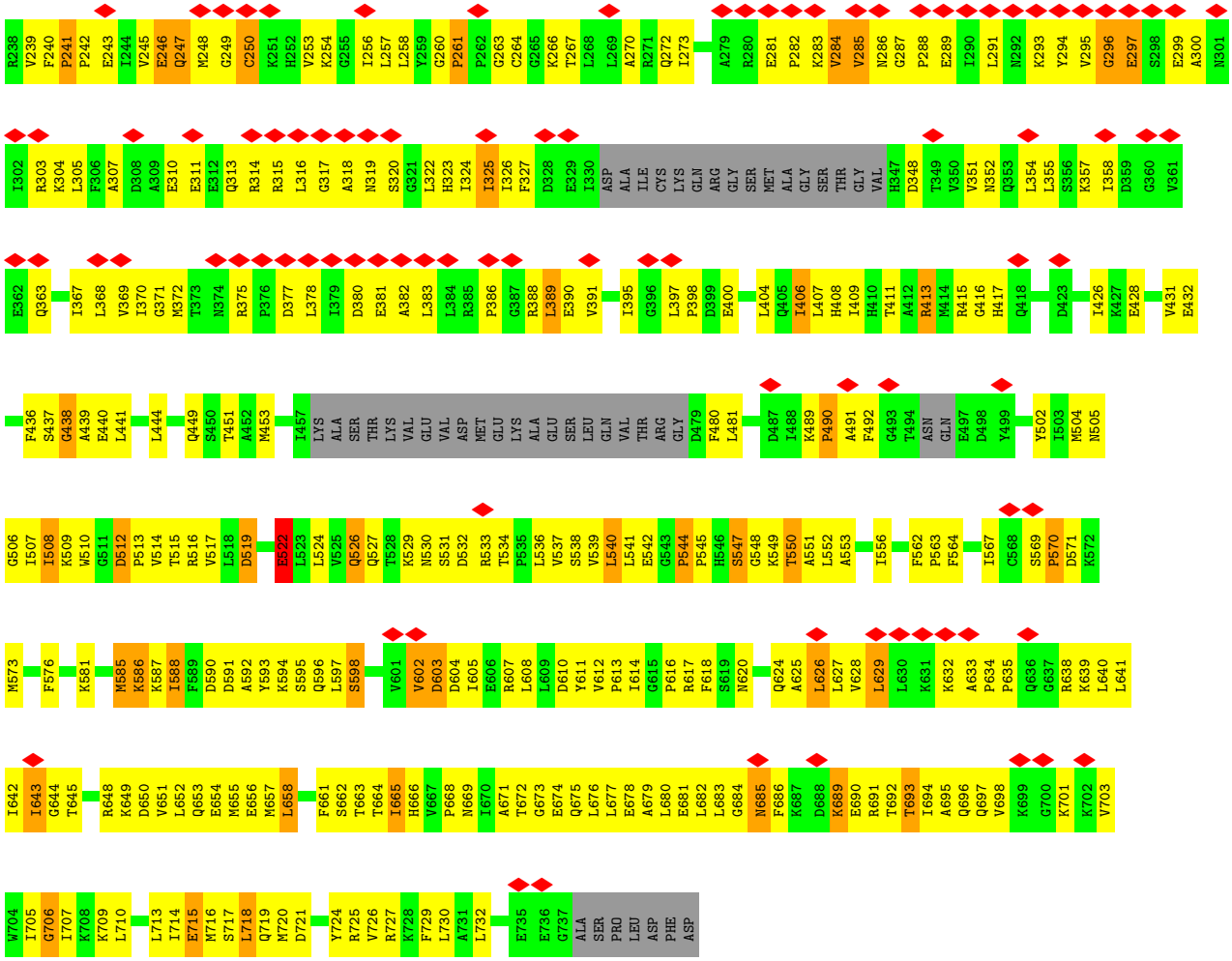




• Molecule 1: Vesicle-fusing ATPase

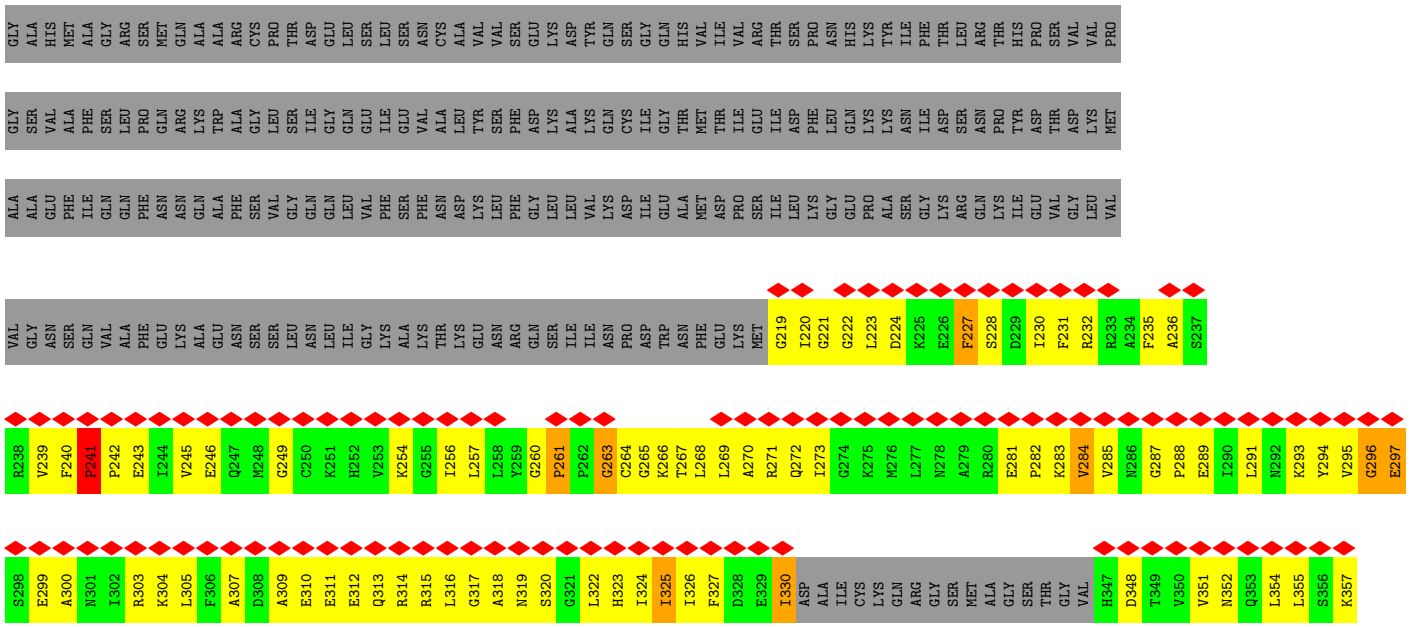
Chain E:

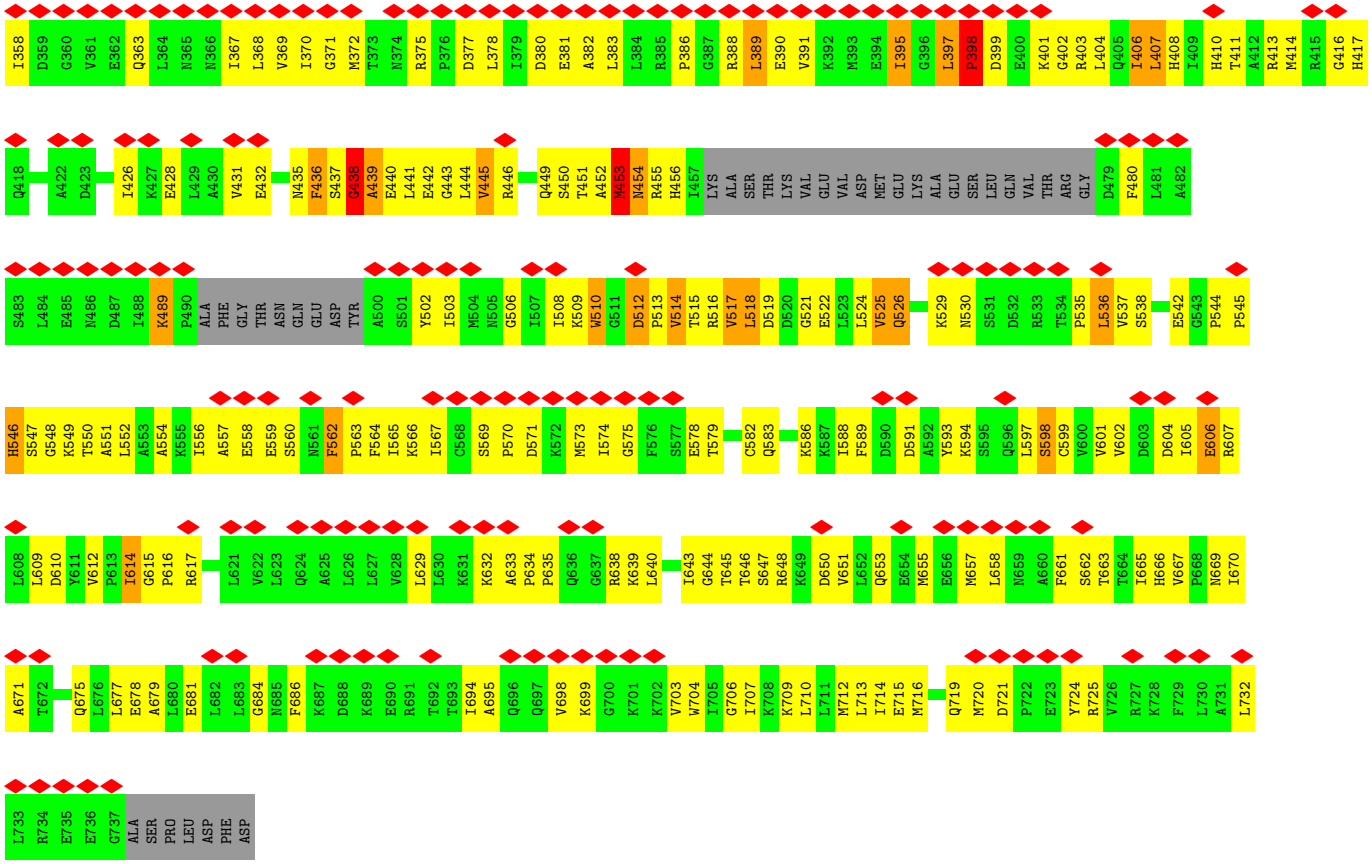




• Molecule 1: Vesicle-fusing ATPase

Chain F:




I358 D359 G360 V361 E362 Q363 L364 N365 N366 I367 L368 V369 I370 G371 M372 T373 N374 R375 P376 D377 L378 I379 D380 E381 A382 L383 L384 R385 P386 G387 R388 L389 E390 V391 K392 M393 E394 I395 G396 L397 P398 D399 E400 K401 G402 R403 L404 Q405 I406 L407 H408 I409 H410 T411 A412 R413 M414 R415 G416 H417
Q418 A422 D423 I426 K427 E428 L429 A430 V431 E432 N435 F436 S437 G438 A439 E440 L441 E442 G443 L444 V445 R446 Q449 S450 T451 A452 M453 N454 R455 H456 I457 LYS ALA SER THR LYS VAL GLU VAL ASP MET GLU LYS ALA GLU SER LEU GLN VAL THR ARG GLY D479 F480 L481 A482
S483 L484 E485 N486 D487 I488 K489 P490 ALA PHE GLY THR ASN GLN GLU ASP TYR A500 S501 Y502 I503 M504 N505 G506 I507 I508 K509 W510 G511 D512 P513 V514 T515 R516 V517 L518 D519 D520 G521 E522 L523 L524 V525 Q526 K529 N530 S531 D532 R533 T534 P535 L536 V537 S538 E542 G543 P544 P545
H546 S547 G548 K549 T550 A551 L552 A553 A554 K555 I556 A557 E558 E559 S560 N561 F562 P563 F564 I565 K566 I567 C568 S569 P570 D571 K572 M573 I574 G575 F576 S577 E578 T579 C582 Q583 K586 K587 I588 F589 D590 D591 A592 Y593 K594 S595 Q596 L597 S598 C599 V600 V601 V602 D603 D604 I605 E606 R607
L608 L609 D610 Y611 V612 P613 I614 G615 P616 R617 L621 V622 L623 Q624 A625 L626 L627 V628 L629 L630 K631 K632 A633 P634 P635 Q636 G637 R638 K639 L640 I643 G644 T645 T646 S647 R648 K649 D650 V651 L652 Q653 E654 M655 E656 M657 L658 N659 A660 F661 S662 T663 T664 I665 H666 V667 P668 N669 I670
A671 T672 Q675 L676 L677 E678 A679 L680 E681 L682 L683 G684 N685 F686 K687 D688 K689 E690 R691 T692 T693 I694 A695 Q696 Q697 V698 K699 G700 K701 K702 V703 W704 I705 G706 I707 K708 K709 L710 L711 M712 L713 I714 E715 M716 Q719 M720 D721 P722 E723 Y724 R725 V726 R727 K728 F729 L730 A731 L732
L733 R734 E735 E736 G737 ALA SER PRO LEU ASP PHE ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	13.843	Depositor
Minimum map value	-5.160	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	Depositor
Map size (Å)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.4312, 2.4312, 2.4312	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.74	4/3559 (0.1%)	1.46	51/4824 (1.1%)
1	B	0.66	2/3566 (0.1%)	1.35	40/4834 (0.8%)
1	C	0.65	1/3584 (0.0%)	1.35	44/4858 (0.9%)
1	D	0.61	0/3516	1.34	36/4775 (0.8%)
1	E	0.69	1/3566 (0.0%)	1.41	50/4833 (1.0%)
1	F	0.69	2/3514 (0.1%)	1.43	53/4759 (1.1%)
All	All	0.68	10/21305 (0.0%)	1.39	274/28883 (0.9%)

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	A	0	1
1	B	0	2
1	E	0	1
1	F	0	2
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	PHE	CA-C	-8.64	1.41	1.52
1	A	236	ALA	CA-CB	-8.41	1.40	1.53
1	C	507	ILE	CA-C	-7.14	1.47	1.53
1	F	456	HIS	CA-C	6.10	1.60	1.52
1	A	330	ILE	CA-CB	5.58	1.61	1.54
1	B	424	VAL	CA-CB	5.49	1.60	1.54
1	E	236	ALA	CA-CB	-5.39	1.44	1.53
1	B	452	ALA	C-O	5.20	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	455	ARG	CA-CB	5.16	1.61	1.53
1	A	235	PHE	CD1-CE1	-5.02	1.23	1.38

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	455	ARG	N-CA-C	12.80	125.31	111.36
1	A	239	VAL	N-CA-C	10.74	121.57	110.72
1	A	261	PRO	CA-C-N	10.72	133.42	120.23
1	A	261	PRO	C-N-CA	10.72	133.42	120.23
1	D	416	GLY	N-CA-C	-10.11	100.25	112.49
1	F	407	LEU	N-CA-C	-9.30	101.14	111.28
1	A	216	GLU	N-CA-C	-9.24	95.76	109.62
1	C	543	GLY	CA-C-N	9.23	126.40	119.66
1	C	543	GLY	C-N-CA	9.23	126.40	119.66
1	B	231	PHE	N-CA-C	-8.98	101.46	111.07
1	F	241	PRO	N-CA-C	8.95	121.62	110.70
1	B	241	PRO	N-CA-C	8.94	121.61	110.70
1	E	241	PRO	N-CA-C	8.92	121.58	110.70
1	C	241	PRO	N-CA-C	8.85	121.50	110.70
1	E	287	GLY	CA-C-N	8.73	128.75	119.05
1	E	287	GLY	C-N-CA	8.73	128.75	119.05
1	A	277	LEU	N-CA-C	8.73	120.88	111.36
1	A	273	ILE	N-CA-C	-8.59	102.46	110.53
1	B	416	GLY	N-CA-C	-8.40	102.32	112.49
1	A	231	PHE	N-CA-C	-8.37	102.16	111.28
1	A	241	PRO	C-N-CD	8.24	138.73	120.60
1	F	452	ALA	N-CA-C	-8.16	102.39	111.28
1	E	416	GLY	N-CA-C	-8.12	102.66	112.49
1	A	694	ILE	N-CA-C	-8.09	102.55	110.72
1	D	261	PRO	O-C-N	8.07	125.02	121.31
1	F	456	HIS	N-CA-C	8.07	120.15	111.36
1	A	260	GLY	CA-C-N	8.02	128.64	120.38
1	A	260	GLY	C-N-CA	8.02	128.64	120.38
1	A	708	LYS	N-CA-C	-7.99	102.57	111.28
1	C	416	GLY	N-CA-C	-7.97	102.85	112.49
1	C	620	ASN	N-CA-C	7.95	119.95	111.28
1	F	445	VAL	N-CA-C	-7.93	102.53	110.62
1	B	530	ASN	N-CA-C	7.93	119.92	111.28
1	F	512	ASP	N-CA-C	-7.83	102.04	113.16
1	E	261	PRO	CA-C-N	-7.81	111.96	119.85
1	E	261	PRO	C-N-CA	-7.81	111.96	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	514	VAL	CB-CA-C	-7.80	101.99	111.97
1	A	235	PHE	N-CA-C	-7.73	102.93	111.36
1	C	231	PHE	N-CA-C	-7.64	102.96	111.28
1	D	241	PRO	N-CA-C	7.54	119.91	110.70
1	D	512	ASP	N-CA-C	-7.54	102.46	113.16
1	F	294	TYR	N-CA-C	7.50	119.53	111.36
1	C	691	ARG	N-CA-C	-7.49	103.12	111.28
1	F	416	GLY	N-CA-C	-7.47	103.45	112.49
1	C	708	LYS	N-CA-C	-7.43	103.26	111.36
1	F	563	PRO	N-CA-C	-7.41	103.47	113.40
1	A	304	LYS	N-CA-C	7.38	118.96	111.07
1	B	406	ILE	CB-CA-C	-7.33	102.11	112.22
1	F	231	PHE	N-CA-C	-7.32	103.24	111.07
1	D	312	GLU	CA-C-N	7.32	130.40	120.38
1	D	312	GLU	C-N-CA	7.32	130.40	120.38
1	F	261	PRO	CA-C-N	-7.30	112.47	119.85
1	F	261	PRO	C-N-CA	-7.30	112.47	119.85
1	E	294	TYR	N-CA-C	7.29	119.30	111.36
1	A	236	ALA	N-CA-C	-7.26	103.30	111.07
1	F	525	VAL	CB-CA-C	-7.26	102.68	111.97
1	C	688	ASP	N-CA-C	7.24	118.82	111.07
1	B	294	TYR	N-CA-C	7.23	119.24	111.36
1	B	295	VAL	N-CA-C	7.20	117.97	110.62
1	F	287	GLY	CA-C-N	7.19	127.03	119.05
1	F	287	GLY	C-N-CA	7.19	127.03	119.05
1	E	649	LYS	N-CA-C	7.18	118.89	111.14
1	B	479	ASP	N-CA-C	-7.17	90.91	111.00
1	F	295	VAL	N-CA-C	7.16	117.92	110.62
1	E	550	THR	N-CA-C	7.09	119.09	111.36
1	B	610	ASP	N-CA-CB	-7.03	101.51	112.13
1	B	436	PHE	N-CA-C	7.03	120.42	110.23
1	D	549	LYS	N-CA-C	6.99	119.93	111.40
1	F	413	ARG	N-CA-C	-6.98	103.67	111.28
1	A	625	ALA	N-CA-C	-6.96	103.70	111.28
1	C	436	PHE	N-CA-C	6.94	120.30	110.23
1	B	651	VAL	CB-CA-C	-6.92	102.80	112.14
1	D	438	GLY	N-CA-C	-6.92	104.27	112.64
1	C	685	ASN	N-CA-C	-6.90	103.89	112.72
1	D	312	GLU	N-CA-C	6.88	118.43	111.07
1	A	238	ARG	N-CA-C	6.86	118.55	111.14
1	D	643	ILE	CB-CA-C	-6.83	100.52	110.63
1	E	633	ALA	CA-C-N	6.82	124.64	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	633	ALA	C-N-CA	6.82	124.64	119.66
1	A	235	PHE	CA-CB-CG	-6.80	107.00	113.80
1	D	592	ALA	N-CA-C	6.78	119.54	111.33
1	B	539	VAL	N-CA-C	6.75	117.56	108.11
1	A	262	PRO	N-CA-C	6.75	121.09	110.50
1	B	705	ILE	N-CA-C	6.72	117.22	108.35
1	C	707	ILE	N-CA-C	6.70	116.83	110.53
1	D	261	PRO	CA-C-N	-6.68	112.90	119.78
1	D	261	PRO	C-N-CA	-6.68	112.90	119.78
1	E	629	LEU	N-CA-C	6.65	118.53	111.28
1	A	440	GLU	N-CA-C	-6.60	104.01	111.07
1	E	585	MET	N-CA-C	-6.59	104.09	111.28
1	A	598	SER	N-CA-C	6.58	119.89	108.76
1	E	603	ASP	N-CA-C	6.53	119.81	109.50
1	F	453	MET	N-CA-C	-6.51	104.18	111.28
1	D	609	LEU	CA-C-N	6.48	131.56	122.36
1	D	609	LEU	C-N-CA	6.48	131.56	122.36
1	E	295	VAL	N-CA-C	6.47	118.00	110.62
1	C	508	ILE	N-CA-C	6.45	117.08	110.05
1	E	547	SER	N-CA-C	6.43	118.29	111.28
1	C	689	LYS	N-CA-C	6.39	118.25	111.28
1	E	237	SER	N-CA-C	-6.38	104.32	111.28
1	C	263	GLY	N-CA-C	-6.38	106.51	115.32
1	F	480	PHE	CB-CA-C	-6.33	109.28	116.63
1	F	395	ILE	N-CA-C	6.32	116.96	108.11
1	F	403	ARG	N-CA-C	-6.31	104.41	111.28
1	C	694	ILE	N-CA-C	-6.30	104.19	110.62
1	A	258	LEU	CA-C-N	-6.26	114.16	122.99
1	A	258	LEU	C-N-CA	-6.26	114.16	122.99
1	C	598	SER	N-CA-C	6.26	118.37	108.79
1	F	598	SER	N-CA-C	6.25	118.36	108.79
1	B	413	ARG	N-CA-C	-6.24	104.47	111.28
1	D	599	CYS	N-CA-C	6.23	119.05	108.90
1	E	240	PHE	CA-C-N	6.19	126.76	120.38
1	E	240	PHE	C-N-CA	6.19	126.76	120.38
1	B	526	GLN	N-CA-C	-6.16	104.48	111.07
1	A	241	PRO	N-CA-C	6.10	118.14	110.70
1	C	726	VAL	N-CA-C	6.10	116.84	110.62
1	C	632	LYS	N-CA-C	6.09	119.09	110.50
1	D	642	ILE	N-CA-C	6.07	116.61	108.11
1	B	348	ASP	CB-CA-C	-6.06	109.60	116.63
1	A	502	TYR	N-CA-C	6.05	117.87	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	348	ASP	CB-CA-C	-6.05	109.61	116.63
1	A	407	LEU	N-CA-C	-6.04	104.69	111.28
1	A	241	PRO	CA-C-N	-6.03	112.54	127.00
1	A	241	PRO	C-N-CA	-6.03	112.54	127.00
1	B	247	GLN	CA-C-N	6.02	128.35	120.28
1	B	247	GLN	C-N-CA	6.02	128.35	120.28
1	C	363	GLN	CB-CA-C	-6.01	109.66	116.63
1	E	250	CYS	N-CA-C	6.00	118.68	108.90
1	E	480	PHE	CB-CA-C	-6.00	109.67	116.63
1	A	363	GLN	CB-CA-C	-6.00	109.67	116.63
1	A	488	ILE	N-CA-C	5.99	121.27	113.07
1	C	705	ILE	N-CA-C	5.99	116.49	108.11
1	E	247	GLN	CA-C-N	5.98	128.29	120.28
1	E	247	GLN	C-N-CA	5.98	128.29	120.28
1	E	706	GLY	N-CA-C	5.97	119.84	112.14
1	F	435	ASN	N-CA-C	5.97	117.87	111.36
1	F	454	ASN	CA-C-N	5.95	128.73	120.29
1	F	454	ASN	C-N-CA	5.95	128.73	120.29
1	F	348	ASP	CB-CA-C	-5.93	109.75	116.63
1	A	426	ILE	N-CA-C	5.92	116.10	110.42
1	E	413	ARG	N-CA-C	-5.92	104.83	111.28
1	A	349	THR	N-CA-C	5.88	117.69	111.28
1	A	279	ALA	N-CA-C	-5.85	100.45	109.52
1	A	707	ILE	N-CA-C	5.83	116.56	110.62
1	F	526	GLN	N-CA-C	-5.82	104.84	111.07
1	E	522	GLU	CA-CB-CG	5.82	125.74	114.10
1	A	530	ASN	N-CA-C	5.80	120.48	113.17
1	D	481	LEU	N-CA-C	-5.79	104.97	111.28
1	B	638	ARG	N-CA-C	5.78	118.89	109.24
1	E	715	GLU	N-CA-C	-5.73	105.03	111.28
1	A	259	TYR	N-CA-C	5.73	118.24	108.90
1	C	678	GLU	N-CA-C	-5.72	105.05	111.28
1	F	263	GLY	N-CA-C	-5.72	107.43	115.32
1	A	678	GLU	N-CA-C	-5.71	105.05	111.28
1	D	238	ARG	N-CA-C	5.71	117.58	111.36
1	D	363	GLN	CB-CA-C	-5.68	110.04	116.63
1	C	239	VAL	N-CA-C	5.67	116.44	110.72
1	F	363	GLN	CB-CA-C	-5.67	110.06	116.63
1	A	227	PHE	N-CA-C	-5.67	105.11	111.28
1	B	544	PRO	CA-C-O	-5.66	116.83	120.90
1	D	403	ARG	N-CA-C	-5.64	105.13	111.28
1	F	546	HIS	N-CA-CB	-5.64	100.91	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	403	ARG	N-CA-C	-5.64	105.14	111.28
1	E	718	LEU	N-CA-C	5.62	117.41	111.28
1	B	544	PRO	O-C-N	5.62	123.89	121.31
1	B	363	GLN	CB-CA-C	-5.62	110.11	116.63
1	E	299	GLU	N-CA-C	-5.61	105.17	111.28
1	F	436	PHE	N-CA-C	5.61	118.36	110.23
1	C	512	ASP	N-CA-C	-5.59	105.86	113.57
1	F	299	GLU	N-CA-C	-5.59	105.19	111.28
1	C	357	LYS	N-CA-C	5.57	117.35	111.28
1	B	480	PHE	N-CA-C	-5.56	99.85	108.31
1	F	235	PHE	N-CA-C	5.56	118.53	111.69
1	A	277	LEU	CB-CA-C	-5.56	101.40	110.85
1	D	311	GLU	N-CA-C	5.55	117.41	111.36
1	A	330	ILE	N-CA-C	-5.55	104.96	110.62
1	C	230	ILE	CA-C-N	5.55	127.72	120.28
1	C	230	ILE	C-N-CA	5.55	127.72	120.28
1	E	678	GLU	N-CA-C	-5.53	105.25	111.28
1	C	295	VAL	N-CA-C	5.53	116.26	110.62
1	B	560	SER	N-CA-C	5.52	117.29	111.28
1	B	498	ASP	N-CA-C	-5.51	105.27	111.28
1	B	299	GLU	N-CA-C	-5.51	105.28	111.28
1	A	255	GLY	N-CA-C	5.50	119.32	110.90
1	B	662	SER	N-CA-C	5.50	117.36	111.36
1	E	629	LEU	CB-CA-C	-5.49	101.67	110.79
1	F	510	TRP	CA-C-N	-5.49	116.86	121.58
1	F	510	TRP	C-N-CA	-5.49	116.86	121.58
1	E	235	PHE	N-CA-C	5.48	118.43	111.69
1	E	363	GLN	CB-CA-C	-5.46	110.29	116.63
1	B	235	PHE	N-CA-C	5.46	118.41	111.69
1	D	594	LYS	N-CA-CB	-5.44	102.12	110.12
1	C	348	ASP	CB-CA-C	-5.44	110.32	116.63
1	D	390	GLU	N-CA-C	5.43	117.20	111.28
1	F	398	PRO	CA-N-CD	-5.43	104.40	112.00
1	A	691	ARG	CA-C-N	5.43	127.55	120.28
1	A	691	ARG	C-N-CA	5.43	127.55	120.28
1	F	517	VAL	CB-CA-C	-5.42	104.83	112.14
1	A	273	ILE	N-CA-CB	5.41	117.49	110.57
1	A	705	ILE	N-CA-C	5.40	115.67	108.11
1	D	486	ASN	N-CA-C	-5.39	105.48	111.36
1	D	276	MET	N-CA-C	5.38	117.22	111.36
1	C	414	MET	CA-C-N	5.36	127.46	120.28
1	C	414	MET	C-N-CA	5.36	127.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	388	ARG	N-CA-C	5.36	117.12	111.28
1	A	525	VAL	CB-CA-C	-5.35	105.13	111.97
1	F	489	LYS	N-CA-C	5.34	121.61	109.81
1	F	562	PHE	CA-C-N	5.33	124.66	118.85
1	F	562	PHE	C-N-CA	5.33	124.66	118.85
1	F	227	PHE	N-CA-C	-5.32	105.48	111.28
1	E	519	ASP	N-CA-CB	5.32	117.94	110.12
1	F	518	LEU	CD1-CG-CD2	-5.32	99.10	110.80
1	D	414	MET	CA-C-N	5.31	127.83	120.29
1	D	414	MET	C-N-CA	5.31	127.83	120.29
1	C	406	ILE	CB-CA-C	-5.31	105.07	112.02
1	B	227	PHE	N-CA-C	-5.30	105.50	111.28
1	A	215	PHE	CA-C-N	-5.29	114.23	122.05
1	A	215	PHE	C-N-CA	-5.29	114.23	122.05
1	B	708	LYS	N-CA-C	-5.29	105.52	111.28
1	B	424	VAL	CB-CA-C	-5.28	102.98	111.59
1	F	514	VAL	CB-CA-C	-5.28	105.21	111.97
1	D	261	PRO	CA-C-O	-5.28	117.10	120.90
1	C	667	VAL	CA-C-N	-5.27	114.55	120.14
1	C	667	VAL	C-N-CA	-5.27	114.55	120.14
1	A	357	LYS	N-CA-C	5.27	118.87	112.23
1	C	234	ALA	N-CA-C	5.27	116.83	111.14
1	F	524	LEU	N-CA-C	-5.26	105.54	111.28
1	D	598	SER	N-CA-C	5.25	117.23	108.99
1	E	526	GLN	N-CA-C	-5.25	105.56	111.28
1	D	294	TYR	N-CA-C	5.25	118.78	112.38
1	F	512	ASP	CA-C-N	-5.24	113.24	119.05
1	F	512	ASP	C-N-CA	-5.24	113.24	119.05
1	E	227	PHE	N-CA-C	-5.23	105.58	111.28
1	A	391	VAL	N-CA-C	5.22	115.41	108.11
1	D	648	ARG	N-CA-C	5.21	116.90	108.41
1	E	235	PHE	CA-C-N	5.21	127.26	120.28
1	E	235	PHE	C-N-CA	5.21	127.26	120.28
1	C	415	ARG	CA-C-N	5.21	125.61	119.94
1	C	415	ARG	C-N-CA	5.21	125.61	119.94
1	E	415	ARG	CA-C-N	5.21	125.61	119.94
1	E	415	ARG	C-N-CA	5.21	125.61	119.94
1	F	406	ILE	CG1-CB-CG2	-5.20	95.09	110.70
1	C	508	ILE	CB-CA-C	-5.18	105.89	111.59
1	B	518	LEU	N-CA-C	5.18	116.92	111.28
1	D	529	LYS	N-CA-C	5.16	116.91	111.28
1	E	570	PRO	N-CA-C	-5.16	106.36	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	516	ARG	N-CA-C	-5.16	105.74	111.36
1	E	544	PRO	CA-C-O	-5.15	117.19	120.90
1	D	379	ILE	N-CA-C	5.14	116.02	110.21
1	E	512	ASP	N-CA-C	-5.13	105.88	113.16
1	B	435	ASN	N-CA-C	5.12	116.94	111.36
1	E	685	ASN	N-CA-C	-5.12	106.17	112.72
1	B	405	GLN	N-CA-C	5.11	116.54	111.07
1	E	727	ARG	N-CA-C	-5.10	105.41	111.69
1	D	233	ARG	N-CA-C	5.10	117.97	111.69
1	B	519	ASP	N-CA-C	-5.09	105.73	111.28
1	C	312	GLU	N-CA-C	-5.08	105.63	111.07
1	C	727	ARG	N-CA-C	-5.08	105.74	111.28
1	E	598	SER	N-CA-C	5.08	116.96	108.99
1	B	594	LYS	N-CA-C	5.08	116.81	111.28
1	E	406	ILE	CB-CA-C	-5.07	105.23	112.22
1	F	442	GLU	N-CA-C	-5.07	105.76	111.28
1	C	322	LEU	CA-CB-CG	5.06	134.00	116.30
1	C	677	LEU	CB-CG-CD2	-5.04	95.58	110.70
1	E	296	GLY	CA-C-N	5.04	130.78	121.70
1	E	296	GLY	C-N-CA	5.04	130.78	121.70
1	C	360	GLY	N-CA-C	-5.04	106.14	111.93
1	F	296	GLY	CA-C-N	5.03	130.76	121.70
1	F	296	GLY	C-N-CA	5.03	130.76	121.70
1	B	296	GLY	CA-C-N	5.03	130.75	121.70
1	B	296	GLY	C-N-CA	5.03	130.75	121.70
1	F	640	LEU	N-CA-C	5.02	117.01	109.23
1	D	489	LYS	N-CA-C	5.01	120.87	109.81
1	A	596	GLN	CB-CA-C	-5.00	103.02	110.88

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	B	438	GLY	Peptide
1	B	546	HIS	Mainchain
1	E	438	GLY	Peptide
1	F	438	GLY	Peptide
1	F	453	MET	Mainchain

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	3513	0	3416	274	0
1	B	3517	0	3436	266	0
1	C	3535	0	3431	286	0
1	D	3467	0	3351	261	0
1	E	3516	0	3424	294	0
1	F	3467	0	3409	271	0
2	B	27	0	10	11	0
2	C	27	0	12	8	0
2	D	27	0	9	11	0
2	E	27	0	10	9	0
All	All	21123	0	20508	1543	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 37.

All (1543) 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:F:222:GLY:H	1:F:402:GLY:HA3	1.24	1.02
1:A:222:GLY:HA3	1:A:402:GLY:HA2	1.51	0.93
1:E:263:GLY:O	1:E:437:SER:HB2	1.71	0.89
1:D:448:ALA:HA	1:D:482:ALA:HB3	1.53	0.89
1:C:490:PRO:HA	1:C:491:ALA:HB3	1.53	0.88
1:F:538:SER:HB3	1:F:662:SER:H	1.40	0.86
1:F:545:PRO:HA	1:F:547:SER:H	1.39	0.85
1:D:527:GLN:HE22	1:E:715:GLU:C	1.83	0.85
1:F:538:SER:HG	1:F:661:PHE:HD1	1.22	0.84
1:C:670:ILE:HD13	1:C:675:GLN:HG2	1.58	0.84
1:E:686:PHE:HE1	1:E:714:ILE:HG23	1.43	0.84
1:F:256:ILE:HG13	1:F:370:ILE:HG22	1.58	0.84
1:A:549:LYS:NZ	1:A:647:SER:OG	2.10	0.83
1:D:507:ILE:HA	2:D:801:ADP:N7	1.93	0.83
1:E:490:PRO:HA	1:E:491:ALA:HB3	1.60	0.83
1:B:490:PRO:HA	1:B:491:ALA:HB3	1.60	0.83
1:F:538:SER:H	1:F:662:SER:HB3	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ILE:HG13	1:C:370:ILE:HG22	1.59	0.83
1:C:687:LYS:N	1:C:690:GLU:OE2	2.12	0.82
1:B:508:ILE:H	2:B:801:ADP:HN61	1.23	0.82
1:A:285:VAL:HG13	1:A:326:ILE:HD11	1.61	0.82
1:E:526:GLN:NE2	1:F:719:GLN:O	2.12	0.81
1:E:527:GLN:O	1:E:531:SER:OG	1.97	0.81
1:B:589:PHE:HE1	1:B:600:VAL:HG11	1.45	0.81
1:A:510:TRP:HA	1:A:682:LEU:HD13	1.61	0.81
1:C:313:GLN:O	1:C:317:GLY:N	2.14	0.81
1:C:407:LEU:HD11	1:C:426:ILE:HG23	1.62	0.81
1:F:525:VAL:HG13	1:F:562:PHE:CE1	2.16	0.80
1:E:707:ILE:HD13	2:E:801:ADP:C8	2.17	0.80
1:F:536:LEU:HD11	1:F:634:PRO:HD3	1.62	0.80
1:B:386:PRO:HA	1:B:390:GLU:HA	1.64	0.80
1:D:568:CYS:SG	1:D:585:MET:HE1	2.21	0.80
1:D:406:ILE:HG22	1:D:441:LEU:HD22	1.61	0.80
1:F:386:PRO:HA	1:F:390:GLU:HA	1.62	0.80
1:A:713:LEU:HD21	1:A:732:LEU:HB3	1.64	0.79
1:E:587:LYS:NZ	1:E:587:LYS:O	2.15	0.79
1:A:542:GLU:HG2	1:A:649:LYS:HD2	1.61	0.79
1:A:546:HIS:C	1:A:708:LYS:HB3	2.07	0.79
1:E:534:THR:HG21	1:F:712:MET:HA	1.63	0.79
1:A:485:GLU:O	1:A:489:LYS:N	2.15	0.79
1:C:497:GLU:O	1:C:499:TYR:N	2.14	0.79
1:B:581:LYS:NZ	1:B:608:LEU:O	2.15	0.79
1:A:557:ALA:O	1:A:560:SER:OG	2.00	0.79
1:C:540:LEU:HB3	1:C:664:THR:HG22	1.63	0.79
1:E:407:LEU:HD11	1:E:426:ILE:HG23	1.65	0.79
1:F:570:PRO:HG2	1:F:604:ASP:HB2	1.65	0.78
1:F:564:PHE:O	1:F:598:SER:OG	2.00	0.78
1:E:627:LEU:HG	1:E:657:MET:HE1	1.63	0.78
1:D:720:MET:HE3	1:D:724:TYR:HE1	1.47	0.78
1:F:517:VAL:HG13	1:F:665:ILE:HG21	1.66	0.78
1:E:680:LEU:HD13	1:E:694:ILE:HD13	1.66	0.78
1:F:222:GLY:N	1:F:402:GLY:HA3	1.97	0.78
1:A:397:LEU:HD13	1:A:435:ASN:HA	1.66	0.78
1:E:386:PRO:HA	1:E:390:GLU:HA	1.63	0.78
1:A:567:ILE:HG13	1:A:601:VAL:HB	1.66	0.77
1:E:706:GLY:O	1:E:710:LEU:N	2.16	0.77
1:D:728:LYS:HE3	1:D:732:LEU:HD11	1.67	0.77
1:E:685:ASN:HB3	1:E:718:LEU:HD11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:LEU:HD12	1:D:607:ARG:HH12	1.50	0.76
1:D:510:TRP:HE3	1:D:675:GLN:HG2	1.51	0.76
1:F:222:GLY:HA2	1:F:399:ASP:HB2	1.67	0.76
1:E:625:ALA:HA	1:F:574:ILE:HD11	1.67	0.76
1:B:627:LEU:HD21	1:B:657:MET:HG3	1.67	0.76
1:F:398:PRO:HG3	1:F:436:PHE:O	1.85	0.76
1:C:652:LEU:HD22	1:C:657:MET:HG2	1.67	0.76
1:B:300:ALA:O	1:B:304:LYS:HG2	1.86	0.76
1:D:502:TYR:O	2:D:801:ADP:O3'	2.03	0.76
1:C:578:GLU:HB3	1:C:621:LEU:HB3	1.68	0.76
1:C:718:LEU:O	1:C:725:ARG:NH1	2.19	0.75
1:A:351:VAL:O	1:A:355:LEU:HG	1.86	0.75
1:A:670:ILE:HG23	1:A:675:GLN:HB2	1.68	0.75
1:E:300:ALA:O	1:E:304:LYS:HG2	1.86	0.75
1:E:686:PHE:HB3	1:E:690:GLU:HB2	1.68	0.75
1:D:448:ALA:HA	1:D:482:ALA:CB	2.16	0.75
1:C:724:TYR:HD2	1:C:727:ARG:HH21	1.35	0.74
1:F:407:LEU:HD11	1:F:426:ILE:HG23	1.67	0.74
1:A:626:LEU:HD21	1:A:657:MET:HE1	1.69	0.74
1:E:552:LEU:HD21	2:E:801:ADP:N6	1.99	0.74
1:F:589:PHE:HD2	1:F:629:LEU:HD13	1.52	0.74
1:B:585:MET:HE1	1:B:626:LEU:HG	1.69	0.74
1:C:691:ARG:HA	1:C:694:ILE:HD12	1.67	0.74
1:F:220:ILE:N	1:F:406:ILE:HD11	2.02	0.74
1:D:313:GLN:HE22	1:D:364:LEU:HA	1.51	0.74
1:A:238:ARG:HA	1:A:252:HIS:CE1	2.21	0.74
1:E:563:PRO:HG2	1:E:595:SER:OG	1.87	0.74
1:C:711:LEU:O	1:C:715:GLU:HG2	1.88	0.74
1:B:540:LEU:HD23	1:B:661:PHE:CD1	2.23	0.74
1:C:544:PRO:O	1:C:547:SER:OG	2.06	0.74
1:C:318:ALA:O	1:C:319:ASN:ND2	2.21	0.74
1:C:386:PRO:HA	1:C:390:GLU:HA	1.70	0.74
1:C:690:GLU:HB2	1:C:726:VAL:HG21	1.69	0.74
1:F:300:ALA:O	1:F:304:LYS:HG2	1.87	0.73
1:A:236:ALA:HB1	1:B:453:MET:HB2	1.70	0.73
1:C:596:GLN:HA	1:C:638:ARG:HD3	1.71	0.73
1:B:524:LEU:HD21	1:B:663:THR:HG21	1.70	0.73
1:C:630:LEU:HD11	1:C:661:PHE:CE1	2.24	0.73
1:A:624:GLN:HG3	1:B:610:ASP:OD2	1.87	0.73
1:A:553:ALA:HA	1:A:556:ILE:HD12	1.69	0.73
1:F:535:PRO:HA	1:F:639:LYS:HG2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LEU:HD11	1:B:649:LYS:NZ	2.04	0.72
1:B:533:ARG:HG3	1:B:534:THR:H	1.53	0.72
1:C:508:ILE:HG13	1:C:510:TRP:HD1	1.53	0.72
1:B:407:LEU:HD11	1:B:426:ILE:HG23	1.71	0.72
1:D:352:ASN:HB3	1:E:288:PRO:HB2	1.70	0.72
1:E:311:GLU:OE1	1:E:314:ARG:NE	2.23	0.72
1:D:301:ASN:HA	1:D:304:LYS:HD3	1.70	0.72
1:E:585:MET:HA	1:E:588:ILE:HD12	1.69	0.72
1:B:508:ILE:N	2:B:801:ADP:HN61	1.88	0.72
1:C:513:PRO:O	1:C:516:ARG:HG2	1.89	0.72
1:E:653:GLN:HA	1:E:658:LEU:HB2	1.71	0.72
1:E:510:TRP:CD1	1:E:707:ILE:HD12	2.25	0.72
1:A:710:LEU:O	1:A:714:ILE:HG13	1.89	0.71
1:C:508:ILE:HD11	1:C:707:ILE:HD11	1.71	0.71
1:F:565:ILE:HG23	1:F:599:CYS:HB3	1.72	0.71
1:C:611:TYR:CE1	1:C:616:PRO:HB2	2.26	0.71
1:D:605:ILE:HD11	1:D:644:GLY:HA3	1.72	0.71
1:E:513:PRO:HA	1:E:516:ARG:HG2	1.70	0.71
1:B:263:GLY:O	1:B:437:SER:HB3	1.91	0.71
1:D:528:THR:OG1	1:D:641:LEU:HD12	1.90	0.71
1:F:569:SER:OG	1:F:571:ASP:OD2	2.05	0.71
1:F:634:PRO:HB2	1:F:638:ARG:HG3	1.73	0.71
1:D:230:ILE:HD11	1:D:256:ILE:HD13	1.72	0.71
1:E:236:ALA:HA	1:E:239:VAL:HG12	1.72	0.71
1:F:606:GLU:N	1:F:606:GLU:OE1	2.24	0.71
1:B:424:VAL:N	1:B:479:ASP:N	2.39	0.70
1:B:656:GLU:OE1	1:C:648:ARG:NH2	2.24	0.70
1:D:386:PRO:HA	1:D:390:GLU:HA	1.73	0.70
1:D:711:LEU:HA	1:D:714:ILE:HD12	1.73	0.70
1:A:221:GLY:HA3	1:A:406:ILE:HG13	1.74	0.70
1:B:303:ARG:HG3	1:B:357:LYS:HE2	1.73	0.70
1:F:510:TRP:CE3	1:F:675:GLN:HB3	2.25	0.70
1:B:507:ILE:HA	2:B:801:ADP:N7	2.06	0.70
1:C:564:PHE:O	1:C:598:SER:OG	2.07	0.70
1:D:513:PRO:HA	1:D:516:ARG:HG2	1.70	0.70
1:E:603:ASP:OD2	1:E:645:THR:OG1	2.06	0.70
1:F:437:SER:OG	1:F:440:GLU:HG2	1.91	0.70
1:A:326:ILE:HG22	1:A:370:ILE:HG12	1.73	0.70
1:F:303:ARG:HG3	1:F:357:LYS:HE2	1.74	0.70
1:C:262:PRO:HD2	1:C:594:LYS:HE2	1.73	0.70
1:E:604:ASP:HB3	1:E:607:ARG:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ALA:HB1	1:A:367:ILE:HG21	1.74	0.70
1:E:514:VAL:HG13	2:E:801:ADP:HN61	1.55	0.70
1:F:721:ASP:HB2	1:F:724:TYR:HD1	1.57	0.70
1:C:669:ASN:OD1	1:C:706:GLY:HA2	1.90	0.70
1:D:348:ASP:O	1:D:352:ASN:ND2	2.25	0.70
1:A:669:ASN:HD22	1:A:706:GLY:HA2	1.57	0.70
1:E:538:SER:OG	1:E:661:PHE:HA	1.92	0.70
1:F:510:TRP:HB3	1:F:679:ALA:HB2	1.74	0.70
1:B:538:SER:HB3	1:B:661:PHE:HD2	1.57	0.69
1:D:510:TRP:CE3	1:D:670:ILE:HG22	2.27	0.69
1:F:224:ASP:O	1:F:228:SER:HB2	1.91	0.69
1:B:648:ARG:NH1	1:B:651:VAL:HG22	2.06	0.69
1:B:311:GLU:OE1	1:B:314:ARG:NE	2.23	0.69
1:F:311:GLU:OE1	1:F:314:ARG:NE	2.22	0.69
1:E:590:ASP:OD2	1:E:594:LYS:NZ	2.25	0.69
1:A:546:HIS:O	1:A:708:LYS:HB3	1.93	0.69
1:B:589:PHE:CE1	1:B:600:VAL:HG11	2.26	0.69
1:C:706:GLY:O	1:C:710:LEU:N	2.24	0.69
1:E:232:ARG:O	1:E:236:ALA:HB3	1.92	0.69
1:F:545:PRO:HA	1:F:547:SER:N	2.06	0.69
1:F:612:VAL:HG12	1:F:617:ARG:HB2	1.73	0.69
1:D:303:ARG:HD3	1:D:353:GLN:CG	2.22	0.69
1:F:536:LEU:HD21	1:F:632:LYS:O	1.92	0.69
1:B:670:ILE:HG22	1:B:672:THR:H	1.58	0.69
1:E:303:ARG:HG3	1:E:357:LYS:HE2	1.74	0.69
1:F:222:GLY:HA3	1:F:399:ASP:H	1.57	0.69
1:A:565:ILE:HG13	1:A:599:CYS:HB3	1.74	0.69
1:A:602:VAL:HG12	1:A:605:ILE:HG12	1.73	0.69
1:D:397:LEU:HD23	1:D:398:PRO:HD2	1.75	0.69
1:E:674:GLU:HA	1:E:677:LEU:HD12	1.75	0.69
1:A:677:LEU:HD21	1:A:695:ALA:HA	1.75	0.68
1:E:652:LEU:CD2	1:E:657:MET:HB3	2.23	0.68
1:F:713:LEU:HD22	1:F:732:LEU:HB3	1.73	0.68
1:D:548:GLY:HA2	2:D:801:ADP:C5'	2.23	0.68
1:E:536:LEU:HD12	1:E:640:LEU:O	1.94	0.68
1:F:546:HIS:CE1	1:F:709:LYS:HB3	2.28	0.68
1:C:533:ARG:HB2	1:D:715:GLU:OE1	1.92	0.68
1:E:652:LEU:HD23	1:E:657:MET:HB3	1.76	0.68
1:C:331:ASP:HA	1:C:379:ILE:HD11	1.76	0.68
1:A:521:GLY:O	1:A:525:VAL:HG23	1.95	0.67
1:E:237:SER:HA	1:F:453:MET:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ILE:HD12	1:D:388:ARG:HB3	1.76	0.67
1:C:542:GLU:CB	1:C:649:LYS:HD3	2.24	0.67
1:D:527:GLN:HE21	1:E:715:GLU:HG3	1.59	0.67
1:A:564:PHE:CE1	1:A:566:LYS:HB2	2.29	0.67
1:B:358:ILE:HD12	1:B:388:ARG:HB3	1.77	0.67
1:C:649:LYS:HE2	1:C:658:LEU:HD13	1.77	0.67
1:F:609:LEU:HD13	1:F:655:MET:HE1	1.77	0.67
1:B:542:GLU:HB3	1:B:649:LYS:HG3	1.77	0.67
1:B:649:LYS:HE3	1:B:658:LEU:HD11	1.76	0.67
1:F:236:ALA:HA	1:F:239:VAL:HG12	1.77	0.67
1:B:258:LEU:HB3	1:B:395:ILE:HD11	1.77	0.67
1:E:510:TRP:CD1	1:E:514:VAL:HG21	2.30	0.67
1:E:618:PHE:HZ	1:F:612:VAL:HG11	1.60	0.67
1:D:312:GLU:OE1	1:D:323:HIS:ND1	2.24	0.66
1:B:224:ASP:O	1:B:228:SER:HB2	1.95	0.66
1:E:624:GLN:NE2	1:F:610:ASP:OD1	2.29	0.66
1:E:681:GLU:HA	1:E:691:ARG:HE	1.59	0.66
1:A:531:SER:OG	1:B:715:GLU:OE1	2.14	0.66
1:A:657:MET:HE3	1:A:661:PHE:CE1	2.31	0.66
1:B:452:ALA:HA	1:B:455:ARG:NH2	2.10	0.66
1:B:528:THR:O	1:B:639:LYS:HD2	1.96	0.66
1:D:627:LEU:HD21	1:D:657:MET:HG3	1.77	0.66
1:E:671:ALA:HA	1:E:703:VAL:O	1.95	0.66
1:B:538:SER:HB3	1:B:661:PHE:CD2	2.30	0.66
1:F:695:ALA:HB1	1:F:699:LYS:HE3	1.78	0.66
1:A:653:GLN:O	1:A:653:GLN:NE2	2.28	0.66
1:C:506:GLY:N	2:C:801:ADP:O2'	2.29	0.66
1:B:589:PHE:HE2	1:B:629:LEU:HB3	1.61	0.66
1:A:526:GLN:HE21	1:A:530:ASN:HD22	1.43	0.65
1:D:245:VAL:O	1:D:249:GLY:N	2.29	0.65
1:E:542:GLU:O	1:E:666:HIS:ND1	2.28	0.65
1:A:510:TRP:HB2	1:A:679:ALA:HA	1.78	0.65
1:D:234:ALA:HA	1:D:253:VAL:HG11	1.78	0.65
1:E:245:VAL:O	1:E:249:GLY:N	2.28	0.65
1:E:592:ALA:HB1	1:E:640:LEU:HD22	1.77	0.65
1:E:437:SER:OG	1:E:440:GLU:HG2	1.96	0.65
1:E:625:ALA:O	1:E:629:LEU:HG	1.97	0.65
1:A:687:LYS:N	1:A:690:GLU:OE1	2.29	0.65
1:D:284:VAL:HG23	1:D:324:ILE:O	1.97	0.65
1:E:640:LEU:HD12	1:E:641:LEU:N	2.12	0.65
1:D:404:LEU:HA	1:D:407:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:MET:SD	1:D:581:LYS:HD3	2.36	0.65
1:D:695:ALA:HB1	1:D:699:LYS:HE3	1.79	0.65
1:F:358:ILE:HD12	1:F:388:ARG:HB3	1.77	0.65
1:A:628:VAL:HG11	1:B:571:ASP:HA	1.79	0.64
1:A:707:ILE:HA	1:A:710:LEU:HB2	1.79	0.64
1:C:261:PRO:HB2	1:C:594:LYS:HG3	1.77	0.64
1:F:510:TRP:HB2	1:F:675:GLN:O	1.97	0.64
1:A:256:ILE:HG13	1:A:370:ILE:HG22	1.80	0.64
1:D:620:ASN:O	1:D:624:GLN:HG2	1.96	0.64
1:E:509:LYS:HD2	1:E:515:THR:HG22	1.79	0.64
1:B:404:LEU:HG	1:B:426:ILE:HG22	1.80	0.64
1:B:548:GLY:HA3	2:B:801:ADP:H2	1.63	0.64
1:B:624:GLN:NE2	1:C:610:ASP:O	2.30	0.64
1:F:438:GLY:O	1:F:441:LEU:N	2.30	0.64
1:E:502:TYR:OH	1:E:569:SER:OG	2.15	0.64
1:F:546:HIS:CD2	1:F:546:HIS:H	2.15	0.64
1:F:570:PRO:HG2	1:F:604:ASP:CB	2.28	0.64
1:D:263:GLY:O	1:D:437:SER:OG	2.12	0.64
1:D:319:ASN:HB3	1:D:320:SER:HB2	1.79	0.64
1:C:358:ILE:CB	1:C:388:ARG:HG3	2.26	0.64
1:A:223:LEU:HD12	1:A:227:PHE:HB2	1.80	0.64
1:E:224:ASP:O	1:E:228:SER:HB2	1.98	0.64
1:E:358:ILE:HD12	1:E:388:ARG:HB3	1.79	0.64
1:E:710:LEU:O	1:E:714:ILE:HG13	1.97	0.64
1:A:617:ARG:HG3	1:A:617:ARG:HH11	1.62	0.64
1:E:505:ASN:HB2	2:E:801:ADP:O3'	1.98	0.64
1:B:533:ARG:HG3	1:B:534:THR:HG23	1.79	0.64
1:C:711:LEU:HA	1:C:714:ILE:HD12	1.80	0.64
1:F:307:ALA:O	1:F:311:GLU:HG2	1.98	0.64
1:B:307:ALA:O	1:B:311:GLU:HG2	1.98	0.63
1:B:540:LEU:HD11	1:B:649:LYS:HZ3	1.60	0.63
1:B:713:LEU:HD22	1:B:732:LEU:HB3	1.79	0.63
1:F:538:SER:O	1:F:663:THR:HG22	1.98	0.63
1:A:232:ARG:O	1:A:236:ALA:HB2	1.97	0.63
1:B:628:VAL:HG13	1:C:571:ASP:OD1	1.97	0.63
1:C:311:GLU:HA	1:C:314:ARG:HG2	1.81	0.63
1:A:258:LEU:HA	1:A:393:MET:O	1.98	0.63
1:A:544:PRO:HG2	1:A:669:ASN:OD1	1.98	0.63
1:C:669:ASN:CG	1:C:706:GLY:HA2	2.24	0.63
1:D:256:ILE:HG22	1:D:391:VAL:HG12	1.80	0.63
1:E:602:VAL:O	1:E:644:GLY:HA2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LYS:HB2	1:A:690:GLU:HG3	1.81	0.63
1:F:562:PHE:CD1	1:F:599:CYS:HB2	2.34	0.63
1:A:597:LEU:HD23	1:A:597:LEU:C	2.23	0.63
1:D:404:LEU:HD11	1:D:427:LYS:HE3	1.81	0.63
1:D:604:ASP:HB3	1:D:607:ARG:CB	2.28	0.63
1:F:635:PRO:O	1:F:638:ARG:HG2	1.98	0.63
1:A:313:GLN:NE2	1:A:365:ASN:O	2.32	0.63
1:D:256:ILE:O	1:D:370:ILE:HA	1.99	0.63
1:E:307:ALA:O	1:E:311:GLU:HG2	1.98	0.63
1:B:570:PRO:HD3	1:B:603:ASP:HB3	1.81	0.63
1:C:383:LEU:HD22	1:C:388:ARG:HD2	1.80	0.63
1:C:511:GLY:HA3	1:C:513:PRO:HD2	1.78	0.62
1:F:546:HIS:O	1:F:546:HIS:ND1	2.32	0.62
1:C:614:ILE:C	1:C:616:PRO:HA	2.24	0.62
1:D:503:ILE:HA	2:D:801:ADP:O2'	1.99	0.62
1:A:563:PRO:HD2	1:A:597:LEU:HD22	1.81	0.62
1:D:521:GLY:O	1:D:525:VAL:HG23	1.98	0.62
1:E:550:THR:HA	1:E:645:THR:HG21	1.81	0.62
1:E:686:PHE:CE1	1:E:714:ILE:HG23	2.31	0.62
1:F:570:PRO:HA	1:F:573:MET:HE2	1.80	0.62
1:D:548:GLY:HA2	2:D:801:ADP:H5'1	1.80	0.62
1:F:268:LEU:HD21	1:F:438:GLY:HA3	1.80	0.62
1:A:508:ILE:HG13	1:A:508:ILE:O	2.00	0.62
1:B:589:PHE:CE2	1:B:629:LEU:HB3	2.34	0.62
1:C:285:VAL:HG13	1:C:326:ILE:HD11	1.81	0.62
1:C:621:LEU:HD11	1:D:575:GLY:HA2	1.82	0.62
1:D:599:CYS:SG	1:D:641:LEU:HD22	2.39	0.62
1:F:404:LEU:O	1:F:408:HIS:HB2	1.99	0.62
1:F:436:PHE:HD2	1:F:444:LEU:HD11	1.64	0.62
1:F:550:THR:HA	1:F:645:THR:HG21	1.81	0.62
1:C:550:THR:HB	2:C:801:ADP:PA	2.39	0.62
1:B:326:ILE:HG22	1:B:370:ILE:HG13	1.82	0.62
1:E:380:ASP:OD1	1:E:382:ALA:N	2.33	0.62
1:F:380:ASP:OD1	1:F:382:ALA:N	2.33	0.62
1:E:326:ILE:HG22	1:E:370:ILE:HG13	1.82	0.62
1:A:231:PHE:CD1	1:A:235:PHE:HE2	2.17	0.61
1:B:527:GLN:HB2	1:C:719:GLN:HG3	1.82	0.61
1:C:624:GLN:O	1:C:628:VAL:HG23	2.00	0.61
1:E:705:ILE:HG13	1:E:709:LYS:HG3	1.81	0.61
1:A:720:MET:O	1:A:725:ARG:NE	2.23	0.61
1:D:286:ASN:HB2	1:D:327:PHE:HD1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:ALA:O	1:D:558:GLU:HG2	2.00	0.61
1:E:532:ASP:OD2	1:E:533:ARG:N	2.32	0.61
1:C:728:LYS:O	1:C:732:LEU:HG	2.00	0.61
1:A:657:MET:HE3	1:A:661:PHE:HE1	1.63	0.61
1:B:245:VAL:O	1:B:249:GLY:N	2.32	0.61
1:B:542:GLU:HG3	1:B:666:HIS:CE1	2.35	0.61
1:C:670:ILE:HG22	1:C:672:THR:H	1.65	0.61
1:D:606:GLU:O	1:D:610:ASP:N	2.33	0.61
1:F:546:HIS:CE1	1:F:709:LYS:CB	2.84	0.61
1:C:542:GLU:HB3	1:C:649:LYS:HD3	1.81	0.61
1:C:334:CYS:HA	1:C:351:VAL:HG22	1.81	0.61
1:D:507:ILE:HA	2:D:801:ADP:C8	2.36	0.61
1:E:581:LYS:NZ	1:E:610:ASP:OD1	2.30	0.61
1:B:380:ASP:OD1	1:B:382:ALA:N	2.33	0.61
1:D:261:PRO:HG2	1:D:264:CYS:HB2	1.82	0.61
1:F:566:LYS:HD2	1:F:567:ILE:N	2.16	0.61
1:B:437:SER:OG	1:B:440:GLU:HG2	2.00	0.60
1:B:625:ALA:O	1:B:629:LEU:HG	2.01	0.60
1:C:579:THR:O	1:C:583:GLN:HG2	2.01	0.60
1:D:513:PRO:HB3	1:D:516:ARG:HE	1.65	0.60
1:D:656:GLU:OE1	1:E:613:PRO:HB3	2.01	0.60
1:E:513:PRO:O	1:E:517:VAL:HG23	2.01	0.60
1:A:408:HIS:HA	1:A:426:ILE:HD12	1.83	0.60
1:F:650:ASP:O	1:F:653:GLN:HG3	2.01	0.60
1:A:223:LEU:CD1	1:A:227:PHE:HB2	2.32	0.60
1:A:299:GLU:HG2	1:A:353:GLN:HG2	1.82	0.60
1:B:421:SER:HB3	1:B:424:VAL:HG23	1.83	0.60
1:C:407:LEU:CD1	1:C:426:ILE:HG23	2.31	0.60
1:D:246:GLU:O	1:E:413:ARG:NH1	2.30	0.60
1:D:249:GLY:HA3	1:E:413:ARG:NH1	2.16	0.60
1:F:326:ILE:HG22	1:F:370:ILE:HG13	1.83	0.60
1:A:598:SER:OG	1:A:640:LEU:HD12	2.01	0.60
1:B:563:PRO:HD2	1:B:597:LEU:HB2	1.82	0.60
1:C:399:ASP:O	1:C:403:ARG:N	2.29	0.60
1:A:677:LEU:HG	1:A:695:ALA:HB2	1.83	0.60
1:C:375:ARG:HH12	1:C:378:LEU:HG	1.65	0.60
1:C:677:LEU:HD11	1:C:698:VAL:HG21	1.84	0.60
1:D:512:ASP:O	1:D:515:THR:OG1	2.18	0.60
1:F:715:GLU:O	1:F:719:GLN:HG2	2.00	0.60
1:C:247:GLN:HA	1:D:417:HIS:CD2	2.36	0.60
1:C:577:SER:O	1:C:580:ALA:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:TRP:CB	1:A:679:ALA:HA	2.31	0.60
1:A:565:ILE:HA	1:A:599:CYS:O	2.02	0.60
1:C:254:LYS:O	1:C:368:LEU:HA	2.02	0.60
1:E:514:VAL:HG13	2:E:801:ADP:N6	2.17	0.60
1:E:544:PRO:O	1:E:547:SER:HB3	2.01	0.60
1:F:268:LEU:CD2	1:F:439:ALA:H	2.15	0.60
1:F:508:ILE:HD11	1:F:510:TRP:HD1	1.67	0.60
1:A:582:CYS:SG	1:A:621:LEU:HG	2.42	0.60
1:C:540:LEU:HD12	1:C:644:GLY:O	2.01	0.60
1:C:606:GLU:HB2	1:C:648:ARG:HD2	1.82	0.60
1:E:247:GLN:HA	1:F:417:HIS:ND1	2.17	0.60
1:B:513:PRO:HD2	1:B:670:ILE:HD11	1.83	0.60
1:B:540:LEU:HA	1:B:644:GLY:O	2.02	0.60
1:C:236:ALA:HB1	1:D:453:MET:HB3	1.84	0.60
1:F:521:GLY:O	1:F:525:VAL:HG23	2.02	0.60
1:A:236:ALA:HB1	1:B:450:SER:HA	1.82	0.60
1:A:270:ALA:O	1:A:273:ILE:HG22	2.01	0.60
1:A:508:ILE:HB	1:A:682:LEU:HB3	1.83	0.60
1:B:407:LEU:CD1	1:B:426:ILE:HG23	2.31	0.60
1:C:590:ASP:HA	1:C:593:TYR:CD2	2.37	0.60
1:D:407:LEU:HG	1:D:441:LEU:HD11	1.83	0.60
1:B:510:TRP:HZ3	1:B:670:ILE:HD12	1.67	0.59
1:B:541:LEU:HD11	1:B:549:LYS:HA	1.83	0.59
1:E:404:LEU:O	1:E:408:HIS:HB2	2.02	0.59
1:E:508:ILE:HD11	1:E:707:ILE:HD11	1.84	0.59
1:F:449:GLN:O	1:F:453:MET:HG2	2.01	0.59
1:E:662:SER:OG	1:F:712:MET:HE3	2.02	0.59
1:B:383:LEU:O	1:B:389:LEU:HB2	2.02	0.59
1:C:695:ALA:HB1	1:C:699:LYS:HE3	1.84	0.59
1:D:527:GLN:NE2	1:E:715:GLU:HG3	2.17	0.59
1:D:585:MET:O	1:D:589:PHE:HD2	1.84	0.59
1:A:571:ASP:HA	1:A:574:ILE:HG23	1.85	0.59
1:D:299:GLU:OE1	1:D:350:VAL:HG13	2.02	0.59
1:D:312:GLU:CG	1:D:313:GLN:H	2.15	0.59
1:E:628:VAL:O	1:E:632:LYS:N	2.36	0.59
1:B:539:VAL:HG21	1:B:665:ILE:HD12	1.84	0.59
1:D:652:LEU:HB3	1:D:658:LEU:HB2	1.83	0.59
1:A:686:PHE:O	1:A:691:ARG:NH2	2.36	0.59
1:A:694:ILE:O	1:A:698:VAL:HG13	2.02	0.59
1:C:606:GLU:HG2	1:C:607:ARG:N	2.18	0.59
1:A:242:PRO:HD2	1:A:243:GLU:CD	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:O	1:B:408:HIS:HB2	2.02	0.59
1:B:548:GLY:HA3	2:B:801:ADP:C2	2.37	0.59
1:B:670:ILE:HD13	1:B:675:GLN:HB3	1.85	0.59
1:A:382:ALA:O	1:A:385:ARG:HG2	2.03	0.59
1:D:593:TYR:O	1:D:638:ARG:HG2	2.01	0.59
1:C:551:ALA:HB2	2:C:801:ADP:H3'	1.84	0.59
1:C:624:GLN:NE2	1:D:610:ASP:HB2	2.18	0.59
1:D:604:ASP:HB3	1:D:607:ARG:HB3	1.84	0.59
1:A:307:ALA:O	1:A:310:GLU:HG3	2.03	0.59
1:B:695:ALA:HB1	1:B:699:LYS:HE3	1.85	0.59
1:E:449:GLN:O	1:E:453:MET:HG2	2.03	0.59
1:F:606:GLU:OE2	1:F:647:SER:HB2	2.02	0.59
1:A:624:GLN:OE1	1:B:607:ARG:NH1	2.36	0.58
1:B:284:VAL:HG23	1:B:324:ILE:O	2.03	0.58
1:E:527:GLN:NE2	1:F:716:MET:HG2	2.18	0.58
1:E:648:ARG:NE	1:E:650:ASP:OD1	2.34	0.58
1:E:697:GLN:HG3	1:E:730:LEU:HD11	1.83	0.58
1:A:671:ALA:HA	1:A:703:VAL:O	2.03	0.58
1:B:261:PRO:HG2	1:B:264:CYS:HB2	1.84	0.58
1:F:562:PHE:HB2	1:F:565:ILE:HG12	1.84	0.58
1:B:571:ASP:OD2	1:B:571:ASP:N	2.35	0.58
1:C:404:LEU:O	1:C:408:HIS:HB2	2.03	0.58
1:C:527:GLN:HB2	1:D:719:GLN:HG3	1.84	0.58
1:D:519:ASP:O	1:D:523:LEU:HG	2.03	0.58
1:E:383:LEU:O	1:E:389:LEU:HB2	2.02	0.58
1:F:549:LYS:HE2	1:F:645:THR:HB	1.86	0.58
1:C:694:ILE:O	1:C:698:VAL:HG22	2.04	0.58
1:E:284:VAL:HG23	1:E:324:ILE:O	2.03	0.58
1:B:449:GLN:O	1:B:453:MET:HG3	2.03	0.58
1:B:526:GLN:HE21	1:C:719:GLN:HB3	1.68	0.58
1:B:533:ARG:HD2	1:C:711:LEU:HD13	1.86	0.58
1:C:540:LEU:HB2	1:C:661:PHE:CD2	2.38	0.58
1:D:513:PRO:O	1:D:516:ARG:HG2	2.03	0.58
1:D:528:THR:HG22	1:D:597:LEU:HD11	1.85	0.58
1:B:236:ALA:HA	1:B:239:VAL:HG12	1.86	0.58
1:C:653:GLN:HG3	1:C:658:LEU:HD23	1.86	0.58
1:F:383:LEU:O	1:F:389:LEU:HB2	2.02	0.58
1:F:407:LEU:CD1	1:F:426:ILE:HG23	2.33	0.58
1:F:513:PRO:O	1:F:517:VAL:HG23	2.03	0.58
1:F:538:SER:OG	1:F:661:PHE:HD1	1.86	0.58
1:A:222:GLY:H	1:A:405:GLN:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:PHE:HB3	1:C:440:GLU:OE1	2.04	0.58
1:C:658:LEU:HD11	1:C:664:THR:HG21	1.85	0.58
1:F:410:HIS:O	1:F:414:MET:HG2	2.02	0.58
1:A:411:THR:OG1	1:A:426:ILE:HD11	2.03	0.58
1:E:236:ALA:HA	1:E:239:VAL:CG1	2.33	0.58
1:E:407:LEU:CD1	1:E:426:ILE:HG23	2.32	0.58
1:E:502:TYR:CZ	1:E:567:ILE:HG21	2.38	0.58
1:A:678:GLU:O	1:A:681:GLU:HG2	2.03	0.58
1:E:548:GLY:HA2	2:E:801:ADP:O5'	2.04	0.58
1:E:624:GLN:OE1	1:E:624:GLN:HA	2.02	0.58
1:E:664:THR:C	1:E:665:ILE:HD13	2.29	0.58
1:A:690:GLU:O	1:A:694:ILE:HG13	2.04	0.57
1:B:236:ALA:O	1:B:239:VAL:HG12	2.04	0.57
1:D:380:ASP:OD1	1:D:382:ALA:N	2.36	0.57
1:D:383:LEU:O	1:D:389:LEU:HB2	2.03	0.57
1:D:711:LEU:O	1:D:715:GLU:HG2	2.04	0.57
1:E:693:THR:O	1:E:697:GLN:NE2	2.20	0.57
1:F:602:VAL:N	1:F:643:ILE:O	2.23	0.57
1:D:527:GLN:OE1	1:E:716:MET:HA	2.04	0.57
1:E:296:GLY:H	1:E:297:GLU:CB	2.18	0.57
1:E:587:LYS:HZ1	1:E:591:ASP:CG	2.12	0.57
1:F:284:VAL:HG23	1:F:324:ILE:O	2.03	0.57
1:A:539:VAL:HG13	1:A:643:ILE:HA	1.87	0.57
1:A:539:VAL:HG23	1:A:665:ILE:HD13	1.85	0.57
1:B:395:ILE:HD12	1:B:395:ILE:H	1.69	0.57
1:B:549:LYS:NZ	1:B:647:SER:HA	2.19	0.57
1:B:670:ILE:HG21	1:B:675:GLN:OE1	2.04	0.57
1:C:688:ASP:OD1	1:C:691:ARG:NH2	2.25	0.57
1:D:524:LEU:O	1:D:527:GLN:HB3	2.04	0.57
1:D:625:ALA:O	1:D:629:LEU:HG	2.05	0.57
1:D:651:VAL:O	1:D:655:MET:HG2	2.03	0.57
1:A:672:THR:OG1	1:A:675:GLN:OE1	2.14	0.57
1:B:605:ILE:HD11	1:B:644:GLY:HA3	1.87	0.57
1:B:620:ASN:HD21	1:B:624:GLN:HE21	1.51	0.57
1:C:449:GLN:O	1:C:453:MET:HG2	2.04	0.57
1:C:508:ILE:HG13	1:C:510:TRP:CD1	2.37	0.57
1:C:509:LYS:O	1:C:682:LEU:HD12	2.04	0.57
1:A:598:SER:O	1:A:640:LEU:HA	2.05	0.57
1:B:552:LEU:O	1:B:556:ILE:HG13	2.04	0.57
1:E:640:LEU:HD12	1:E:641:LEU:H	1.68	0.57
1:A:257:LEU:HG	1:A:389:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:THR:OG1	1:A:328:ASP:OD2	2.21	0.57
1:E:354:LEU:O	1:E:358:ILE:HG12	2.05	0.57
1:F:222:GLY:CA	1:F:399:ASP:HB2	2.33	0.57
1:F:554:ALA:O	1:F:558:GLU:HG3	2.05	0.57
1:B:593:TYR:O	1:B:638:ARG:NE	2.38	0.57
1:C:375:ARG:NH2	1:C:377:ASP:OD1	2.38	0.57
1:D:267:THR:HA	1:D:372:MET:SD	2.45	0.57
1:E:721:ASP:O	1:E:725:ARG:HG3	2.05	0.57
1:F:354:LEU:O	1:F:358:ILE:HG12	2.05	0.57
1:B:510:TRP:CZ3	1:B:670:ILE:HD12	2.40	0.57
1:D:543:GLY:N	1:D:549:LYS:HD3	2.19	0.57
1:D:551:ALA:HB3	2:D:801:ADP:N3	2.20	0.57
1:D:648:ARG:HG3	1:D:651:VAL:HG23	1.87	0.57
1:F:604:ASP:HB3	1:F:607:ARG:HB2	1.85	0.57
1:F:653:GLN:HB3	1:F:658:LEU:HD23	1.87	0.57
1:B:578:GLU:HG3	1:B:619:SER:HB2	1.86	0.57
1:D:303:ARG:HD3	1:D:353:GLN:HG3	1.87	0.57
1:F:508:ILE:C	1:F:509:LYS:HD3	2.30	0.57
1:C:677:LEU:HD11	1:C:698:VAL:CG2	2.34	0.56
1:A:546:HIS:ND1	1:A:709:LYS:HE3	2.20	0.56
1:B:221:GLY:HA3	1:B:406:ILE:CD1	2.35	0.56
1:C:536:LEU:HD12	1:C:640:LEU:HB3	1.87	0.56
1:C:613:PRO:HD3	1:C:648:ARG:HH22	1.70	0.56
1:D:528:THR:CB	1:D:641:LEU:HD12	2.34	0.56
1:D:531:SER:HG	1:D:534:THR:HG1	1.51	0.56
1:E:652:LEU:HD22	1:E:658:LEU:HD13	1.86	0.56
1:F:245:VAL:O	1:F:249:GLY:N	2.36	0.56
1:A:549:LYS:HB3	1:A:667:VAL:HG21	1.86	0.56
1:B:242:PRO:HD2	1:B:243:GLU:H	1.70	0.56
1:B:354:LEU:O	1:B:358:ILE:HG12	2.06	0.56
1:B:546:HIS:O	1:B:547:SER:OG	2.17	0.56
1:D:284:VAL:HB	1:D:325:ILE:HA	1.86	0.56
1:E:242:PRO:HD2	1:E:243:GLU:H	1.70	0.56
1:E:713:LEU:HD22	1:E:732:LEU:HD13	1.87	0.56
1:F:508:ILE:CD1	1:F:510:TRP:HD1	2.18	0.56
1:A:263:GLY:C	1:A:437:SER:HB3	2.30	0.56
1:A:676:LEU:CD1	1:A:710:LEU:HD11	2.36	0.56
1:D:312:GLU:HG2	1:D:313:GLN:H	1.67	0.56
1:D:720:MET:HE3	1:D:724:TYR:CE1	2.36	0.56
1:C:542:GLU:HG2	1:C:666:HIS:HA	1.88	0.56
1:D:312:GLU:CG	1:D:313:GLN:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:LEU:HB2	1:D:691:ARG:HH21	1.69	0.56
1:F:635:PRO:HD2	1:F:638:ARG:HD2	1.86	0.56
1:A:407:LEU:HD12	1:A:426:ILE:HG23	1.87	0.56
1:A:549:LYS:HE3	1:A:646:THR:C	2.31	0.56
1:C:281:GLU:CB	1:C:324:ILE:HD13	2.36	0.56
1:C:688:ASP:O	1:C:692:THR:HG23	2.05	0.56
1:E:267:THR:HA	1:E:372:MET:SD	2.44	0.56
1:E:550:THR:HB	2:E:801:ADP:O1A	2.05	0.56
1:F:296:GLY:H	1:F:297:GLU:CB	2.18	0.56
1:F:518:LEU:H	1:F:518:LEU:HD12	1.70	0.56
1:B:296:GLY:H	1:B:297:GLU:CB	2.18	0.56
1:B:654:GLU:O	1:C:613:PRO:HG3	2.05	0.56
1:D:686:PHE:HB2	1:D:691:ARG:HG2	1.87	0.56
1:E:573:MET:SD	1:E:581:LYS:HG2	2.45	0.56
1:F:546:HIS:CE1	1:F:706:GLY:N	2.74	0.56
1:A:585:MET:HE1	1:A:626:LEU:HD12	1.86	0.56
1:D:242:PRO:HD2	1:D:243:GLU:H	1.69	0.56
1:D:687:LYS:O	1:D:691:ARG:HG3	2.06	0.56
1:A:293:LYS:O	1:A:294:TYR:CG	2.59	0.56
1:A:513:PRO:O	1:A:517:VAL:HG23	2.05	0.56
1:A:536:LEU:HD23	1:A:633:ALA:HA	1.88	0.56
1:A:683:LEU:HD12	1:A:714:ILE:HD13	1.87	0.56
1:A:688:ASP:OD1	1:A:689:LYS:N	2.39	0.56
1:D:657:MET:HG2	1:D:661:PHE:CE2	2.41	0.56
1:E:527:GLN:CD	1:F:716:MET:HG2	2.31	0.56
1:F:261:PRO:HG2	1:F:264:CYS:HB2	1.87	0.56
1:A:231:PHE:CE1	1:A:235:PHE:HE2	2.24	0.55
1:B:582:CYS:SG	1:C:574:ILE:HG22	2.46	0.55
1:B:596:GLN:HA	1:B:638:ARG:HG2	1.87	0.55
1:E:551:ALA:HB2	2:E:801:ADP:H3'	1.88	0.55
1:B:270:ALA:O	1:B:273:ILE:HG22	2.06	0.55
1:B:571:ASP:O	1:B:574:ILE:HG13	2.05	0.55
1:B:621:LEU:HD11	1:C:575:GLY:HA2	1.87	0.55
1:E:549:LYS:HA	1:E:552:LEU:HD12	1.87	0.55
1:A:383:LEU:O	1:A:389:LEU:HB2	2.06	0.55
1:C:686:PHE:CE1	1:C:714:ILE:HG23	2.42	0.55
1:E:264:CYS:SG	1:E:395:ILE:HG21	2.46	0.55
1:F:404:LEU:HG	1:F:426:ILE:HG22	1.88	0.55
1:A:726:VAL:O	1:A:730:LEU:HG	2.05	0.55
1:B:508:ILE:O	2:B:801:ADP:N6	2.40	0.55
1:D:632:LYS:NZ	1:E:571:ASP:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:TRP:HB2	1:E:679:ALA:CB	2.36	0.55
1:A:521:GLY:HA2	1:A:524:LEU:HD12	1.88	0.55
1:A:683:LEU:HB3	1:A:685:ASN:ND2	2.21	0.55
1:C:589:PHE:CD2	1:C:629:LEU:HD13	2.42	0.55
1:F:503:ILE:HG22	1:F:506:GLY:H	1.71	0.55
1:A:678:GLU:O	1:A:682:LEU:HD12	2.07	0.55
1:C:531:SER:OG	1:D:715:GLU:OE1	2.25	0.55
1:D:257:LEU:HB2	1:D:389:LEU:HD13	1.88	0.55
1:D:681:GLU:HG2	1:D:691:ARG:NH1	2.22	0.55
1:E:270:ALA:O	1:E:273:ILE:HG22	2.06	0.55
1:F:437:SER:O	1:F:440:GLU:HB2	2.06	0.55
1:A:531:SER:O	1:A:639:LYS:HE2	2.07	0.55
1:C:616:PRO:HG2	1:D:614:ILE:HD13	1.88	0.55
1:E:232:ARG:O	1:E:236:ALA:CB	2.54	0.55
1:E:689:LYS:O	1:E:692:THR:OG1	2.25	0.55
1:F:544:PRO:O	1:F:547:SER:OG	2.25	0.55
1:A:231:PHE:CD1	1:A:235:PHE:CE2	2.95	0.55
1:A:352:ASN:HA	1:A:355:LEU:HD12	1.89	0.55
1:C:347:HIS:O	1:C:350:VAL:HG22	2.06	0.55
1:E:437:SER:O	1:E:440:GLU:HB2	2.07	0.55
1:A:300:ALA:HA	1:A:303:ARG:HG2	1.89	0.55
1:A:540:LEU:HD11	1:A:646:THR:HG22	1.88	0.55
1:F:605:ILE:HD11	1:F:644:GLY:HA3	1.88	0.55
1:A:222:GLY:O	1:A:224:ASP:N	2.40	0.55
1:B:289:GLU:O	1:B:291:LEU:N	2.32	0.55
1:D:534:THR:OG1	1:E:715:GLU:HG2	2.07	0.55
1:E:674:GLU:O	1:E:677:LEU:HB2	2.06	0.55
1:B:533:ARG:HG3	1:B:534:THR:N	2.21	0.54
1:C:375:ARG:NH1	1:C:378:LEU:HG	2.21	0.54
1:C:546:HIS:HB2	1:C:709:LYS:HB2	1.89	0.54
1:D:528:THR:OG1	1:D:537:VAL:HG21	2.07	0.54
1:E:673:GLY:HA3	1:E:698:VAL:HB	1.88	0.54
1:F:559:GLU:HA	1:F:559:GLU:OE1	2.07	0.54
1:A:625:ALA:O	1:A:629:LEU:HG	2.08	0.54
1:A:627:LEU:HD13	1:B:607:ARG:HH12	1.72	0.54
1:B:508:ILE:H	2:B:801:ADP:N6	2.01	0.54
1:B:508:ILE:HD13	1:B:683:LEU:HD21	1.88	0.54
1:C:555:LYS:HA	1:C:558:GLU:OE1	2.06	0.54
1:F:397:LEU:CB	1:F:398:PRO:CD	2.86	0.54
1:F:512:ASP:OD1	1:F:513:PRO:HD3	2.08	0.54
1:A:247:GLN:C	1:B:414:MET:HE1	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:HB2	1:A:327:PHE:CB	2.38	0.54
1:A:315:ARG:HG2	1:A:316:LEU:CD1	2.37	0.54
1:C:511:GLY:C	1:C:513:PRO:HD2	2.33	0.54
1:C:538:SER:O	1:C:662:SER:OG	2.25	0.54
1:F:407:LEU:O	1:F:411:THR:OG1	2.19	0.54
1:A:437:SER:OG	1:A:440:GLU:HG2	2.07	0.54
1:A:535:PRO:HB3	1:B:504:MET:SD	2.47	0.54
1:C:284:VAL:HG11	1:C:305:LEU:HD11	1.89	0.54
1:D:512:ASP:N	1:D:513:PRO:CD	2.71	0.54
1:E:310:GLU:OE2	1:E:357:LYS:NZ	2.40	0.54
1:E:595:SER:HB3	1:E:598:SER:HB3	1.89	0.54
1:F:411:THR:O	1:F:414:MET:HB2	2.07	0.54
1:F:436:PHE:HB3	1:F:440:GLU:CB	2.37	0.54
1:F:548:GLY:HA3	1:F:707:ILE:CG2	2.38	0.54
1:F:612:VAL:CG1	1:F:617:ARG:HB2	2.38	0.54
1:A:724:TYR:HD1	1:A:727:ARG:HH12	1.54	0.54
1:C:577:SER:O	1:C:579:THR:N	2.40	0.54
1:D:677:LEU:O	1:D:691:ARG:NH2	2.40	0.54
1:F:223:LEU:HD21	1:F:397:LEU:O	2.06	0.54
1:A:227:PHE:CE2	1:A:231:PHE:HD1	2.26	0.54
1:A:563:PRO:HG2	1:A:597:LEU:O	2.08	0.54
1:D:657:MET:HG2	1:D:661:PHE:HE2	1.73	0.54
1:A:355:LEU:HB3	1:A:388:ARG:NH1	2.23	0.54
1:A:683:LEU:HD11	1:A:711:LEU:HD23	1.89	0.54
1:B:651:VAL:HG12	1:B:655:MET:HE3	1.89	0.54
1:D:657:MET:HE2	1:D:661:PHE:CZ	2.43	0.54
1:D:686:PHE:CE1	1:D:714:ILE:HG23	2.42	0.54
1:E:510:TRP:HB2	1:E:679:ALA:HB2	1.88	0.54
1:E:705:ILE:HD13	1:E:710:LEU:HD13	1.89	0.54
1:F:686:PHE:HE1	1:F:714:ILE:HG23	1.73	0.54
1:C:728:LYS:HE3	1:C:732:LEU:HD21	1.90	0.54
1:D:310:GLU:O	1:D:313:GLN:NE2	2.40	0.54
1:D:670:ILE:HG12	1:D:705:ILE:O	2.08	0.54
1:A:235:PHE:CE1	1:A:277:LEU:CB	2.90	0.54
1:B:315:ARG:HG3	1:B:316:LEU:HD12	1.90	0.54
1:C:245:VAL:O	1:C:249:GLY:N	2.36	0.54
1:E:516:ARG:O	1:E:519:ASP:OD1	2.25	0.54
1:F:267:THR:HA	1:F:372:MET:SD	2.48	0.54
1:F:546:HIS:CE1	1:F:706:GLY:H	2.26	0.54
1:A:611:TYR:HD1	1:A:618:PHE:HB3	1.72	0.54
1:B:479:ASP:O	1:B:482:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:HIS:CB	1:C:709:LYS:HB2	2.38	0.54
1:C:677:LEU:HD21	1:C:695:ALA:CB	2.38	0.54
1:E:662:SER:HA	1:F:709:LYS:NZ	2.23	0.54
1:A:716:MET:HG2	1:A:732:LEU:HD11	1.88	0.53
1:B:576:PHE:HB2	1:B:581:LYS:HG3	1.90	0.53
1:B:648:ARG:HG3	1:B:651:VAL:HG23	1.90	0.53
1:C:686:PHE:HE1	1:C:714:ILE:HG23	1.73	0.53
1:F:562:PHE:HE2	1:F:597:LEU:HD12	1.73	0.53
1:A:227:PHE:CE1	1:A:273:ILE:HD13	2.44	0.53
1:B:569:SER:HA	1:B:603:ASP:HB3	1.88	0.53
1:C:521:GLY:HA3	1:C:556:ILE:HD13	1.91	0.53
1:C:540:LEU:HD23	1:C:649:LYS:HE3	1.90	0.53
1:F:582:CYS:SG	1:F:586:LYS:HE3	2.48	0.53
1:A:264:CYS:SG	1:A:265:GLY:N	2.80	0.53
1:A:548:GLY:N	1:A:708:LYS:HB2	2.22	0.53
1:B:267:THR:HA	1:B:372:MET:SD	2.47	0.53
1:C:591:ASP:O	1:C:594:LYS:HB3	2.08	0.53
1:B:527:GLN:NE2	1:C:716:MET:SD	2.77	0.53
1:C:308:ASP:OD1	1:C:309:ALA:N	2.41	0.53
1:F:510:TRP:HZ3	1:F:675:GLN:NE2	2.06	0.53
1:A:406:ILE:O	1:A:409:ILE:HG22	2.07	0.53
1:C:227:PHE:O	1:C:231:PHE:HB2	2.09	0.53
1:C:256:ILE:HA	1:C:391:VAL:HG13	1.90	0.53
1:F:315:ARG:HG3	1:F:316:LEU:HD12	1.90	0.53
1:F:522:GLU:OE2	1:F:526:GLN:HG2	2.08	0.53
1:C:570:PRO:HG2	1:C:604:ASP:HB2	1.91	0.53
1:C:690:GLU:CB	1:C:726:VAL:HG21	2.38	0.53
1:D:265:GLY:O	1:D:268:LEU:HG	2.09	0.53
1:A:536:LEU:HD23	1:A:634:PRO:HD3	1.90	0.53
1:B:310:GLU:OE2	1:B:357:LYS:NZ	2.40	0.53
1:C:410:HIS:O	1:C:414:MET:HG2	2.09	0.53
1:C:444:LEU:HD12	1:C:445:VAL:HG23	1.91	0.53
1:C:708:LYS:HA	1:C:711:LEU:HG	1.90	0.53
1:D:527:GLN:NE2	1:E:716:MET:HA	2.24	0.53
1:D:618:PHE:CE2	1:E:614:ILE:HD12	2.43	0.53
1:F:450:SER:O	1:F:453:MET:HB2	2.09	0.53
1:F:721:ASP:HB2	1:F:724:TYR:CD1	2.42	0.53
1:C:508:ILE:O	2:C:801:ADP:N6	2.42	0.53
1:F:263:GLY:O	1:F:437:SER:HB3	2.08	0.53
1:E:604:ASP:O	1:E:608:LEU:N	2.38	0.53
1:F:242:PRO:HD2	1:F:243:GLU:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:O	1:A:246:GLU:HG2	2.09	0.53
1:A:306:PHE:CD1	1:A:357:LYS:HB3	2.43	0.53
1:C:611:TYR:HE1	1:C:616:PRO:HB2	1.74	0.53
1:D:375:ARG:NH2	1:D:377:ASP:OD2	2.42	0.53
1:B:479:ASP:O	1:B:480:PHE:C	2.51	0.52
1:C:242:PRO:HD2	1:C:243:GLU:H	1.73	0.52
1:F:310:GLU:OE2	1:F:357:LYS:NZ	2.41	0.52
1:F:436:PHE:CD2	1:F:444:LEU:HD11	2.44	0.52
1:F:503:ILE:HD11	1:F:551:ALA:HA	1.90	0.52
1:D:523:LEU:HD13	1:E:720:MET:SD	2.49	0.52
1:D:560:SER:HB2	1:D:562:PHE:CD1	2.45	0.52
1:F:260:GLY:N	1:F:266:LYS:HD3	2.25	0.52
1:F:440:GLU:O	1:F:444:LEU:HG	2.09	0.52
1:F:515:THR:HA	1:F:518:LEU:CD1	2.39	0.52
1:A:706:GLY:O	1:A:710:LEU:N	2.43	0.52
1:B:589:PHE:HD2	1:B:629:LEU:HD22	1.74	0.52
1:C:377:ASP:OD2	1:C:377:ASP:N	2.36	0.52
1:C:612:VAL:HG12	1:C:617:ARG:HB3	1.91	0.52
1:D:604:ASP:HB3	1:D:607:ARG:HB2	1.91	0.52
1:D:731:ALA:HA	1:D:734:ARG:NH1	2.23	0.52
1:E:696:GLN:HB3	1:E:697:GLN:NE2	2.24	0.52
1:A:286:ASN:HB2	1:A:327:PHE:HB3	1.91	0.52
1:B:576:PHE:HB3	1:B:580:ALA:HB3	1.90	0.52
1:D:628:VAL:HG13	1:E:571:ASP:OD1	2.08	0.52
1:E:684:GLY:HA2	1:E:691:ARG:NH2	2.25	0.52
1:C:490:PRO:HB2	1:C:492:PHE:N	2.25	0.52
1:C:681:GLU:HG3	1:C:691:ARG:HD2	1.91	0.52
1:D:686:PHE:HB3	1:D:690:GLU:HG3	1.91	0.52
1:F:270:ALA:O	1:F:273:ILE:HG22	2.09	0.52
1:F:529:LYS:HG3	1:F:597:LEU:HD11	1.90	0.52
1:F:617:ARG:HG3	1:F:617:ARG:HH11	1.74	0.52
1:C:510:TRP:CZ3	1:C:670:ILE:HD12	2.45	0.52
1:C:613:PRO:HD3	1:C:648:ARG:NH2	2.24	0.52
1:E:315:ARG:HG3	1:E:316:LEU:HD12	1.90	0.52
1:F:593:TYR:O	1:F:638:ARG:HD3	2.10	0.52
1:C:388:ARG:NH1	1:C:388:ARG:HB2	2.24	0.52
1:C:715:GLU:OE1	1:C:715:GLU:HA	2.09	0.52
1:F:268:LEU:HD23	1:F:439:ALA:H	1.75	0.52
1:F:517:VAL:HG21	1:F:667:VAL:HG21	1.91	0.52
1:A:673:GLY:O	1:A:677:LEU:HD22	2.10	0.52
1:D:313:GLN:OE1	1:D:365:ASN:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:LEU:HD13	1:E:607:ARG:HH12	1.74	0.52
1:D:686:PHE:HE1	1:D:714:ILE:HG23	1.75	0.52
1:A:222:GLY:HA3	1:A:402:GLY:CA	2.32	0.52
1:B:263:GLY:C	1:B:437:SER:HB3	2.35	0.52
1:C:611:TYR:CZ	1:C:651:VAL:HG11	2.45	0.52
1:E:289:GLU:C	1:E:291:LEU:H	2.17	0.52
1:F:236:ALA:HA	1:F:239:VAL:CG1	2.39	0.52
1:A:568:CYS:O	1:A:603:ASP:HB3	2.10	0.52
1:C:256:ILE:HG22	1:C:391:VAL:HG11	1.92	0.52
1:F:525:VAL:HG13	1:F:562:PHE:HE1	1.73	0.52
1:F:635:PRO:HB2	1:F:638:ARG:NH1	2.25	0.52
1:A:398:PRO:HG3	1:A:436:PHE:O	2.09	0.51
1:D:567:ILE:HG23	1:D:601:VAL:HB	1.92	0.51
1:A:258:LEU:O	1:A:372:MET:HA	2.10	0.51
1:A:300:ALA:O	1:A:304:LYS:HG3	2.10	0.51
1:A:548:GLY:CA	1:A:708:LYS:HB2	2.39	0.51
1:A:611:TYR:CE2	1:A:651:VAL:HG11	2.44	0.51
1:B:527:GLN:HA	1:C:719:GLN:CD	2.36	0.51
1:E:327:PHE:CZ	1:E:369:VAL:HG21	2.45	0.51
1:A:683:LEU:HB3	1:A:685:ASN:HD22	1.73	0.51
1:B:406:ILE:HD12	1:B:406:ILE:H	1.74	0.51
1:B:728:LYS:HE3	1:B:732:LEU:HD21	1.91	0.51
1:D:527:GLN:HA	1:E:719:GLN:HG3	1.92	0.51
1:D:592:ALA:HB1	1:D:640:LEU:HD13	1.93	0.51
1:A:231:PHE:CE2	1:A:235:PHE:HD2	2.29	0.51
1:A:255:GLY:HA3	1:A:389:LEU:HD13	1.91	0.51
1:A:503:ILE:HG22	1:A:506:GLY:H	1.75	0.51
1:C:256:ILE:O	1:C:370:ILE:HA	2.10	0.51
1:D:527:GLN:NE2	1:E:715:GLU:O	2.40	0.51
1:A:222:GLY:H	1:A:405:GLN:CB	2.23	0.51
1:D:254:LYS:O	1:D:368:LEU:HA	2.10	0.51
1:B:542:GLU:CD	1:B:649:LYS:HD3	2.35	0.51
1:C:231:PHE:O	1:C:235:PHE:HB2	2.11	0.51
1:C:445:VAL:HG12	1:C:449:GLN:HE22	1.75	0.51
1:D:522:GLU:OE2	1:D:556:ILE:HA	2.10	0.51
1:D:527:GLN:CD	1:E:716:MET:HA	2.36	0.51
1:E:717:SER:OG	1:E:729:PHE:HB2	2.11	0.51
1:A:681:GLU:HA	1:A:691:ARG:CZ	2.41	0.51
1:B:221:GLY:HA3	1:B:406:ILE:HD11	1.92	0.51
1:D:298:SER:O	1:D:301:ASN:HB3	2.10	0.51
1:D:531:SER:OG	1:D:534:THR:OG1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ALA:O	1:C:273:ILE:HG22	2.11	0.51
1:C:510:TRP:HB2	1:C:679:ALA:CB	2.41	0.51
1:C:547:SER:HB2	1:C:549:LYS:HG3	1.93	0.51
1:C:688:ASP:HA	1:C:691:ARG:NH1	2.26	0.51
1:D:627:LEU:CD1	1:E:607:ARG:HH12	2.24	0.51
1:A:550:THR:HG23	1:A:603:ASP:OD1	2.11	0.51
1:C:285:VAL:HA	1:C:326:ILE:HG13	1.93	0.51
1:C:499:TYR:HB3	1:C:558:GLU:OE2	2.11	0.51
1:D:260:GLY:HA3	1:D:266:LYS:HD3	1.92	0.51
1:A:235:PHE:CD1	1:A:235:PHE:N	2.71	0.50
1:A:527:GLN:HB2	1:B:719:GLN:HG3	1.93	0.50
1:C:542:GLU:HB2	1:C:649:LYS:HD3	1.91	0.50
1:D:570:PRO:HA	1:D:573:MET:HB3	1.93	0.50
1:E:585:MET:HE1	1:E:602:VAL:HG13	1.93	0.50
1:F:303:ARG:CG	1:F:357:LYS:HE2	2.41	0.50
1:F:428:GLU:O	1:F:432:GLU:HG2	2.11	0.50
1:B:507:ILE:HA	2:B:801:ADP:C5	2.45	0.50
1:F:265:GLY:CA	1:F:437:SER:HB2	2.41	0.50
1:B:348:ASP:O	1:B:352:ASN:ND2	2.45	0.50
1:C:525:VAL:HG13	1:C:562:PHE:CZ	2.46	0.50
1:D:260:GLY:N	1:D:266:LYS:HD3	2.26	0.50
1:F:658:LEU:HA	1:F:661:PHE:HD2	1.75	0.50
1:B:428:GLU:O	1:B:432:GLU:HG2	2.12	0.50
1:B:570:PRO:HG3	1:B:608:LEU:HD23	1.93	0.50
1:C:261:PRO:CB	1:C:594:LYS:HG3	2.41	0.50
1:D:310:GLU:O	1:D:313:GLN:HG2	2.12	0.50
1:D:325:ILE:O	1:D:369:VAL:HA	2.12	0.50
1:A:222:GLY:H	1:A:405:GLN:CG	2.25	0.50
1:A:270:ALA:HA	1:A:273:ILE:HG22	1.93	0.50
1:A:411:THR:HG21	1:A:426:ILE:HD11	1.93	0.50
1:C:511:GLY:CA	1:C:513:PRO:HD2	2.41	0.50
1:A:687:LYS:NZ	1:A:722:PRO:HB3	2.26	0.50
1:B:606:GLU:OE1	1:B:606:GLU:N	2.45	0.50
1:B:627:LEU:CD2	1:B:657:MET:HG3	2.40	0.50
1:C:584:ALA:O	1:C:588:ILE:HG13	2.11	0.50
1:E:261:PRO:HB3	1:E:594:LYS:HE2	1.93	0.50
1:E:404:LEU:HG	1:E:426:ILE:HG22	1.94	0.50
1:E:586:LYS:NZ	1:F:574:ILE:O	2.36	0.50
1:E:627:LEU:HD13	1:F:607:ARG:CZ	2.42	0.50
1:F:268:LEU:HD12	1:F:269:LEU:N	2.27	0.50
1:A:428:GLU:O	1:A:431:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:TRP:HB2	1:A:679:ALA:CA	2.42	0.50
1:C:331:ASP:HA	1:C:379:ILE:CD1	2.42	0.50
1:C:730:LEU:O	1:C:734:ARG:HG3	2.12	0.50
1:D:236:ALA:HB1	1:E:453:MET:HG3	1.93	0.50
1:D:313:GLN:HG3	1:D:314:ARG:N	2.27	0.50
1:D:543:GLY:H	1:D:549:LYS:HD3	1.76	0.50
1:A:399:ASP:O	1:A:403:ARG:N	2.22	0.50
1:B:423:ASP:HB2	1:B:479:ASP:N	2.27	0.50
1:E:612:VAL:HG11	1:E:617:ARG:HH21	1.76	0.50
1:C:568:CYS:HB2	1:C:602:VAL:HA	1.93	0.49
1:D:330:ILE:HD12	1:D:331:ASP:N	2.27	0.49
1:E:553:ALA:HA	1:E:556:ILE:HD12	1.94	0.49
1:E:684:GLY:HA2	1:E:691:ARG:HH21	1.77	0.49
1:A:509:LYS:HD2	1:A:509:LYS:N	2.26	0.49
1:A:626:LEU:CD2	1:A:657:MET:HE1	2.41	0.49
1:B:303:ARG:CG	1:B:357:LYS:HE2	2.41	0.49
1:B:516:ARG:O	1:B:519:ASP:OD1	2.30	0.49
1:B:631:LYS:NZ	1:C:604:ASP:OD2	2.38	0.49
1:C:707:ILE:HD12	1:C:710:LEU:HD23	1.94	0.49
1:A:326:ILE:HG22	1:A:370:ILE:CG1	2.39	0.49
1:B:626:LEU:O	1:B:630:LEU:HG	2.11	0.49
1:B:648:ARG:HH11	1:B:651:VAL:HG22	1.75	0.49
1:D:690:GLU:O	1:D:693:THR:OG1	2.23	0.49
1:E:233:ARG:HG2	1:F:454:ASN:HB2	1.94	0.49
1:E:563:PRO:HD2	1:E:597:LEU:O	2.11	0.49
1:F:514:VAL:O	1:F:518:LEU:HD12	2.12	0.49
1:A:261:PRO:HD2	1:A:396:GLY:HA2	1.94	0.49
1:C:612:VAL:CG1	1:C:617:ARG:HB3	2.41	0.49
1:D:681:GLU:HG2	1:D:691:ARG:CZ	2.42	0.49
1:E:510:TRP:CE2	1:E:707:ILE:HB	2.47	0.49
1:E:519:ASP:O	1:E:522:GLU:HB2	2.13	0.49
1:E:540:LEU:HD12	1:E:644:GLY:O	2.13	0.49
1:B:256:ILE:O	1:B:370:ILE:HA	2.13	0.49
1:B:455:ARG:NH2	1:B:481:LEU:CB	2.75	0.49
1:C:513:PRO:HA	1:C:516:ARG:HG2	1.94	0.49
1:C:513:PRO:HD3	1:C:675:GLN:NE2	2.28	0.49
1:D:402:GLY:HA2	1:D:405:GLN:OE1	2.12	0.49
1:D:548:GLY:HA2	2:D:801:ADP:H5'2	1.91	0.49
1:D:628:VAL:O	1:D:632:LYS:N	2.46	0.49
1:E:303:ARG:CG	1:E:357:LYS:HE2	2.41	0.49
1:E:524:LEU:HD11	1:E:663:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:PRO:HB3	1:F:594:LYS:CB	2.43	0.49
1:F:544:PRO:HD2	1:F:669:ASN:OD1	2.13	0.49
1:B:436:PHE:HB3	1:B:440:GLU:CB	2.42	0.49
1:C:322:LEU:HD22	1:C:366:ASN:O	2.13	0.49
1:C:428:GLU:O	1:C:432:GLU:HG2	2.12	0.49
1:C:703:VAL:O	1:C:704:TRP:HD1	1.95	0.49
1:D:268:LEU:HA	1:D:271:ARG:CD	2.43	0.49
1:D:527:GLN:HE22	1:E:716:MET:HA	1.78	0.49
1:E:221:GLY:HA3	1:E:406:ILE:HD12	1.94	0.49
1:E:590:ASP:O	1:E:593:TYR:HB2	2.13	0.49
1:F:549:LYS:HE3	1:F:646:THR:C	2.38	0.49
1:A:222:GLY:H	1:A:405:GLN:HG2	1.76	0.49
1:A:313:GLN:OE1	1:A:317:GLY:HA2	2.13	0.49
1:A:509:LYS:HG2	1:A:515:THR:OG1	2.12	0.49
1:C:237:SER:OG	1:C:252:HIS:ND1	2.44	0.49
1:C:671:ALA:HA	1:C:703:VAL:O	2.13	0.49
1:C:717:SER:OG	1:C:725:ARG:O	2.30	0.49
1:D:581:LYS:O	1:D:585:MET:HG2	2.13	0.49
1:E:313:GLN:O	1:E:317:GLY:N	2.45	0.49
1:E:653:GLN:OE1	1:E:658:LEU:HD23	2.12	0.49
1:F:510:TRP:HA	1:F:678:GLU:HG3	1.95	0.49
1:C:325:ILE:HG13	1:C:369:VAL:HG23	1.93	0.49
1:C:512:ASP:N	1:C:513:PRO:CD	2.76	0.49
1:D:589:PHE:CE2	1:D:629:LEU:HD13	2.48	0.49
1:D:602:VAL:O	1:D:644:GLY:HA2	2.13	0.49
1:E:428:GLU:O	1:E:432:GLU:HG2	2.12	0.49
1:E:672:THR:OG1	1:E:675:GLN:HB2	2.13	0.49
1:F:236:ALA:O	1:F:239:VAL:HG12	2.13	0.49
1:A:283:LYS:HA	1:A:324:ILE:O	2.13	0.49
1:B:313:GLN:O	1:B:317:GLY:N	2.45	0.49
1:B:352:ASN:HA	1:B:355:LEU:HD12	1.95	0.49
1:C:352:ASN:HD22	1:D:289:GLU:CB	2.26	0.49
1:C:540:LEU:HD11	1:C:646:THR:HG22	1.94	0.49
1:D:242:PRO:HD2	1:D:243:GLU:N	2.28	0.49
1:D:539:VAL:HG13	1:D:643:ILE:HG13	1.94	0.49
1:E:585:MET:HE2	1:E:626:LEU:HD21	1.94	0.49
1:A:652:LEU:HA	1:A:655:MET:SD	2.53	0.49
1:C:560:SER:HB2	1:C:562:PHE:CE1	2.48	0.49
1:C:573:MET:HB3	1:C:576:PHE:CD2	2.48	0.49
1:D:241:PRO:HA	1:D:242:PRO:HA	1.66	0.49
1:D:424:VAL:HG21	1:D:480:PHE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:ASN:O	1:D:490:PRO:HD3	2.13	0.49
1:D:540:LEU:HD12	1:D:661:PHE:CE1	2.48	0.49
1:E:587:LYS:HZ3	1:E:587:LYS:C	2.14	0.49
1:F:223:LEU:O	1:F:227:PHE:HB3	2.13	0.49
1:F:313:GLN:O	1:F:317:GLY:N	2.45	0.49
1:A:624:GLN:HG3	1:B:610:ASP:CG	2.37	0.48
1:B:222:GLY:HA3	1:B:399:ASP:HB2	1.95	0.48
1:B:406:ILE:HB	1:B:441:LEU:HD13	1.95	0.48
1:B:437:SER:O	1:B:440:GLU:HB2	2.13	0.48
1:C:691:ARG:HH11	1:C:691:ARG:HB2	1.76	0.48
1:D:284:VAL:HG21	1:D:325:ILE:HG22	1.95	0.48
1:F:256:ILE:O	1:F:370:ILE:HA	2.13	0.48
1:F:526:GLN:O	1:F:530:ASN:HB2	2.11	0.48
1:F:677:LEU:O	1:F:681:GLU:HG3	2.13	0.48
1:B:281:GLU:N	1:B:282:PRO:HA	2.28	0.48
1:C:404:LEU:HG	1:C:426:ILE:HG22	1.95	0.48
1:D:721:ASP:O	1:D:725:ARG:HG3	2.13	0.48
1:E:254:LYS:O	1:E:368:LEU:HA	2.13	0.48
1:E:256:ILE:O	1:E:370:ILE:HA	2.13	0.48
1:F:436:PHE:CD1	1:F:436:PHE:N	2.80	0.48
1:A:508:ILE:HD12	1:A:682:LEU:HB2	1.96	0.48
1:A:517:VAL:HG13	1:A:665:ILE:CG2	2.43	0.48
1:B:289:GLU:C	1:B:291:LEU:H	2.16	0.48
1:B:541:LEU:HD12	1:B:541:LEU:O	2.13	0.48
1:C:497:GLU:OE1	1:C:498:ASP:N	2.46	0.48
1:D:260:GLY:CA	1:D:266:LYS:HD3	2.43	0.48
1:D:264:CYS:SG	1:D:395:ILE:HG21	2.53	0.48
1:E:596:GLN:O	1:E:638:ARG:HA	2.13	0.48
1:E:714:ILE:O	1:E:718:LEU:HG	2.13	0.48
1:F:566:LYS:HD2	1:F:567:ILE:H	1.77	0.48
1:F:609:LEU:CD1	1:F:655:MET:HE1	2.42	0.48
1:C:322:LEU:HD12	1:C:324:ILE:HD11	1.95	0.48
1:C:614:ILE:O	1:C:616:PRO:HA	2.12	0.48
1:C:657:MET:HE3	1:C:661:PHE:CZ	2.49	0.48
1:F:552:LEU:O	1:F:556:ILE:HG13	2.14	0.48
1:A:436:PHE:CD2	1:A:444:LEU:HD11	2.48	0.48
1:A:567:ILE:HG13	1:A:601:VAL:CB	2.41	0.48
1:B:236:ALA:HA	1:B:239:VAL:CG1	2.43	0.48
1:D:694:ILE:O	1:D:698:VAL:HG22	2.13	0.48
1:A:428:GLU:O	1:A:432:GLU:HG2	2.14	0.48
1:B:246:GLU:HG2	1:B:247:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLU:O	1:B:490:PRO:HD3	2.13	0.48
1:C:596:GLN:HA	1:C:638:ARG:CD	2.41	0.48
1:C:603:ASP:HA	1:C:645:THR:HG1	1.77	0.48
1:E:281:GLU:N	1:E:282:PRO:HA	2.27	0.48
1:F:720:MET:HB3	1:F:724:TYR:HB2	1.95	0.48
1:A:690:GLU:HB3	1:A:726:VAL:HG22	1.95	0.48
1:B:452:ALA:HA	1:B:455:ARG:CZ	2.44	0.48
1:C:289:GLU:O	1:C:291:LEU:N	2.34	0.48
1:C:326:ILE:HB	1:C:370:ILE:HD11	1.95	0.48
1:C:604:ASP:N	1:C:645:THR:OG1	2.43	0.48
1:E:289:GLU:O	1:E:291:LEU:N	2.32	0.48
1:E:662:SER:HA	1:F:709:LYS:HZ3	1.78	0.48
1:F:438:GLY:O	1:F:441:LEU:HB2	2.13	0.48
1:B:307:ALA:HA	1:B:310:GLU:HG2	1.96	0.48
1:C:311:GLU:O	1:C:314:ARG:HG2	2.14	0.48
1:C:589:PHE:CE1	1:C:600:VAL:HG11	2.49	0.48
1:D:331:ASP:HA	1:D:379:ILE:HD11	1.96	0.48
1:E:705:ILE:HD12	1:E:713:LEU:HD12	1.96	0.48
1:F:281:GLU:N	1:F:282:PRO:HA	2.28	0.48
1:A:407:LEU:CD1	1:A:426:ILE:HG23	2.44	0.48
1:A:499:TYR:OH	1:A:565:ILE:HB	2.14	0.48
1:A:677:LEU:HG	1:A:695:ALA:CB	2.43	0.48
1:E:257:LEU:HG	1:E:371:GLY:O	2.14	0.48
1:E:562:PHE:CD1	1:E:597:LEU:HG	2.49	0.48
1:F:570:PRO:CG	1:F:604:ASP:HB2	2.41	0.48
1:E:286:ASN:OD1	1:E:327:PHE:HD1	1.97	0.48
1:E:352:ASN:HA	1:E:355:LEU:HD12	1.96	0.48
1:F:257:LEU:HG	1:F:371:GLY:O	2.14	0.48
1:A:241:PRO:HA	1:A:242:PRO:HA	1.39	0.47
1:A:517:VAL:HG13	1:A:665:ILE:HG21	1.96	0.47
1:A:543:GLY:O	1:A:647:SER:HA	2.14	0.47
1:B:230:ILE:HD11	1:B:391:VAL:HG11	1.96	0.47
1:B:670:ILE:HG21	1:B:675:GLN:HB2	1.96	0.47
1:E:508:ILE:HD13	1:E:683:LEU:HD21	1.95	0.47
1:F:629:LEU:O	1:F:632:LYS:HB3	2.14	0.47
1:A:398:PRO:HD2	1:A:434:LYS:O	2.14	0.47
1:A:540:LEU:HD12	1:A:644:GLY:O	2.14	0.47
1:B:428:GLU:O	1:B:431:VAL:HG12	2.14	0.47
1:B:438:GLY:O	1:B:441:LEU:N	2.42	0.47
1:C:318:ALA:C	1:C:319:ASN:HD22	2.21	0.47
1:C:538:SER:OG	1:C:662:SER:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:GLU:OE1	1:D:621:LEU:HD13	2.14	0.47
1:A:242:PRO:O	1:A:246:GLU:OE1	2.32	0.47
1:A:388:ARG:O	1:A:389:LEU:HD22	2.14	0.47
1:A:650:ASP:OD1	1:A:650:ASP:N	2.46	0.47
1:B:407:LEU:O	1:B:411:THR:OG1	2.27	0.47
1:C:576:PHE:HB3	1:C:580:ALA:HB3	1.96	0.47
1:D:268:LEU:HA	1:D:271:ARG:HD2	1.96	0.47
1:D:593:TYR:OH	1:D:632:LYS:HD2	2.14	0.47
1:D:627:LEU:CD2	1:D:657:MET:HG3	2.45	0.47
1:D:670:ILE:HD11	1:D:705:ILE:CG2	2.44	0.47
1:E:428:GLU:O	1:E:431:VAL:HG12	2.14	0.47
1:F:327:PHE:CB	1:F:330:ILE:HG22	2.44	0.47
1:C:510:TRP:CD1	1:C:510:TRP:H	2.32	0.47
1:C:633:ALA:HB1	1:D:504:MET:HE1	1.96	0.47
1:D:397:LEU:HD23	1:D:398:PRO:CD	2.42	0.47
1:E:440:GLU:O	1:E:444:LEU:HG	2.14	0.47
1:E:677:LEU:HD11	1:E:695:ALA:HA	1.95	0.47
1:F:510:TRP:CB	1:F:679:ALA:HB2	2.43	0.47
1:F:525:VAL:HG11	1:F:560:SER:CB	2.45	0.47
1:F:579:THR:O	1:F:583:GLN:HG2	2.14	0.47
1:F:710:LEU:O	1:F:714:ILE:HG13	2.14	0.47
1:A:237:SER:OG	1:A:252:HIS:HA	2.14	0.47
1:B:540:LEU:HD11	1:B:649:LYS:HZ2	1.79	0.47
1:C:513:PRO:HD3	1:C:675:GLN:HE22	1.80	0.47
1:C:609:LEU:O	1:C:610:ASP:HB2	2.13	0.47
1:C:666:HIS:CE1	1:C:668:PRO:HB3	2.49	0.47
1:D:310:GLU:O	1:D:313:GLN:CG	2.63	0.47
1:F:609:LEU:HD13	1:F:655:MET:CE	2.43	0.47
1:B:241:PRO:HA	1:B:242:PRO:HA	1.58	0.47
1:B:503:ILE:HG22	1:B:506:GLY:H	1.79	0.47
1:B:540:LEU:O	1:B:540:LEU:HD12	2.15	0.47
1:C:536:LEU:CD1	1:C:640:LEU:HB3	2.44	0.47
1:C:721:ASP:O	1:C:725:ARG:HG3	2.13	0.47
1:D:303:ARG:HH11	1:D:357:LYS:CE	2.28	0.47
1:D:510:TRP:CE3	1:D:675:GLN:HG2	2.40	0.47
1:D:564:PHE:HB3	1:D:598:SER:HB3	1.97	0.47
1:D:652:LEU:HD13	1:D:657:MET:HB3	1.95	0.47
1:E:508:ILE:HG13	1:E:510:TRP:HB3	1.95	0.47
1:E:612:VAL:HG22	1:E:613:PRO:HD2	1.97	0.47
1:E:705:ILE:CD1	1:E:713:LEU:HD12	2.45	0.47
1:F:428:GLU:O	1:F:431:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ARG:HG3	1:A:617:ARG:NH1	2.28	0.47
1:A:683:LEU:HD13	1:A:685:ASN:HD22	1.79	0.47
1:C:510:TRP:CD2	1:C:707:ILE:HD13	2.50	0.47
1:D:281:GLU:N	1:D:282:PRO:HA	2.30	0.47
1:E:311:GLU:O	1:E:314:ARG:HG2	2.15	0.47
1:E:531:SER:HB3	1:E:534:THR:O	2.14	0.47
1:F:548:GLY:HA3	1:F:707:ILE:HG22	1.95	0.47
1:B:272:GLN:OE1	1:B:272:GLN:HA	2.15	0.47
1:C:428:GLU:O	1:C:431:VAL:HG12	2.15	0.47
1:D:247:GLN:HA	1:E:417:HIS:CE1	2.50	0.47
1:D:257:LEU:HG	1:D:371:GLY:O	2.14	0.47
1:E:272:GLN:OE1	1:E:272:GLN:HA	2.15	0.47
1:E:526:GLN:HA	1:E:529:LYS:HG2	1.96	0.47
1:F:311:GLU:O	1:F:314:ARG:HG2	2.15	0.47
1:F:535:PRO:HB2	1:F:536:LEU:HD13	1.97	0.47
1:B:237:SER:HA	1:C:453:MET:HG3	1.97	0.47
1:B:402:GLY:O	1:B:406:ILE:HD12	2.15	0.47
1:B:523:LEU:HA	1:B:526:GLN:HG2	1.96	0.47
1:B:533:ARG:CG	1:B:534:THR:H	2.18	0.47
1:B:640:LEU:CD2	1:B:642:ILE:HG13	2.45	0.47
1:C:355:LEU:O	1:C:388:ARG:NH2	2.40	0.47
1:E:233:ARG:CG	1:F:454:ASN:HB2	2.45	0.47
1:E:549:LYS:O	1:E:552:LEU:HB2	2.15	0.47
1:B:710:LEU:O	1:B:714:ILE:HG13	2.15	0.47
1:C:490:PRO:HA	1:C:491:ALA:CB	2.29	0.47
1:C:550:THR:HB	2:C:801:ADP:O2A	2.15	0.47
1:C:582:CYS:SG	1:C:621:LEU:HG	2.55	0.47
1:D:536:LEU:HD21	1:D:630:LEU:O	2.15	0.47
1:D:654:GLU:HB3	1:E:614:ILE:HD11	1.96	0.47
1:D:688:ASP:O	1:D:692:THR:HG23	2.14	0.47
1:E:697:GLN:HG3	1:E:730:LEU:CD1	2.45	0.47
1:B:319:ASN:HB3	1:B:320:SER:HB2	1.97	0.46
1:B:503:ILE:HG12	1:B:551:ALA:HA	1.96	0.46
1:C:540:LEU:HD22	1:C:661:PHE:CD2	2.50	0.46
1:E:307:ALA:HA	1:E:310:GLU:HG2	1.96	0.46
1:E:540:LEU:HD12	1:E:541:LEU:N	2.30	0.46
1:A:222:GLY:N	1:A:405:GLN:HB3	2.31	0.46
1:A:263:GLY:CA	1:A:264:CYS:HB2	2.45	0.46
1:B:257:LEU:HG	1:B:371:GLY:O	2.15	0.46
1:B:513:PRO:CD	1:B:670:ILE:HD11	2.44	0.46
1:D:286:ASN:HB2	1:D:327:PHE:CD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:LEU:O	1:D:411:THR:HG23	2.14	0.46
1:F:307:ALA:HA	1:F:310:GLU:HG2	1.96	0.46
1:A:315:ARG:C	1:A:316:LEU:HD12	2.40	0.46
1:A:347:HIS:N	1:A:348:ASP:HA	2.31	0.46
1:B:311:GLU:O	1:B:314:ARG:HG2	2.15	0.46
1:B:499:TYR:HA	1:B:502:TYR:CE2	2.49	0.46
1:B:568:CYS:SG	1:B:588:ILE:HD12	2.56	0.46
1:B:614:ILE:O	1:B:616:PRO:HA	2.14	0.46
1:C:670:ILE:HD13	1:C:675:GLN:CG	2.38	0.46
1:C:721:ASP:HB2	1:C:724:TYR:CD1	2.50	0.46
1:D:528:THR:HG21	1:D:641:LEU:HB2	1.97	0.46
1:D:589:PHE:CD2	1:D:629:LEU:HD13	2.50	0.46
1:E:564:PHE:HB3	1:E:595:SER:HB2	1.97	0.46
1:F:557:ALA:HB2	1:F:601:VAL:HG21	1.98	0.46
1:B:438:GLY:O	1:B:441:LEU:HB2	2.15	0.46
1:B:512:ASP:N	1:B:513:PRO:CD	2.78	0.46
1:B:523:LEU:O	1:B:526:GLN:HG2	2.14	0.46
1:B:578:GLU:CG	1:B:619:SER:HB2	2.45	0.46
1:F:223:LEU:N	1:F:223:LEU:HD23	2.31	0.46
1:F:261:PRO:O	1:F:264:CYS:HB2	2.15	0.46
1:A:258:LEU:O	1:A:258:LEU:HD12	2.15	0.46
1:A:322:LEU:HD12	1:A:323:HIS:H	1.80	0.46
1:B:513:PRO:O	1:B:517:VAL:HG23	2.15	0.46
1:C:436:PHE:N	1:C:436:PHE:CD1	2.82	0.46
1:C:510:TRP:NE1	1:C:514:VAL:HG21	2.30	0.46
1:C:546:HIS:HA	1:C:708:LYS:HE2	1.98	0.46
1:C:612:VAL:CG2	1:C:613:PRO:HD2	2.46	0.46
1:D:609:LEU:O	1:D:610:ASP:OD1	2.34	0.46
1:E:683:LEU:HB3	1:E:685:ASN:OD1	2.16	0.46
1:E:713:LEU:HD23	1:E:713:LEU:HA	1.75	0.46
1:A:231:PHE:CE1	1:A:235:PHE:CE2	3.04	0.46
1:A:403:ARG:O	1:A:407:LEU:HG	2.15	0.46
1:B:222:GLY:N	1:B:402:GLY:HA3	2.31	0.46
1:B:576:PHE:HB2	1:B:581:LYS:CG	2.46	0.46
1:C:510:TRP:HA	1:C:679:ALA:HA	1.98	0.46
1:D:453:MET:O	1:D:457:ILE:HG13	2.16	0.46
1:D:510:TRP:CB	1:D:679:ALA:HB2	2.46	0.46
1:D:550:THR:HG23	2:D:801:ADP:PA	2.56	0.46
1:E:397:LEU:HG	1:E:398:PRO:HD2	1.96	0.46
1:E:451:THR:HB	1:E:481:LEU:CB	2.45	0.46
1:F:230:ILE:HD11	1:F:391:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:LEU:HA	1:F:271:ARG:HG2	1.98	0.46
1:F:571:ASP:HA	1:F:574:ILE:HB	1.97	0.46
1:F:653:GLN:HA	1:F:658:LEU:HB3	1.97	0.46
1:C:380:ASP:OD1	1:C:382:ALA:N	2.44	0.46
1:C:539:VAL:HG23	1:C:663:THR:HG23	1.96	0.46
1:E:261:PRO:HG2	1:E:264:CYS:HB2	1.96	0.46
1:E:593:TYR:CD2	1:E:635:PRO:HD3	2.50	0.46
1:B:325:ILE:HG13	1:B:369:VAL:HB	1.98	0.46
1:C:233:ARG:HB2	1:C:233:ARG:CZ	2.45	0.46
1:C:674:GLU:O	1:C:677:LEU:HB2	2.16	0.46
1:D:312:GLU:CD	1:D:323:HIS:ND1	2.74	0.46
1:E:261:PRO:HB3	1:E:594:LYS:CE	2.46	0.46
1:E:490:PRO:HA	1:E:491:ALA:CB	2.34	0.46
1:E:527:GLN:HA	1:F:719:GLN:HG3	1.96	0.46
1:A:628:VAL:CG1	1:B:571:ASP:HA	2.45	0.46
1:F:261:PRO:HD2	1:F:264:CYS:SG	2.56	0.46
1:D:627:LEU:HD23	1:D:627:LEU:HA	1.68	0.46
1:D:635:PRO:O	1:D:638:ARG:HB2	2.15	0.46
1:D:636:GLN:NE2	1:E:504:MET:SD	2.82	0.46
1:E:327:PHE:CE2	1:E:369:VAL:HG21	2.50	0.46
1:F:694:ILE:O	1:F:698:VAL:HG22	2.17	0.46
1:A:624:GLN:OE1	1:A:624:GLN:HA	2.16	0.45
1:A:709:LYS:HE2	1:A:709:LYS:HA	1.97	0.45
1:B:436:PHE:N	1:B:436:PHE:CD1	2.83	0.45
1:B:440:GLU:O	1:B:444:LEU:HG	2.16	0.45
1:C:263:GLY:C	1:C:437:SER:HB3	2.41	0.45
1:E:648:ARG:NE	1:E:651:VAL:HG13	2.32	0.45
1:E:655:MET:C	1:E:656:GLU:HG3	2.41	0.45
1:F:589:PHE:CD2	1:F:629:LEU:HD22	2.50	0.45
1:A:510:TRP:O	1:A:678:GLU:HB3	2.17	0.45
1:A:627:LEU:O	1:A:631:LYS:NZ	2.49	0.45
1:B:507:ILE:HG13	1:B:555:LYS:HD3	1.97	0.45
1:B:707:ILE:O	1:B:711:LEU:HG	2.15	0.45
1:D:657:MET:HE2	1:D:661:PHE:HZ	1.81	0.45
1:D:686:PHE:HB2	1:D:691:ARG:CG	2.46	0.45
1:E:218:MET:HA	1:E:219:GLY:HA2	1.74	0.45
1:E:319:ASN:HB3	1:E:320:SER:HB2	1.97	0.45
1:F:712:MET:O	1:F:716:MET:HG3	2.15	0.45
1:A:239:VAL:O	1:A:240:PHE:C	2.57	0.45
1:A:620:ASN:ND2	1:B:610:ASP:OD1	2.49	0.45
1:B:527:GLN:CB	1:C:719:GLN:HG3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:ILE:HD11	1:E:707:ILE:CD1	2.46	0.45
1:E:611:TYR:CE1	1:E:616:PRO:HB2	2.51	0.45
1:F:289:GLU:C	1:F:291:LEU:H	2.21	0.45
1:F:502:TYR:CD2	1:F:503:ILE:HG13	2.51	0.45
1:A:261:PRO:CG	1:A:397:LEU:H	2.30	0.45
1:A:721:ASP:O	1:A:725:ARG:HG3	2.16	0.45
1:D:247:GLN:HA	1:E:417:HIS:ND1	2.31	0.45
1:D:318:ALA:O	1:D:319:ASN:ND2	2.49	0.45
1:D:399:ASP:HB3	1:D:401:LYS:HG2	1.98	0.45
1:D:564:PHE:HD2	1:D:598:SER:HB2	1.81	0.45
1:E:586:LYS:NZ	1:F:575:GLY:HA3	2.32	0.45
1:F:307:ALA:O	1:F:310:GLU:HG2	2.17	0.45
1:F:510:TRP:HB3	1:F:679:ALA:CB	2.43	0.45
1:C:352:ASN:ND2	1:D:289:GLU:H	2.14	0.45
1:D:327:PHE:HB2	1:D:330:ILE:CG2	2.47	0.45
1:F:241:PRO:HA	1:F:242:PRO:HA	1.63	0.45
1:F:686:PHE:CE1	1:F:714:ILE:HG23	2.50	0.45
1:B:307:ALA:O	1:B:310:GLU:HG2	2.16	0.45
1:C:247:GLN:HA	1:D:417:HIS:NE2	2.31	0.45
1:C:562:PHE:O	1:C:565:ILE:HD11	2.17	0.45
1:E:325:ILE:HG13	1:E:369:VAL:HB	1.97	0.45
1:F:319:ASN:HB3	1:F:320:SER:HB2	1.97	0.45
1:F:510:TRP:CE2	1:F:670:ILE:HG12	2.52	0.45
1:F:670:ILE:O	1:F:704:TRP:HA	2.16	0.45
1:A:315:ARG:O	1:A:316:LEU:HD12	2.17	0.45
1:A:612:VAL:HG12	1:A:617:ARG:HB2	1.99	0.45
1:C:320:SER:O	1:C:320:SER:OG	2.31	0.45
1:F:612:VAL:HG13	1:F:614:ILE:O	2.17	0.45
1:A:713:LEU:CD2	1:A:732:LEU:HB3	2.42	0.45
1:B:539:VAL:HA	1:B:663:THR:O	2.16	0.45
1:C:236:ALA:HB1	1:D:453:MET:CB	2.47	0.45
1:C:550:THR:H	2:C:801:ADP:PB	2.40	0.45
1:C:593:TYR:CE2	1:C:632:LYS:NZ	2.84	0.45
1:F:632:LYS:HD2	1:F:633:ALA:H	1.81	0.45
1:A:220:ILE:HG22	1:A:221:GLY:N	2.32	0.45
1:D:303:ARG:HH11	1:D:357:LYS:HE3	1.82	0.45
1:D:542:GLU:OE2	1:D:649:LYS:HD2	2.17	0.45
1:E:538:SER:OG	1:E:662:SER:N	2.47	0.45
1:E:732:LEU:HD23	1:E:732:LEU:HA	1.71	0.45
1:A:299:GLU:CD	1:A:303:ARG:HH21	2.24	0.45
1:A:508:ILE:CD1	1:A:683:LEU:HG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:HD11	1:B:554:ALA:HB3	1.99	0.45
1:B:519:ASP:O	1:B:523:LEU:HG	2.17	0.45
1:B:545:PRO:O	1:B:546:HIS:HB2	2.17	0.45
1:D:218:MET:HA	1:D:219:GLY:HA2	1.77	0.45
1:D:550:THR:HG23	2:D:801:ADP:O2A	2.16	0.45
1:D:573:MET:CE	1:D:585:MET:HE3	2.47	0.45
1:E:618:PHE:CD1	1:E:618:PHE:C	2.95	0.45
1:E:713:LEU:CD2	1:E:732:LEU:HD13	2.47	0.45
1:E:714:ILE:HG12	1:E:729:PHE:HE1	1.82	0.45
1:E:726:VAL:O	1:E:730:LEU:HG	2.17	0.45
1:F:297:GLU:O	1:F:300:ALA:HB3	2.17	0.45
1:A:646:THR:HG21	1:A:652:LEU:HD22	1.99	0.44
1:D:424:VAL:CG2	1:D:480:PHE:HA	2.46	0.44
1:D:522:GLU:CD	1:D:559:GLU:HB2	2.42	0.44
1:D:564:PHE:HB3	1:D:598:SER:CB	2.46	0.44
1:E:230:ILE:HD11	1:E:391:VAL:HG11	1.98	0.44
1:E:236:ALA:CA	1:E:239:VAL:HG12	2.44	0.44
1:E:297:GLU:O	1:E:300:ALA:HB3	2.17	0.44
1:E:436:PHE:CD1	1:E:436:PHE:N	2.85	0.44
1:E:512:ASP:N	1:E:513:PRO:CD	2.79	0.44
1:F:441:LEU:O	1:F:445:VAL:HG23	2.16	0.44
1:B:549:LYS:HZ2	1:B:647:SER:HA	1.83	0.44
1:D:231:PHE:HA	1:D:235:PHE:CD2	2.53	0.44
1:D:312:GLU:HG3	1:D:313:GLN:N	2.32	0.44
1:F:325:ILE:HG13	1:F:369:VAL:HB	1.98	0.44
1:C:555:LYS:O	1:C:559:GLU:HG2	2.18	0.44
1:E:307:ALA:O	1:E:310:GLU:HG2	2.16	0.44
1:E:573:MET:O	1:E:576:PHE:HB2	2.16	0.44
1:F:289:GLU:O	1:F:291:LEU:N	2.35	0.44
1:B:436:PHE:HB3	1:B:440:GLU:HB2	1.99	0.44
1:C:355:LEU:HA	1:C:388:ARG:NE	2.31	0.44
1:D:626:LEU:O	1:D:630:LEU:HG	2.18	0.44
1:E:506:GLY:O	1:E:508:ILE:N	2.49	0.44
1:F:525:VAL:HG11	1:F:560:SER:HB2	1.99	0.44
1:F:602:VAL:O	1:F:644:GLY:HA2	2.17	0.44
1:A:220:ILE:HD11	1:A:227:PHE:CZ	2.53	0.44
1:A:236:ALA:CB	1:B:453:MET:HB2	2.43	0.44
1:A:355:LEU:HD22	1:A:388:ARG:NH1	2.32	0.44
1:B:297:GLU:O	1:B:300:ALA:HB3	2.17	0.44
1:D:300:ALA:O	1:D:303:ARG:HB3	2.18	0.44
1:D:573:MET:SD	1:D:608:LEU:HD22	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:721:ASP:HB2	1:E:724:TYR:CD2	2.52	0.44
1:F:240:PHE:HA	1:F:241:PRO:HD3	1.82	0.44
1:F:546:HIS:CE1	1:F:709:LYS:HB2	2.51	0.44
1:A:215:PHE:C	1:A:217:LYS:N	2.74	0.44
1:B:284:VAL:O	1:B:326:ILE:HG12	2.18	0.44
1:C:546:HIS:O	1:C:708:LYS:HG2	2.17	0.44
1:D:655:MET:O	1:D:656:GLU:HB2	2.18	0.44
1:B:240:PHE:HA	1:B:241:PRO:HD3	1.88	0.44
1:B:536:LEU:HD12	1:B:640:LEU:O	2.18	0.44
1:D:361:VAL:CB	1:E:285:VAL:HG21	2.48	0.44
1:E:246:GLU:HG2	1:E:247:GLN:N	2.33	0.44
1:E:586:LYS:NZ	1:F:574:ILE:HG23	2.32	0.44
1:E:696:GLN:HA	1:E:696:GLN:OE1	2.18	0.44
1:B:503:ILE:HD11	1:B:551:ALA:O	2.17	0.44
1:B:537:VAL:HG12	1:C:712:MET:HE1	1.98	0.44
1:D:510:TRP:HB3	1:D:679:ALA:HB2	1.99	0.44
1:D:546:HIS:HB3	1:D:708:LYS:CB	2.47	0.44
1:F:223:LEU:HD22	1:F:395:ILE:HG23	1.99	0.44
1:F:272:GLN:HA	1:F:272:GLN:OE1	2.16	0.44
1:F:443:GLY:O	1:F:446:ARG:HB3	2.18	0.44
1:F:593:TYR:O	1:F:638:ARG:CD	2.66	0.44
1:A:508:ILE:HD11	1:A:683:LEU:HG	2.00	0.44
1:A:526:GLN:NE2	1:A:530:ASN:HD22	2.13	0.44
1:B:531:SER:HA	1:B:639:LYS:HD3	1.99	0.44
1:C:514:VAL:HG11	2:C:801:ADP:N6	2.33	0.44
1:C:726:VAL:H	1:C:726:VAL:HG23	1.62	0.44
1:B:221:GLY:HA3	1:B:406:ILE:HD12	2.00	0.43
1:B:510:TRP:CE2	1:B:514:VAL:CG2	3.01	0.43
1:B:533:ARG:HH21	1:C:685:ASN:HD21	1.65	0.43
1:D:527:GLN:HE22	1:E:716:MET:N	2.13	0.43
1:E:250:CYS:SG	1:F:446:ARG:HA	2.58	0.43
1:F:436:PHE:HB3	1:F:440:GLU:HB2	1.98	0.43
1:A:397:LEU:CD1	1:A:435:ASN:HA	2.43	0.43
1:A:564:PHE:CZ	1:A:566:LYS:HB2	2.53	0.43
1:B:375:ARG:NH2	1:B:377:ASP:OD2	2.50	0.43
1:B:507:ILE:CG1	1:B:555:LYS:HD3	2.48	0.43
1:B:548:GLY:HA2	2:B:801:ADP:O1A	2.18	0.43
1:C:220:ILE:HD11	1:C:272:GLN:HG3	1.99	0.43
1:C:519:ASP:O	1:C:523:LEU:HG	2.18	0.43
1:E:242:PRO:HD2	1:E:243:GLU:N	2.33	0.43
1:F:352:ASN:HA	1:F:355:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:536:LEU:HD11	1:F:633:ALA:HA	2.00	0.43
1:A:300:ALA:O	1:A:303:ARG:HG2	2.17	0.43
1:A:402:GLY:O	1:A:406:ILE:HD12	2.18	0.43
1:A:611:TYR:HA	1:A:617:ARG:O	2.19	0.43
1:B:533:ARG:HD2	1:C:711:LEU:CD1	2.48	0.43
1:B:542:GLU:OE1	1:B:649:LYS:HD3	2.18	0.43
1:B:612:VAL:HG13	1:B:614:ILE:O	2.17	0.43
1:C:218:MET:HA	1:C:219:GLY:HA2	1.75	0.43
1:D:690:GLU:O	1:D:694:ILE:HG13	2.18	0.43
1:E:248:MET:HA	1:F:449:GLN:OE1	2.18	0.43
1:B:499:TYR:HA	1:B:502:TYR:CD2	2.53	0.43
1:C:265:GLY:O	1:C:268:LEU:HG	2.18	0.43
1:C:676:LEU:O	1:C:679:ALA:HB3	2.18	0.43
1:F:589:PHE:O	1:F:593:TYR:CD1	2.71	0.43
1:A:357:LYS:HE3	1:A:357:LYS:HA	2.00	0.43
1:A:410:HIS:NE2	1:A:442:GLU:HG2	2.33	0.43
1:A:593:TYR:HB3	1:A:635:PRO:HD3	2.00	0.43
1:B:539:VAL:CG2	1:B:665:ILE:HD12	2.47	0.43
1:C:510:TRP:CG	1:C:707:ILE:HD13	2.53	0.43
1:C:540:LEU:HD22	1:C:661:PHE:CE2	2.53	0.43
1:D:626:LEU:HD13	1:D:657:MET:HE1	2.01	0.43
1:F:657:MET:SD	1:F:661:PHE:CE2	3.11	0.43
1:A:322:LEU:HD13	1:A:366:ASN:O	2.18	0.43
1:B:254:LYS:O	1:B:368:LEU:HA	2.18	0.43
1:B:490:PRO:HA	1:B:491:ALA:CB	2.34	0.43
1:B:541:LEU:HA	1:B:665:ILE:O	2.19	0.43
1:C:319:ASN:HA	1:C:320:SER:HA	1.88	0.43
1:C:547:SER:O	1:C:707:ILE:HG22	2.19	0.43
1:D:240:PHE:HA	1:D:241:PRO:HD3	1.79	0.43
1:E:221:GLY:HA3	1:E:406:ILE:CD1	2.49	0.43
1:E:375:ARG:NH2	1:E:377:ASP:OD2	2.51	0.43
1:F:219:GLY:C	1:F:220:ILE:HD12	2.43	0.43
1:A:573:MET:HA	1:A:576:PHE:CD2	2.54	0.43
1:A:687:LYS:HZ3	1:A:722:PRO:HB3	1.82	0.43
1:B:510:TRP:CE2	1:B:514:VAL:HG22	2.53	0.43
1:B:670:ILE:HG22	1:B:672:THR:N	2.30	0.43
1:C:407:LEU:O	1:C:411:THR:OG1	2.29	0.43
1:D:538:SER:OG	1:D:661:PHE:HA	2.18	0.43
1:D:573:MET:HE1	1:D:585:MET:HE3	2.01	0.43
1:E:406:ILE:HB	1:E:441:LEU:HD13	2.00	0.43
1:A:632:LYS:HE3	1:A:633:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:GLN:OE1	1:C:530:ASN:ND2	2.51	0.43
1:C:677:LEU:O	1:C:681:GLU:OE1	2.35	0.43
1:D:227:PHE:O	1:D:230:ILE:HG22	2.19	0.43
1:F:265:GLY:HA3	1:F:437:SER:HB2	1.99	0.43
1:A:299:GLU:OE1	1:A:303:ARG:NH2	2.48	0.43
1:A:659:ASN:HD21	1:B:545:PRO:HB2	1.84	0.43
1:A:676:LEU:O	1:A:679:ALA:HB3	2.19	0.43
1:B:609:LEU:HD23	1:B:609:LEU:HA	1.67	0.43
1:C:521:GLY:O	1:C:525:VAL:HG23	2.18	0.43
1:C:596:GLN:O	1:C:638:ARG:HA	2.19	0.43
1:E:352:ASN:CB	1:F:288:PRO:HG2	2.49	0.43
1:E:654:GLU:CD	1:F:614:ILE:HD11	2.44	0.43
1:E:658:LEU:HD12	1:E:658:LEU:HA	1.61	0.43
1:F:257:LEU:HB2	1:F:389:LEU:HD13	2.00	0.43
1:F:320:SER:O	1:F:320:SER:OG	2.36	0.43
1:F:510:TRP:HB3	1:F:679:ALA:CA	2.49	0.43
1:C:576:PHE:HB2	1:C:581:LYS:HE3	2.00	0.43
1:C:635:PRO:HB2	1:C:638:ARG:NH1	2.33	0.43
1:D:303:ARG:HG3	1:D:357:LYS:HG3	2.00	0.43
1:E:549:LYS:HE2	1:E:645:THR:HB	2.00	0.43
1:F:677:LEU:HD21	1:F:695:ALA:HA	2.01	0.43
1:A:313:GLN:NE2	1:A:365:ASN:OD1	2.52	0.42
1:A:315:ARG:HG2	1:A:316:LEU:HD12	2.00	0.42
1:B:232:ARG:O	1:B:236:ALA:HB3	2.19	0.42
1:B:536:LEU:HD22	1:B:632:LYS:O	2.19	0.42
1:E:676:LEU:HD22	1:E:703:VAL:HG11	2.01	0.42
1:F:270:ALA:HA	1:F:273:ILE:HG22	1.99	0.42
1:F:397:LEU:CB	1:F:398:PRO:HD3	2.49	0.42
1:A:227:PHE:CE2	1:A:231:PHE:CD1	3.07	0.42
1:B:406:ILE:O	1:B:409:ILE:HG22	2.20	0.42
1:C:324:ILE:HD12	1:C:324:ILE:N	2.34	0.42
1:C:554:ALA:O	1:C:558:GLU:OE1	2.37	0.42
1:C:656:GLU:OE1	1:D:613:PRO:HD3	2.19	0.42
1:D:377:ASP:OD1	1:D:378:LEU:N	2.52	0.42
1:E:253:VAL:HA	1:F:446:ARG:HH21	1.83	0.42
1:E:377:ASP:OD1	1:E:378:LEU:N	2.53	0.42
1:E:388:ARG:O	1:E:389:LEU:HD23	2.20	0.42
1:F:254:LYS:O	1:F:368:LEU:HA	2.18	0.42
1:F:395:ILE:HD12	1:F:395:ILE:N	2.34	0.42
1:A:242:PRO:HD2	1:A:243:GLU:OE1	2.19	0.42
1:A:380:ASP:OD1	1:A:381:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:HA	1:A:713:LEU:HD23	1.69	0.42
1:B:257:LEU:HB2	1:B:389:LEU:HD13	2.01	0.42
1:B:377:ASP:OD1	1:B:378:LEU:N	2.53	0.42
1:B:526:GLN:NE2	1:C:719:GLN:HB3	2.33	0.42
1:B:541:LEU:HD13	1:B:667:VAL:HG21	2.01	0.42
1:E:605:ILE:HA	1:E:608:LEU:HB3	2.01	0.42
1:A:708:LYS:O	1:A:711:LEU:HB2	2.19	0.42
1:B:543:GLY:O	1:B:549:LYS:NZ	2.50	0.42
1:B:579:THR:O	1:B:583:GLN:HG2	2.20	0.42
1:B:677:LEU:O	1:B:681:GLU:HG3	2.19	0.42
1:D:407:LEU:HA	1:D:441:LEU:HD21	2.01	0.42
1:D:539:VAL:HG23	1:D:663:THR:HG23	2.01	0.42
1:A:664:THR:C	1:A:665:ILE:HD12	2.44	0.42
1:B:242:PRO:CD	1:B:243:GLU:H	2.32	0.42
1:B:520:ASP:OD2	1:B:665:ILE:HG12	2.20	0.42
1:B:531:SER:CB	1:B:639:LYS:HD3	2.49	0.42
1:B:548:GLY:CA	2:B:801:ADP:H2	2.31	0.42
1:B:620:ASN:ND2	1:B:624:GLN:HE21	2.16	0.42
1:B:621:LEU:HD21	1:C:575:GLY:HA2	2.01	0.42
1:C:445:VAL:O	1:C:449:GLN:OE1	2.38	0.42
1:C:499:TYR:OH	1:C:565:ILE:HB	2.20	0.42
1:C:528:THR:O	1:C:639:LYS:HD3	2.19	0.42
1:C:682:LEU:N	1:C:682:LEU:HD23	2.34	0.42
1:C:688:ASP:HA	1:C:691:ARG:CZ	2.49	0.42
1:F:388:ARG:O	1:F:389:LEU:HD23	2.19	0.42
1:F:401:LYS:O	1:F:404:LEU:HB3	2.19	0.42
1:F:597:LEU:HA	1:F:639:LYS:O	2.19	0.42
1:A:219:GLY:O	1:A:220:ILE:HG13	2.20	0.42
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.89	0.42
1:A:706:GLY:O	1:A:709:LYS:HB3	2.20	0.42
1:B:593:TYR:OH	1:B:632:LYS:HG2	2.19	0.42
1:C:386:PRO:HG2	1:D:440:GLU:OE1	2.20	0.42
1:D:331:ASP:CA	1:D:379:ILE:HD11	2.50	0.42
1:E:607:ARG:HA	1:E:607:ARG:HD3	1.88	0.42
1:E:632:LYS:HB3	1:E:632:LYS:HE3	1.87	0.42
1:E:691:ARG:HA	1:E:694:ILE:HD12	2.02	0.42
1:F:721:ASP:O	1:F:725:ARG:HG3	2.19	0.42
1:B:347:HIS:O	1:B:350:VAL:HG22	2.20	0.42
1:C:349:THR:O	1:C:352:ASN:HB3	2.20	0.42
1:C:498:ASP:O	1:C:500:ALA:N	2.53	0.42
1:C:560:SER:HB2	1:C:562:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:ASP:HB3	1:C:607:ARG:HB3	2.02	0.42
1:D:304:LYS:HA	1:D:307:ALA:HB3	2.02	0.42
1:D:527:GLN:NE2	1:E:715:GLU:C	2.64	0.42
1:D:608:LEU:O	1:D:622:VAL:HG11	2.20	0.42
1:D:626:LEU:HD23	1:D:626:LEU:HA	1.72	0.42
1:E:612:VAL:CG2	1:E:613:PRO:HD2	2.49	0.42
1:A:222:GLY:C	1:A:224:ASP:N	2.78	0.42
1:A:377:ASP:OD2	1:A:378:LEU:HD23	2.20	0.42
1:B:395:ILE:HD12	1:B:395:ILE:N	2.34	0.42
1:B:662:SER:OG	1:C:712:MET:HE3	2.20	0.42
1:C:707:ILE:O	1:C:711:LEU:HG	2.19	0.42
1:D:236:ALA:HA	1:D:239:VAL:HG12	2.01	0.42
1:E:236:ALA:O	1:E:239:VAL:HG12	2.20	0.42
1:E:242:PRO:CD	1:E:243:GLU:H	2.31	0.42
1:F:221:GLY:N	1:F:406:ILE:HD13	2.35	0.42
1:A:255:GLY:C	1:A:389:LEU:HD13	2.44	0.42
1:B:324:ILE:HG12	1:B:368:LEU:HD11	2.01	0.42
1:B:388:ARG:O	1:B:389:LEU:HD23	2.20	0.42
1:B:502:TYR:CE2	1:B:567:ILE:HD13	2.54	0.42
1:C:603:ASP:HA	1:C:645:THR:OG1	2.20	0.42
1:D:388:ARG:O	1:D:389:LEU:HD23	2.20	0.42
1:E:547:SER:OG	1:E:549:LYS:HG2	2.19	0.42
1:F:232:ARG:O	1:F:236:ALA:HB3	2.20	0.42
1:F:284:VAL:O	1:F:326:ILE:HG12	2.19	0.42
1:F:589:PHE:CD2	1:F:629:LEU:HD13	2.43	0.42
1:F:653:GLN:CB	1:F:658:LEU:HD23	2.50	0.42
1:A:256:ILE:CG1	1:A:370:ILE:HG22	2.47	0.42
1:A:627:LEU:HD23	1:A:627:LEU:HA	1.94	0.42
1:B:323:HIS:HB2	1:B:367:ILE:HG22	2.02	0.42
1:B:398:PRO:HG2	1:B:434:LYS:O	2.19	0.42
1:B:712:MET:O	1:B:716:MET:HG3	2.19	0.42
1:E:319:ASN:HA	1:E:320:SER:HA	1.90	0.42
1:E:530:ASN:O	1:E:639:LYS:HE3	2.19	0.42
1:E:536:LEU:HD22	1:E:634:PRO:HD3	2.02	0.42
1:A:534:THR:HG23	1:B:715:GLU:HG3	2.01	0.41
1:E:260:GLY:HA3	1:E:266:LYS:HD3	2.01	0.41
1:E:270:ALA:HA	1:E:273:ILE:HG22	2.02	0.41
1:E:547:SER:N	2:E:801:ADP:O2B	2.53	0.41
1:A:254:LYS:O	1:A:368:LEU:HA	2.20	0.41
1:A:285:VAL:HG13	1:A:326:ILE:CD1	2.43	0.41
1:A:566:LYS:HD3	1:A:566:LYS:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LEU:O	1:A:725:ARG:NE	2.54	0.41
1:C:284:VAL:HB	1:C:325:ILE:HA	2.01	0.41
1:C:510:TRP:HB2	1:C:679:ALA:HB2	2.03	0.41
1:C:653:GLN:HA	1:C:658:LEU:HB3	2.02	0.41
1:D:560:SER:HB2	1:D:562:PHE:CE1	2.55	0.41
1:E:406:ILE:O	1:E:409:ILE:HG22	2.20	0.41
1:E:407:LEU:O	1:E:411:THR:OG1	2.30	0.41
1:E:510:TRP:HA	1:E:679:ALA:HA	2.01	0.41
1:E:593:TYR:CE1	1:E:632:LYS:NZ	2.88	0.41
1:F:324:ILE:HG12	1:F:368:LEU:HD11	2.01	0.41
1:F:451:THR:O	1:F:454:ASN:HB3	2.20	0.41
1:F:615:GLY:HA3	1:F:616:PRO:C	2.44	0.41
1:A:396:GLY:O	1:A:397:LEU:HB2	2.20	0.41
1:A:499:TYR:CE2	1:A:565:ILE:HB	2.55	0.41
1:B:268:LEU:HD12	1:B:269:LEU:N	2.35	0.41
1:D:620:ASN:OD1	1:E:617:ARG:NH1	2.53	0.41
1:D:659:ASN:HD21	1:E:545:PRO:HB3	1.85	0.41
1:D:710:LEU:HG	1:D:714:ILE:HD11	2.02	0.41
1:E:540:LEU:HD12	1:E:541:LEU:H	1.84	0.41
1:F:542:GLU:OE1	1:F:666:HIS:HB2	2.19	0.41
1:F:658:LEU:O	1:F:658:LEU:HD12	2.21	0.41
1:A:498:ASP:OD2	1:A:567:ILE:HD13	2.21	0.41
1:B:715:GLU:O	1:B:719:GLN:HG2	2.21	0.41
1:C:638:ARG:HG3	1:C:638:ARG:HH11	1.85	0.41
1:C:690:GLU:HB2	1:C:726:VAL:CG2	2.44	0.41
1:D:223:LEU:O	1:D:223:LEU:HD23	2.20	0.41
1:D:397:LEU:HD12	1:D:594:LYS:O	2.20	0.41
1:D:544:PRO:O	1:D:547:SER:HB3	2.21	0.41
1:E:219:GLY:C	1:E:220:ILE:HD12	2.46	0.41
1:E:324:ILE:HG12	1:E:368:LEU:HD11	2.01	0.41
1:E:682:LEU:HD23	1:E:682:LEU:HA	1.72	0.41
1:F:609:LEU:HD23	1:F:609:LEU:HA	1.86	0.41
1:A:407:LEU:O	1:A:411:THR:HG23	2.21	0.41
1:A:411:THR:CG2	1:A:426:ILE:HD11	2.50	0.41
1:C:331:ASP:CA	1:C:379:ILE:HD11	2.47	0.41
1:C:507:ILE:HG23	2:C:801:ADP:C6	2.56	0.41
1:C:687:LYS:HB2	1:C:690:GLU:OE1	2.21	0.41
1:D:231:PHE:O	1:D:235:PHE:HB2	2.20	0.41
1:E:440:GLU:OE2	1:E:492:PHE:HA	2.20	0.41
1:E:669:ASN:ND2	1:E:706:GLY:N	2.69	0.41
1:E:676:LEU:O	1:E:680:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:705:ILE:CG1	1:E:709:LYS:HG3	2.49	0.41
1:F:560:SER:HB2	1:F:562:PHE:CD1	2.54	0.41
1:A:219:GLY:C	1:A:220:ILE:HG13	2.45	0.41
1:A:236:ALA:HA	1:B:453:MET:HB3	2.03	0.41
1:A:560:SER:O	1:A:561:ASN:OD1	2.39	0.41
1:C:577:SER:O	1:C:578:GLU:C	2.64	0.41
1:E:257:LEU:HB2	1:E:389:LEU:HD13	2.02	0.41
1:F:502:TYR:HD2	1:F:503:ILE:HG13	1.85	0.41
1:F:508:ILE:CD1	1:F:510:TRP:CD1	3.02	0.41
1:F:525:VAL:CG1	1:F:560:SER:HB2	2.51	0.41
1:A:233:ARG:O	1:A:236:ALA:HB3	2.20	0.41
1:A:683:LEU:HD13	1:A:685:ASN:ND2	2.36	0.41
1:B:621:LEU:HD11	1:C:575:GLY:H	1.86	0.41
1:B:648:ARG:HG3	1:B:651:VAL:CG2	2.51	0.41
1:C:498:ASP:O	1:C:501:SER:N	2.45	0.41
1:C:595:SER:O	1:C:638:ARG:HD2	2.20	0.41
1:C:691:ARG:NH1	1:C:691:ARG:HB2	2.35	0.41
1:F:323:HIS:HB2	1:F:367:ILE:HG22	2.02	0.41
1:F:377:ASP:OD1	1:F:378:LEU:N	2.53	0.41
1:B:218:MET:HA	1:B:219:GLY:HA2	1.70	0.41
1:C:322:LEU:HD22	1:C:366:ASN:C	2.46	0.41
1:E:564:PHE:CB	1:E:595:SER:HB2	2.50	0.41
1:F:512:ASP:N	1:F:513:PRO:CD	2.84	0.41
1:A:219:GLY:O	1:A:272:GLN:HG2	2.21	0.41
1:A:262:PRO:CG	1:A:374:ASN:OD1	2.69	0.41
1:A:538:SER:O	1:A:662:SER:HB2	2.20	0.41
1:A:636:GLN:HA	1:A:637:GLY:HA2	1.49	0.41
1:A:693:THR:O	1:A:697:GLN:OE1	2.38	0.41
1:B:289:GLU:C	1:B:291:LEU:N	2.78	0.41
1:B:488:ILE:O	1:B:490:PRO:N	2.54	0.41
1:D:331:ASP:O	1:D:332:ALA:HB3	2.20	0.41
1:D:529:LYS:HD3	1:D:597:LEU:CD2	2.51	0.41
1:D:569:SER:HA	1:D:570:PRO:HD3	1.90	0.41
1:E:620:ASN:O	1:E:624:GLN:HG2	2.21	0.41
1:F:671:ALA:HA	1:F:703:VAL:O	2.21	0.41
1:A:284:VAL:O	1:A:326:ILE:HG13	2.21	0.41
1:A:564:PHE:HE1	1:A:566:LYS:HB2	1.83	0.41
1:A:676:LEU:HD23	1:A:698:VAL:HG11	2.03	0.41
1:B:242:PRO:HD2	1:B:243:GLU:N	2.34	0.41
1:D:309:ALA:HA	1:D:312:GLU:OE2	2.20	0.41
1:E:258:LEU:HB3	1:E:395:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:VAL:O	1:E:326:ILE:HG12	2.20	0.41
1:E:513:PRO:HA	1:E:516:ARG:CG	2.46	0.41
1:E:569:SER:HA	1:E:570:PRO:HD3	1.95	0.41
1:E:673:GLY:O	1:E:676:LEU:HB3	2.20	0.41
1:F:525:VAL:HG11	1:F:560:SER:HA	2.03	0.41
1:A:375:ARG:HA	1:A:376:PRO:HD2	1.97	0.40
1:B:516:ARG:O	1:B:520:ASP:HB2	2.22	0.40
1:C:242:PRO:HD2	1:C:243:GLU:N	2.36	0.40
1:C:411:THR:O	1:C:414:MET:HB2	2.20	0.40
1:C:626:LEU:HD23	1:C:626:LEU:HA	1.85	0.40
1:C:627:LEU:O	1:C:631:LYS:HG3	2.21	0.40
1:D:331:ASP:HA	1:D:379:ILE:CD1	2.51	0.40
1:E:323:HIS:HB2	1:E:367:ILE:HG22	2.02	0.40
1:F:542:GLU:C	1:F:666:HIS:HD1	2.27	0.40
1:A:215:PHE:N	1:A:231:PHE:CZ	2.89	0.40
1:A:259:TYR:HB2	1:A:373:THR:O	2.21	0.40
1:B:549:LYS:HB2	2:B:801:ADP:O1B	2.20	0.40
1:C:633:ALA:HA	1:C:634:PRO:HD3	1.90	0.40
1:D:278:ASN:O	1:D:279:ALA:C	2.63	0.40
1:E:532:ASP:OD2	1:E:533:ARG:HG2	2.20	0.40
1:E:721:ASP:HB2	1:E:724:TYR:HD2	1.87	0.40
1:F:562:PHE:H	1:F:565:ILE:HD11	1.87	0.40
1:A:549:LYS:HG3	1:A:550:THR:N	2.35	0.40
1:D:527:GLN:O	1:D:527:GLN:HG3	2.20	0.40
1:E:656:GLU:HG2	1:F:648:ARG:NH2	2.36	0.40
1:F:375:ARG:NH2	1:F:377:ASP:OD2	2.51	0.40
1:A:423:ASP:C	1:A:479:ASP:N	2.80	0.40
1:A:653:GLN:HB2	1:A:658:LEU:HD23	2.04	0.40
1:A:716:MET:HG2	1:A:732:LEU:CD1	2.52	0.40
1:B:326:ILE:HG22	1:B:370:ILE:CG1	2.51	0.40
1:B:534:THR:HA	1:B:535:PRO:HD3	1.98	0.40
1:C:709:LYS:HA	1:C:709:LYS:HD2	1.93	0.40
1:D:258:LEU:HD11	1:D:372:MET:HG2	2.04	0.40
1:E:513:PRO:O	1:E:516:ARG:HG2	2.22	0.40
1:F:544:PRO:HA	1:F:545:PRO:HD3	1.98	0.40
1:F:588:ILE:O	1:F:591:ASP:HB2	2.21	0.40
1:A:436:PHE:HA	1:A:440:GLU:OE2	2.22	0.40
1:B:531:SER:CA	1:B:639:LYS:HD3	2.52	0.40
1:C:620:ASN:O	1:C:624:GLN:HG2	2.21	0.40
1:C:675:GLN:O	1:C:678:GLU:HB3	2.21	0.40
1:C:677:LEU:HD21	1:C:695:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ASN:HA	1:D:320:SER:HA	1.86	0.40
1:D:549:LYS:HE2	2:D:801:ADP:O1B	2.22	0.40
1:D:562:PHE:CD2	1:D:597:LEU:HG	2.56	0.40
1:E:640:LEU:HG	1:E:642:ILE:CD1	2.51	0.40
1:E:641:LEU:HD12	1:E:641:LEU:O	2.22	0.40
1:E:643:ILE:N	1:E:643:ILE:HD12	2.36	0.40
1:E:698:VAL:O	1:E:701:LYS:HB2	2.22	0.40
1:F:309:ALA:HA	1:F:312:GLU:OE1	2.22	0.40
1:F:605:ILE:N	1:F:606:GLU:OE1	2.54	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	475/747 (64%)	443 (93%)	20 (4%)	12 (2%)	4 26
1	B	473/747 (63%)	429 (91%)	32 (7%)	12 (2%)	4 26
1	C	477/747 (64%)	450 (94%)	18 (4%)	9 (2%)	6 32
1	D	471/747 (63%)	439 (93%)	27 (6%)	5 (1%)	11 46
1	E	474/747 (64%)	441 (93%)	22 (5%)	11 (2%)	5 28
1	F	465/747 (62%)	428 (92%)	26 (6%)	11 (2%)	4 27
All	All	2835/4482 (63%)	2630 (93%)	145 (5%)	60 (2%)	8 30

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	293	LYS
1	A	294	TYR

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Mol	Chain	Res	Type
1	A	318	ALA
1	A	320	SER
1	A	333	ILE
1	B	283	LYS
1	B	297	GLU
1	B	318	ALA
1	B	439	ALA
1	B	489	LYS
1	C	297	GLU
1	C	318	ALA
1	C	498	ASP
1	C	578	GLU
1	D	283	LYS
1	D	318	ALA
1	D	489	LYS
1	E	283	LYS
1	E	297	GLU
1	E	318	ALA
1	E	439	ALA
1	E	489	LYS
1	F	283	LYS
1	F	297	GLU
1	F	318	ALA
1	F	397	LEU
1	F	439	ALA
1	F	489	LYS
1	A	264	CYS
1	A	397	LEU
1	C	293	LYS
1	C	499	TYR
1	E	507	ILE
1	A	241	PRO
1	B	241	PRO
1	B	293	LYS
1	B	502	TYR
1	C	241	PRO
1	C	610	ASP
1	D	293	LYS
1	E	241	PRO
1	E	293	LYS
1	F	241	PRO
1	F	293	LYS

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Mol	Chain	Res	Type
1	A	242	PRO
1	F	398	PRO
1	B	490	PRO
1	B	546	HIS
1	D	241	PRO
1	E	438	GLY
1	B	438	GLY
1	E	490	PRO
1	F	438	GLY
1	A	398	PRO
1	B	668	PRO
1	E	668	PRO
1	F	684	GLY
1	C	490	PRO
1	A	668	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/638 (54%)	323 (94%)	21 (6%)	17	38
1	B	349/638 (55%)	334 (96%)	15 (4%)	26	47
1	C	347/638 (54%)	324 (93%)	23 (7%)	15	37
1	D	340/638 (53%)	327 (96%)	13 (4%)	29	50
1	E	345/638 (54%)	321 (93%)	24 (7%)	14	35
1	F	345/638 (54%)	328 (95%)	17 (5%)	22	43
All	All	2070/3828 (54%)	1957 (94%)	113 (6%)	21	41

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	GLU
1	A	253	VAL
1	A	284	VAL

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Mol	Chain	Res	Type
1	A	322	LEU
1	A	326	ILE
1	A	367	ILE
1	A	375	ARG
1	A	395	ILE
1	A	409	ILE
1	A	445	VAL
1	A	537	VAL
1	A	539	VAL
1	A	566	LYS
1	A	573	MET
1	A	581	LYS
1	A	586	LYS
1	A	631	LYS
1	A	651	VAL
1	A	658	LEU
1	A	677	LEU
1	A	690	GLU
1	B	246	GLU
1	B	284	VAL
1	B	285	VAL
1	B	305	LEU
1	B	322	LEU
1	B	325	ILE
1	B	351	VAL
1	B	381	GLU
1	B	389	LEU
1	B	508	ILE
1	B	567	ILE
1	B	623	LEU
1	B	626	LEU
1	B	651	VAL
1	B	659	ASN
1	C	246	GLU
1	C	256	ILE
1	C	268	LEU
1	C	273	ILE
1	C	305	LEU
1	C	312	GLU
1	C	316	LEU
1	C	322	LEU
1	C	324	ILE

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Mol	Chain	Res	Type
1	C	326	ILE
1	C	367	ILE
1	C	457	ILE
1	C	541	LEU
1	C	573	MET
1	C	587	LYS
1	C	602	VAL
1	C	609	LEU
1	C	623	LEU
1	C	632	LYS
1	C	651	VAL
1	C	682	LEU
1	C	691	ARG
1	C	711	LEU
1	D	246	GLU
1	D	273	ILE
1	D	284	VAL
1	D	305	LEU
1	D	311	GLU
1	D	389	LEU
1	D	407	LEU
1	D	424	VAL
1	D	602	VAL
1	D	614	ILE
1	D	645	THR
1	D	681	GLU
1	D	716	MET
1	E	246	GLU
1	E	284	VAL
1	E	285	VAL
1	E	305	LEU
1	E	322	LEU
1	E	325	ILE
1	E	351	VAL
1	E	381	GLU
1	E	389	LEU
1	E	400	GLU
1	E	508	ILE
1	E	522	GLU
1	E	537	VAL
1	E	539	VAL
1	E	540	LEU

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Mol	Chain	Res	Type
1	E	586	LYS
1	E	588	ILE
1	E	602	VAL
1	E	626	LEU
1	E	643	ILE
1	E	658	LEU
1	E	665	ILE
1	E	689	LYS
1	E	693	THR
1	F	246	GLU
1	F	284	VAL
1	F	285	VAL
1	F	305	LEU
1	F	322	LEU
1	F	325	ILE
1	F	330	ILE
1	F	351	VAL
1	F	381	GLU
1	F	389	LEU
1	F	519	ASP
1	F	536	LEU
1	F	537	VAL
1	F	578	GLU
1	F	606	GLU
1	F	614	ILE
1	F	651	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	408	HIS
1	A	418	GLN
1	A	530	ASN
1	A	583	GLN
1	A	596	GLN
1	A	659	ASN
1	A	666	HIS
1	A	685	ASN
1	B	374	ASN
1	B	405	GLN
1	B	418	GLN

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Mol	Chain	Res	Type
1	B	526	GLN
1	B	546	HIS
1	B	620	ASN
1	C	319	ASN
1	C	352	ASN
1	C	405	GLN
1	C	418	GLN
1	C	675	GLN
1	C	685	ASN
1	D	313	GLN
1	D	319	ASN
1	D	352	ASN
1	D	449	GLN
1	D	527	GLN
1	D	596	GLN
1	E	405	GLN
1	E	418	GLN
1	F	286	ASN
1	F	405	GLN
1	F	418	GLN
1	F	546	HIS
1	F	624	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	E	801	-	28,29,29	1.89	5 (17%)	43,45,45	2.11	13 (30%)
2	ADP	C	801	-	28,29,29	1.81	6 (21%)	43,45,45	2.23	16 (37%)
2	ADP	D	801	-	28,29,29	1.44	5 (17%)	43,45,45	2.64	13 (30%)
2	ADP	B	801	-	28,29,29	1.57	5 (17%)	43,45,45	2.11	11 (25%)

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	ADP	E	801	-	-	4/16/32/32	0/3/3/3
2	ADP	C	801	-	-	2/16/32/32	0/3/3/3
2	ADP	D	801	-	-	4/16/32/32	0/3/3/3
2	ADP	B	801	-	-	7/16/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ADP	C5-C4	6.22	1.50	1.39
2	E	801	ADP	C5-C4	5.44	1.48	1.39
2	E	801	ADP	PA-O3A	5.37	1.65	1.59
2	B	801	ADP	C5-C4	4.62	1.47	1.39
2	D	801	ADP	C5-C4	4.00	1.46	1.39
2	B	801	ADP	PA-O3A	3.63	1.63	1.59
2	C	801	ADP	C5-C6	3.52	1.50	1.41
2	C	801	ADP	C8-N7	3.46	1.38	1.31
2	B	801	ADP	C5-C6	3.22	1.50	1.41
2	D	801	ADP	C8-N7	3.14	1.37	1.31
2	D	801	ADP	C5-C6	2.89	1.49	1.41
2	E	801	ADP	C5-C6	2.89	1.49	1.41
2	D	801	ADP	PA-O3A	2.71	1.62	1.59
2	C	801	ADP	PA-O3A	2.56	1.62	1.59
2	C	801	ADP	C4-N9	-2.54	1.32	1.37
2	B	801	ADP	C5-N7	-2.43	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	ADP	C5-N7	-2.42	1.34	1.39
2	C	801	ADP	C1'-N9	2.22	1.52	1.46
2	D	801	ADP	C5-N7	-2.14	1.35	1.39
2	E	801	ADP	C8-N7	2.12	1.35	1.31
2	B	801	ADP	C8-N7	2.07	1.35	1.31

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	801	ADP	C5-C4-N3	-6.69	117.50	126.72
2	D	801	ADP	C5-C4-N3	-6.49	117.78	126.72
2	B	801	ADP	C5-C4-N3	-6.49	117.78	126.72
2	D	801	ADP	N3-C2-N1	-5.73	119.91	128.58
2	D	801	ADP	C4-N9-C8	5.65	111.67	105.74
2	C	801	ADP	C5-C4-N3	-5.59	119.02	126.72
2	D	801	ADP	N3-C4-N9	5.57	136.63	127.17
2	D	801	ADP	N9-C8-N7	-5.45	106.21	113.94
2	E	801	ADP	N3-C4-N9	5.40	136.36	127.17
2	B	801	ADP	C4-C5-N7	-5.37	104.45	110.58
2	D	801	ADP	C2-N3-C4	5.05	124.17	111.83
2	D	801	ADP	C5-N7-C8	4.60	110.67	103.45
2	B	801	ADP	N3-C4-N9	4.46	134.76	127.17
2	D	801	ADP	C4-C5-N7	-4.20	105.78	110.58
2	B	801	ADP	C5-N7-C8	4.18	110.02	103.45
2	C	801	ADP	C2-N3-C4	4.12	121.89	111.83
2	C	801	ADP	C1'-N9-C8	4.11	136.22	127.09
2	C	801	ADP	C5-C4-N9	4.09	110.27	105.81
2	C	801	ADP	C3'-C2'-C1'	4.04	109.11	101.46
2	B	801	ADP	C2-N3-C4	3.68	120.81	111.83
2	C	801	ADP	C4-C5-N7	-3.67	106.39	110.58
2	C	801	ADP	C6-C5-N7	3.59	139.01	132.09
2	E	801	ADP	C4-C5-N7	-3.55	106.53	110.58
2	C	801	ADP	N3-C2-N1	-3.54	123.23	128.58
2	E	801	ADP	C2-N3-C4	3.41	120.17	111.83
2	B	801	ADP	C6-C5-N7	3.20	138.26	132.09
2	B	801	ADP	N9-C8-N7	-3.09	109.55	113.94
2	D	801	ADP	C3'-C2'-C1'	3.02	107.17	101.46
2	E	801	ADP	C2'-C3'-C4'	2.94	108.30	102.61
2	D	801	ADP	C6-C5-N7	2.92	137.72	132.09
2	E	801	ADP	C2'-C1'-N9	2.86	120.42	113.30
2	E	801	ADP	N6-C6-N1	2.85	124.72	118.38
2	C	801	ADP	C4-N9-C8	-2.82	102.77	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	ADP	N9-C8-N7	2.79	117.89	113.94
2	D	801	ADP	C2'-C1'-N9	-2.75	106.48	113.30
2	E	801	ADP	O4'-C4'-C5'	2.67	117.88	109.33
2	B	801	ADP	C4-N9-C8	2.63	108.50	105.74
2	E	801	ADP	O4'-C1'-N9	-2.60	103.10	108.09
2	B	801	ADP	C3'-C2'-C1'	2.49	106.18	101.46
2	C	801	ADP	C4-N9-C1'	-2.48	120.83	126.63
2	D	801	ADP	C2-N1-C6	2.47	122.78	118.73
2	E	801	ADP	C1'-N9-C8	-2.45	121.66	127.09
2	E	801	ADP	C5-C6-N6	-2.44	117.25	123.29
2	B	801	ADP	O5'-C5'-C4'	2.41	117.21	108.99
2	C	801	ADP	C2-N1-C6	2.40	122.67	118.73
2	E	801	ADP	C5-N7-C8	2.36	107.16	103.45
2	C	801	ADP	O2'-C2'-C3'	-2.24	104.64	111.82
2	E	801	ADP	O5'-C5'-C4'	2.19	116.45	108.99
2	C	801	ADP	N3-C4-N9	2.08	130.71	127.17
2	B	801	ADP	N3-C2-N1	-2.06	125.47	128.58
2	C	801	ADP	C2'-C1'-N9	2.06	118.42	113.30
2	D	801	ADP	O2A-PA-O5'	-2.04	98.30	107.57
2	C	801	ADP	C4'-O4'-C1'	2.03	113.94	109.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ADP	C5'-O5'-PA-O1A
2	B	801	ADP	C5'-O5'-PA-O3A
2	E	801	ADP	C5'-O5'-PA-O2A
2	E	801	ADP	C5'-O5'-PA-O3A
2	B	801	ADP	O4'-C4'-C5'-O5'
2	B	801	ADP	C3'-C4'-C5'-O5'
2	B	801	ADP	O4'-C1'-N9-C4
2	B	801	ADP	O4'-C1'-N9-C8
2	B	801	ADP	C5'-O5'-PA-O2A
2	D	801	ADP	C5'-O5'-PA-O1A
2	D	801	ADP	O4'-C4'-C5'-O5'
2	C	801	ADP	O4'-C1'-N9-C4
2	C	801	ADP	O4'-C1'-N9-C8
2	E	801	ADP	O4'-C1'-N9-C4
2	D	801	ADP	O4'-C1'-N9-C8
2	E	801	ADP	O4'-C1'-N9-C8
2	D	801	ADP	C3'-C4'-C5'-O5'

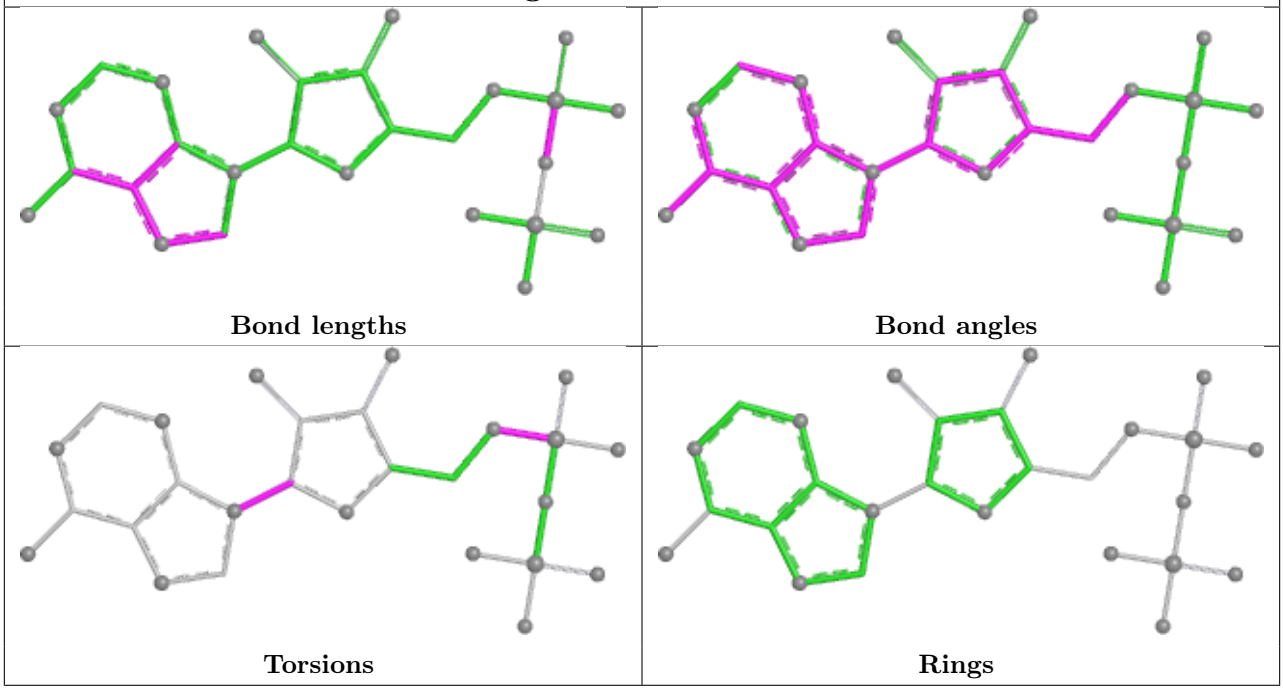
There are no ring outliers.

4 monomers are involved in 39 short contacts:

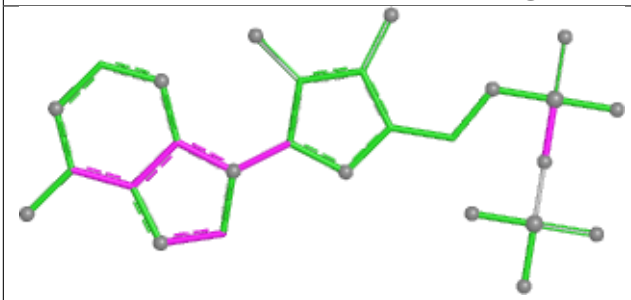
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	ADP	9	0
2	C	801	ADP	8	0
2	D	801	ADP	11	0
2	B	801	ADP	11	0

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.

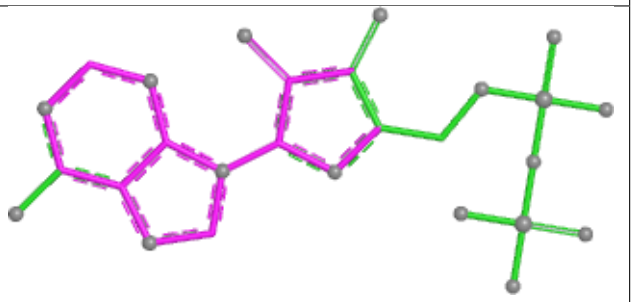
Ligand ADP E 801



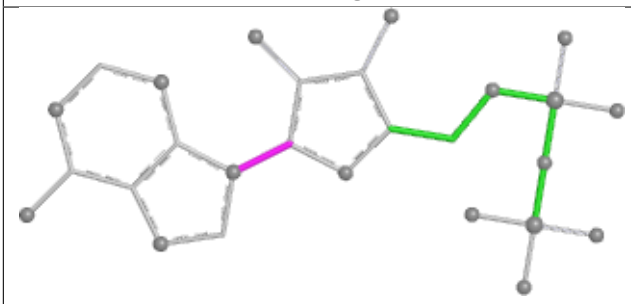
Ligand ADP C 801



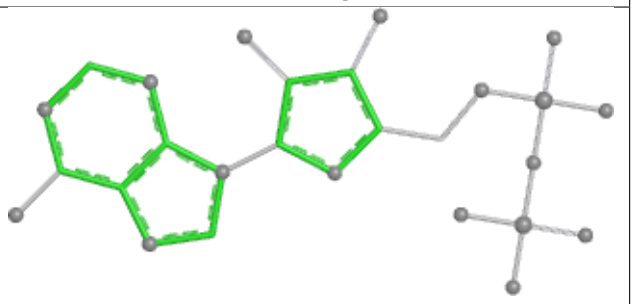
Bond lengths



Bond angles

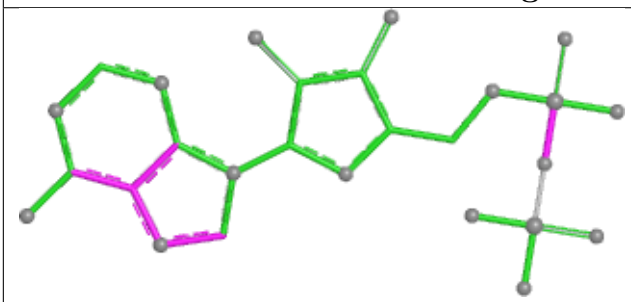


Torsions

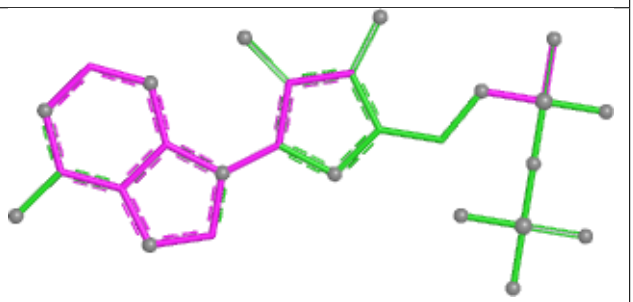


Rings

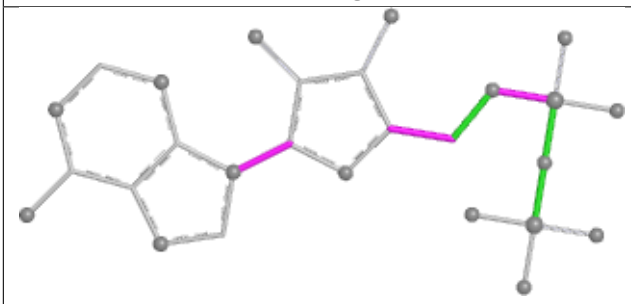
Ligand ADP D 801



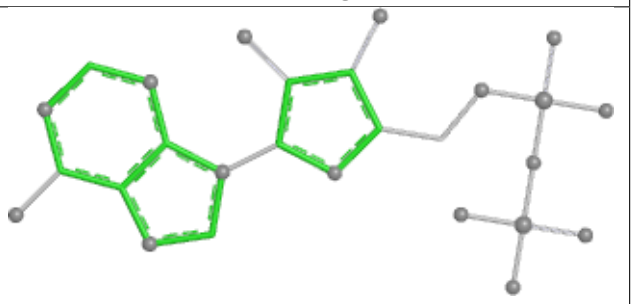
Bond lengths



Bond angles

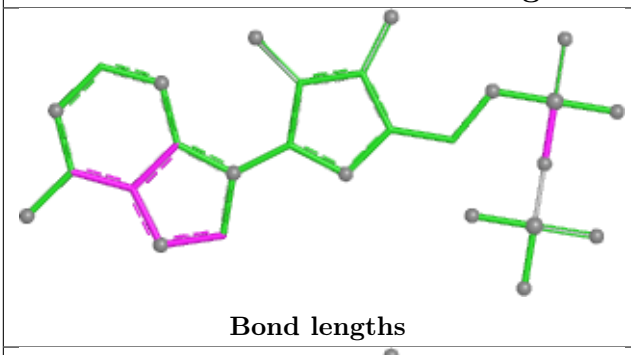


Torsions

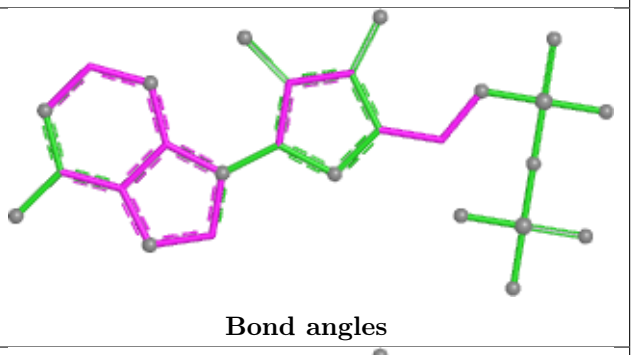


Rings

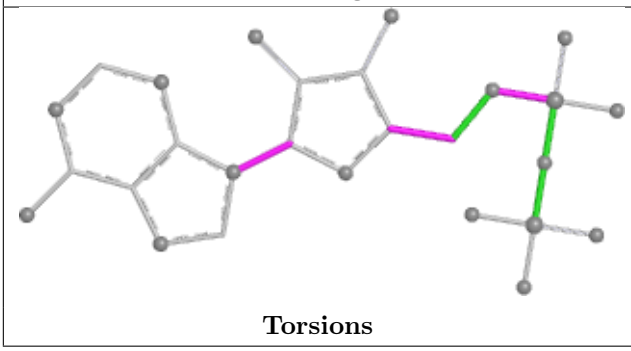
Ligand ADP B 801



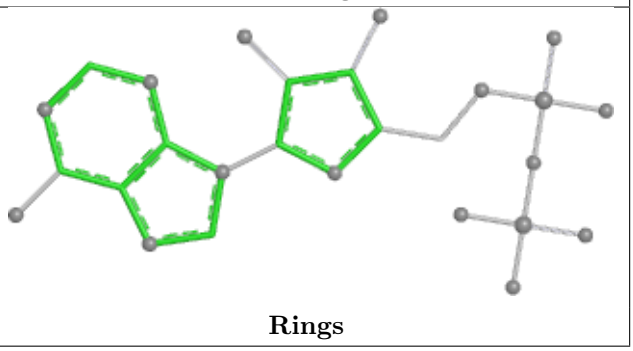
Bond lengths



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.

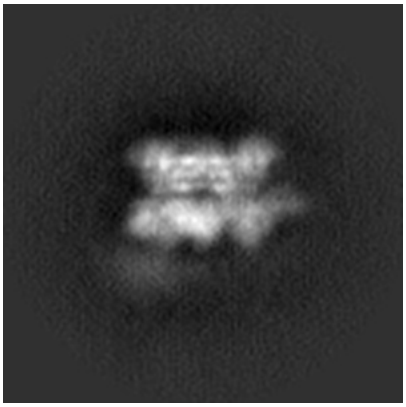
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6205. These allow visual inspection of the internal detail of the map and identification of artifacts.

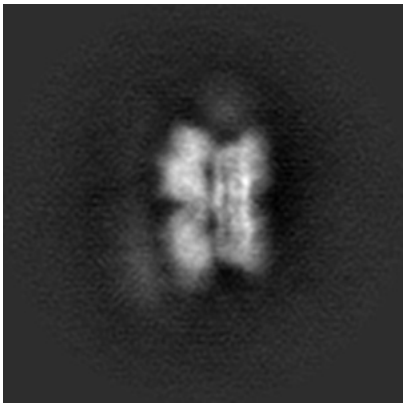
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

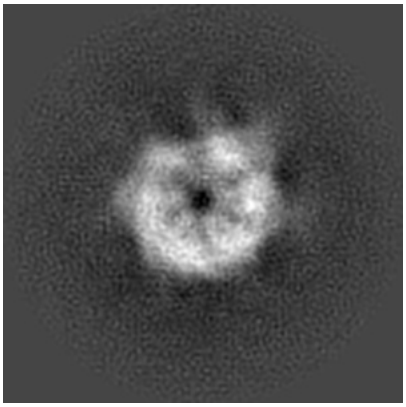
6.1.1 Primary map



X



Y

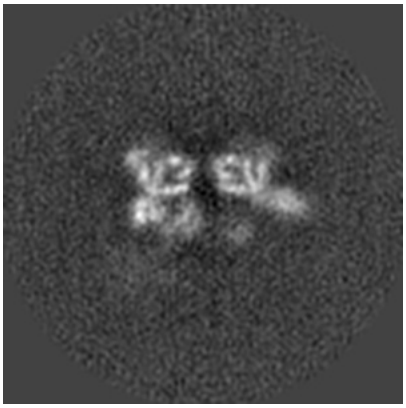


Z

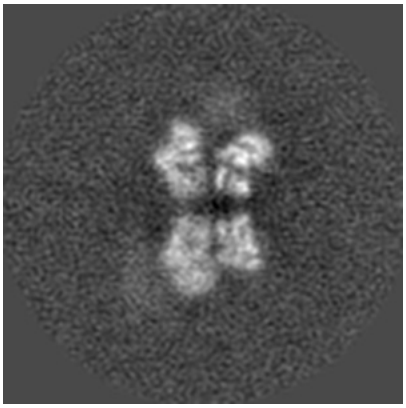
The images above show the map projected in three orthogonal directions.

6.2 Central slices

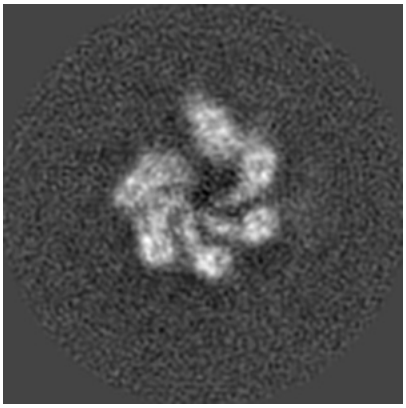
6.2.1 Primary map



X Index: 64



Y Index: 64

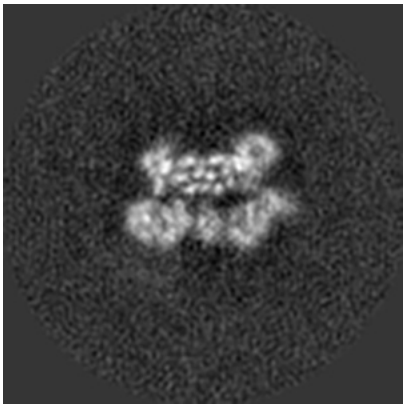


Z Index: 64

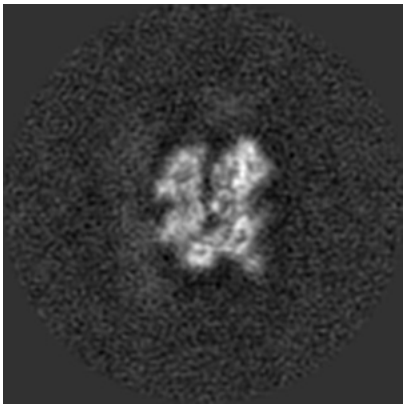
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

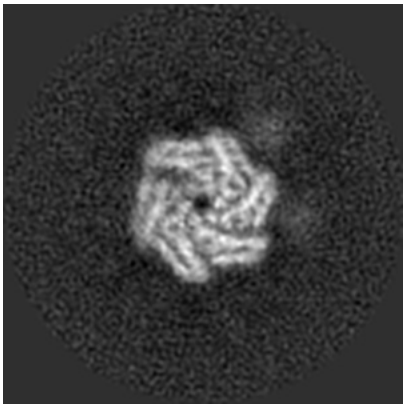
6.3.1 Primary map



X Index: 71



Y Index: 51

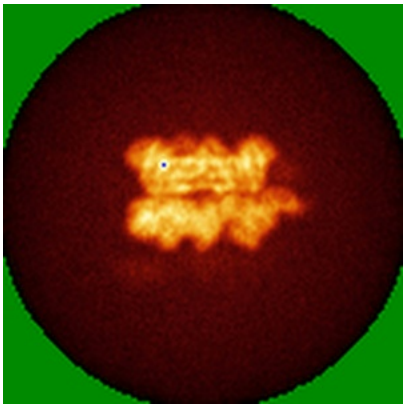


Z Index: 77

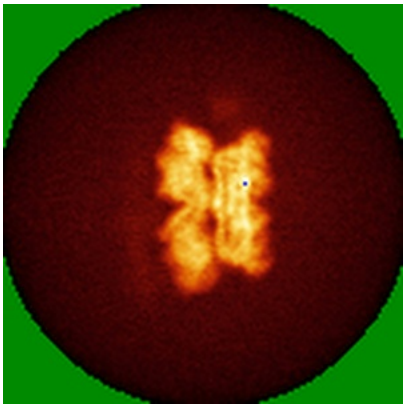
The images above show the largest variance slices of the map in three orthogonal directions.

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

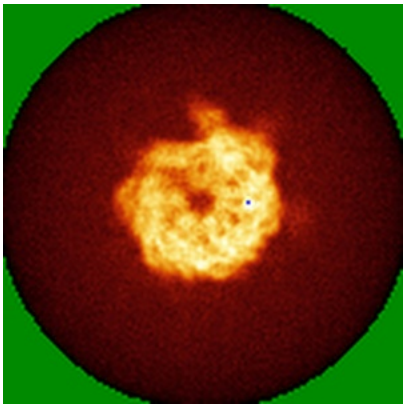
6.4.1 Primary map



X



Y

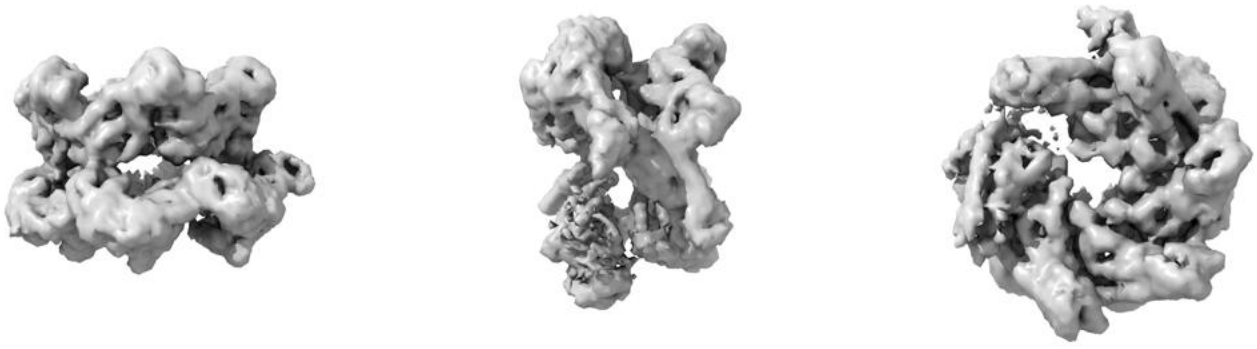


Z

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 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

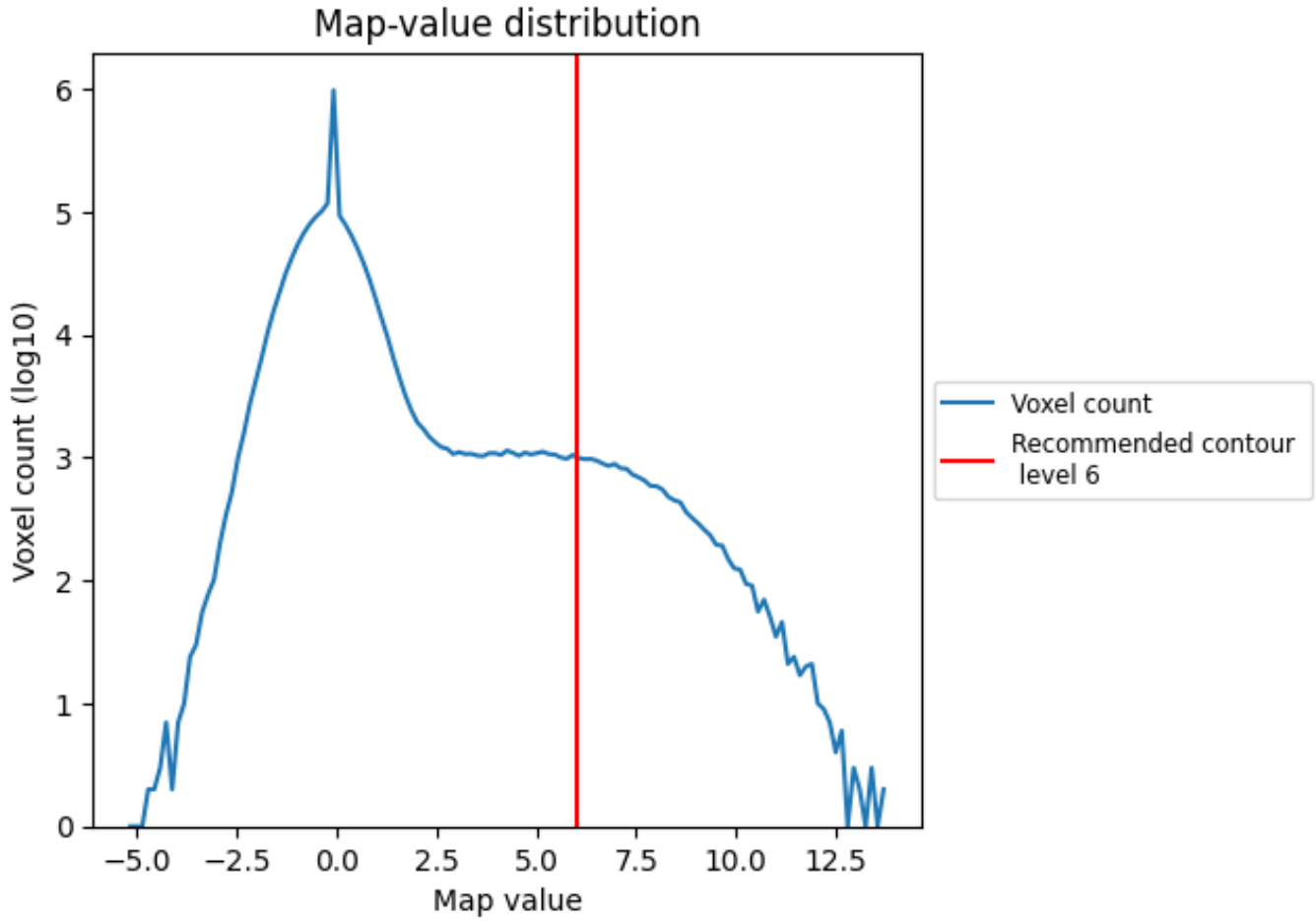
6.6 Mask visualisation (i)

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

7 Map analysis

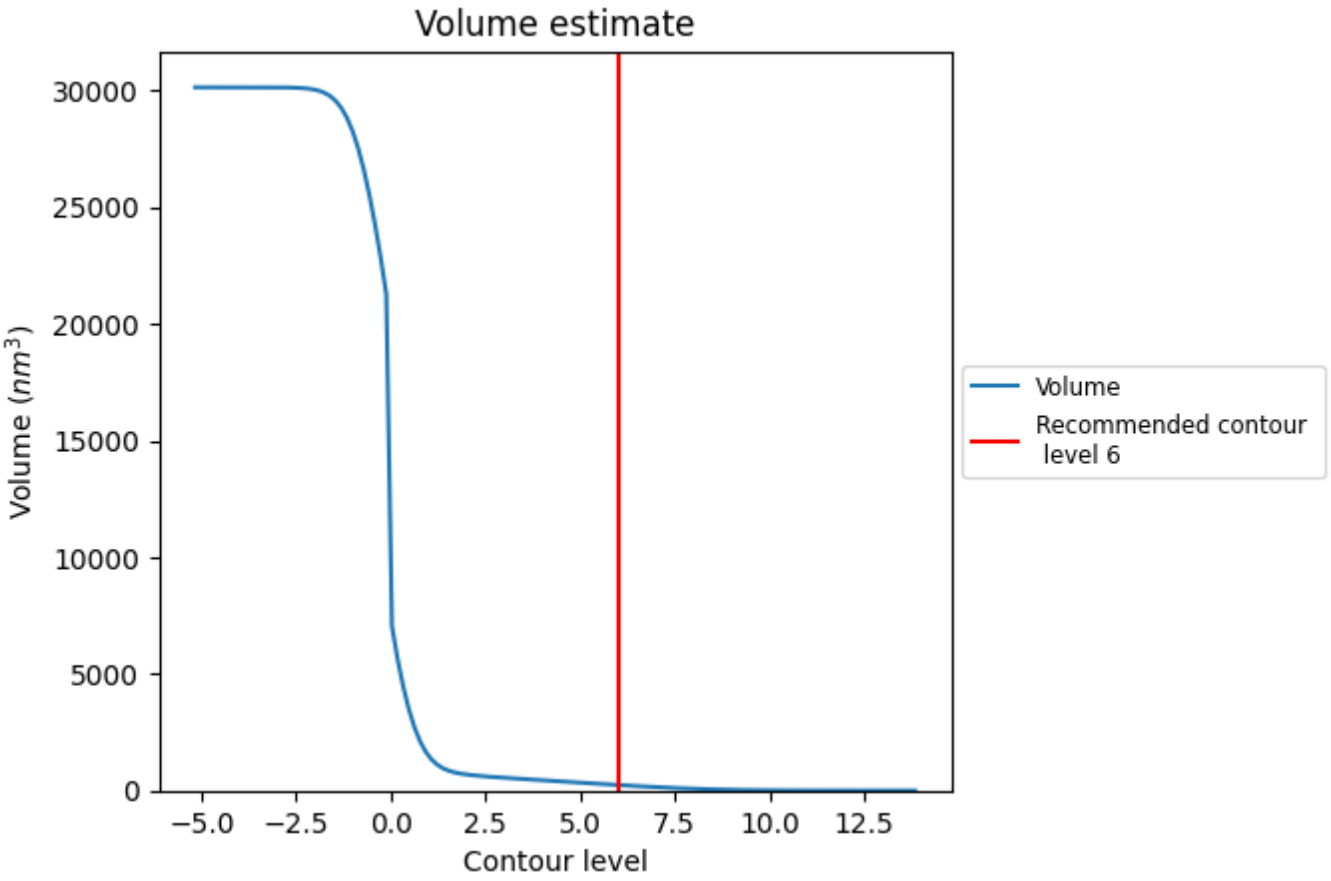
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

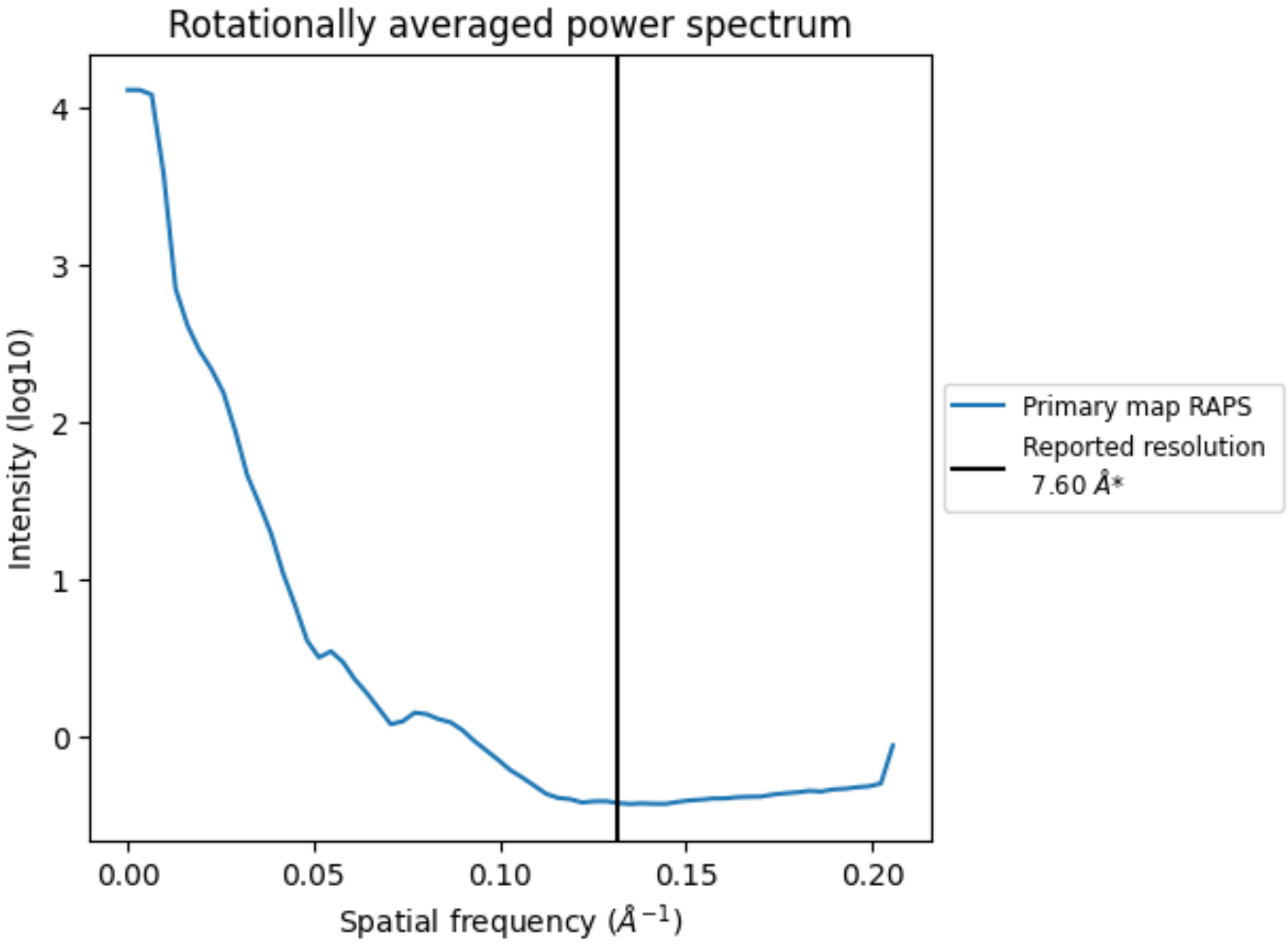
7.2 Volume estimate



The volume at the recommended contour level is 239 nm^3; this corresponds to an approximate mass of 216 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 0.132 $Å^{-1}$

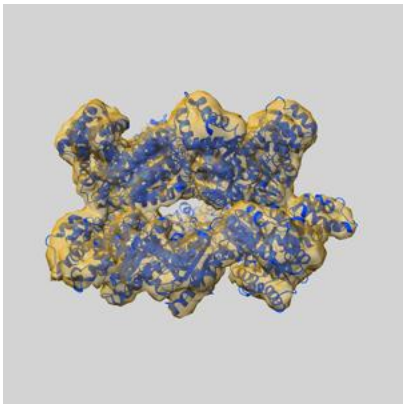
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

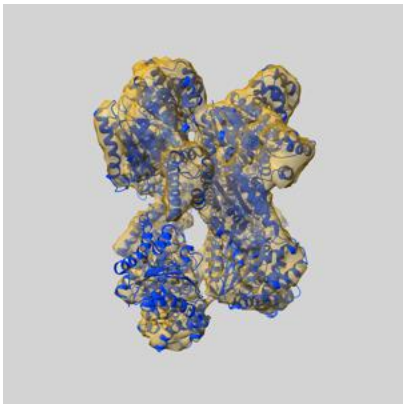
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6205 and PDB model 3J95. Per-residue inclusion information can be found in section 3 on page 6.

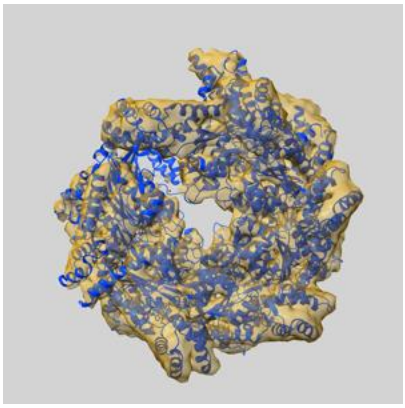
9.1 Map-model overlay



X



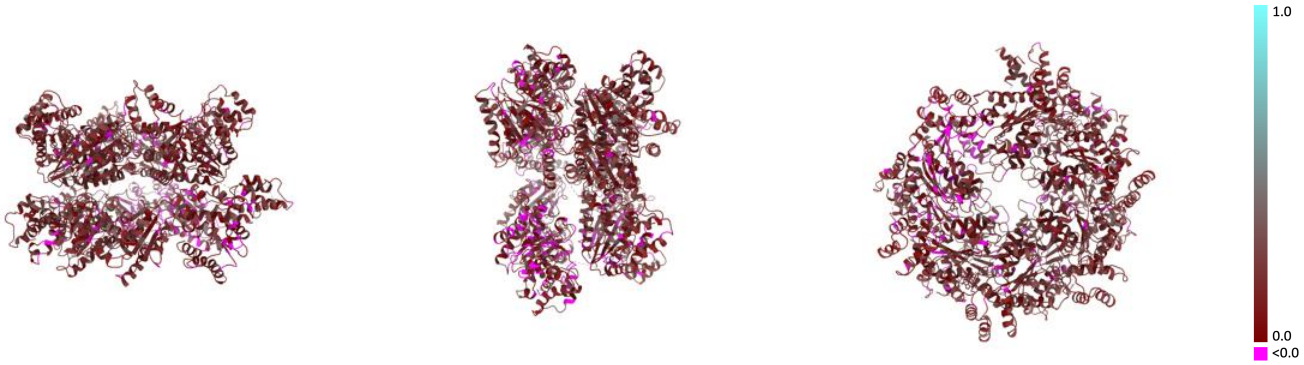
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

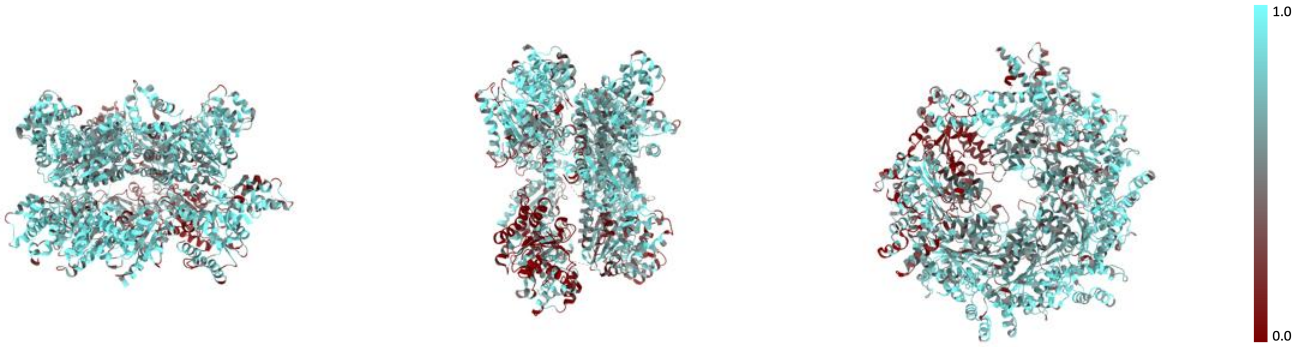
9.2 Q-score mapped to coordinate model (i)



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.

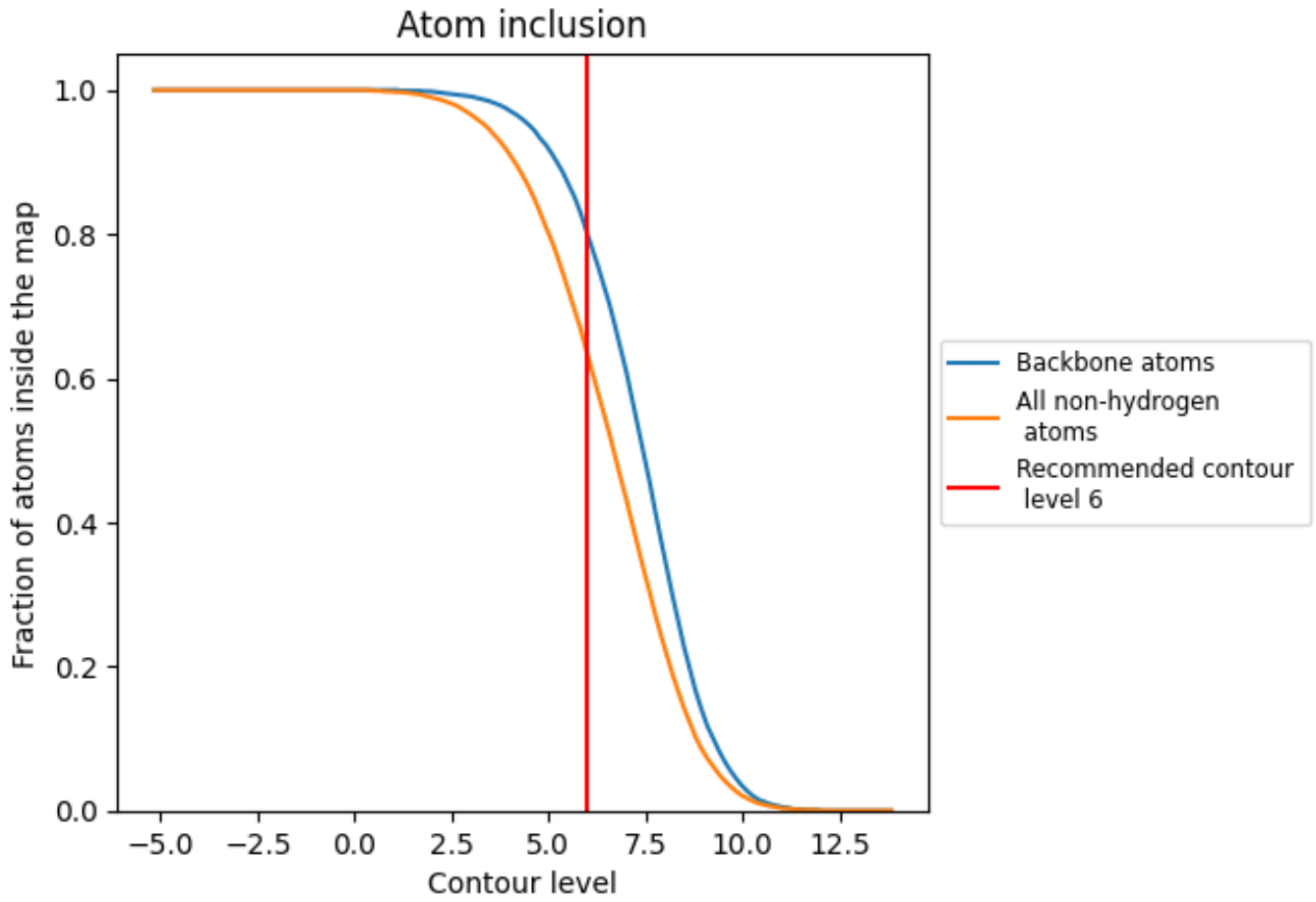
9.3 Atom inclusion mapped to coordinate model (i)



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 (6).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 63% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6340	0.1590
A	0.6410	0.1540
B	0.6920	0.1590
C	0.7250	0.1840
D	0.7220	0.1800
E	0.6600	0.1560
F	0.3590	0.1170