Full wwPDB EM Validation Report

Nov 19, 2022 – 09:26 PM EST

PDB ID	:	1Q5A
EMDB ID	:	EMD-1052
Title	:	S-shaped trans interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors	:	He, W.; Cowin, P.; Stokes, D.L.
Deposited on	:	2003-08-06
Resolution	:	30.00 Å(reported)
Based on initial model	:	1L3W

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

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

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

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

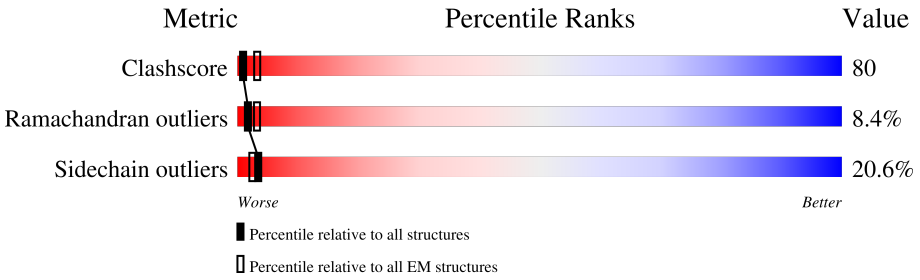
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance

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

The reported resolution of this entry is 30.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	880	61% 17% 30% 10% · 39%
1	B	880	61% 16% 30% 11% · 39%

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	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	902	X	-	X	-
2	NAG	A	903	X	-	-	-
2	NAG	A	904	-	-	X	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	902	X	-	X	-
2	NAG	B	903	X	-	-	-
2	NAG	B	904	-	-	X	-
3	NDG	A	811	-	-	X	-
3	NDG	B	811	-	-	X	-

2 Entry composition (i)

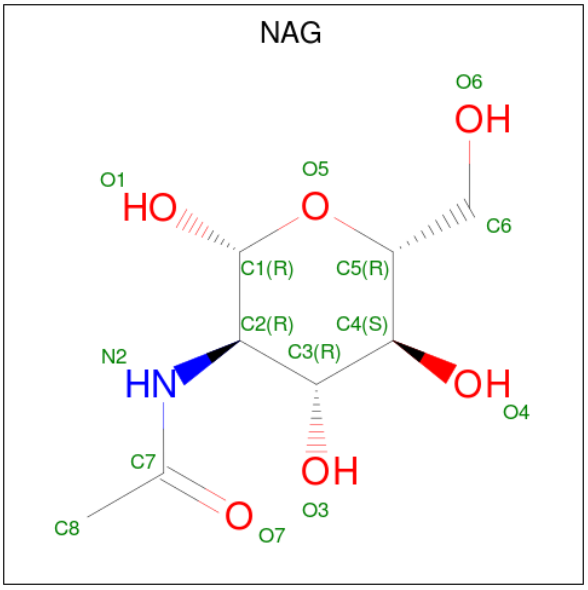
There are 4 unique types of molecules in this entry. The entry contains 8826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EP-cadherin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total 4191	C 2635	N 695	O 850	S 11	0	0
1	B	540	Total 4191	C 2635	N 695	O 850	S 11	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0
2	A	1	Total 182	C 104	N 13	O 65	0

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	A	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0
2	B	1	Total C N O 182 104 13 65	0

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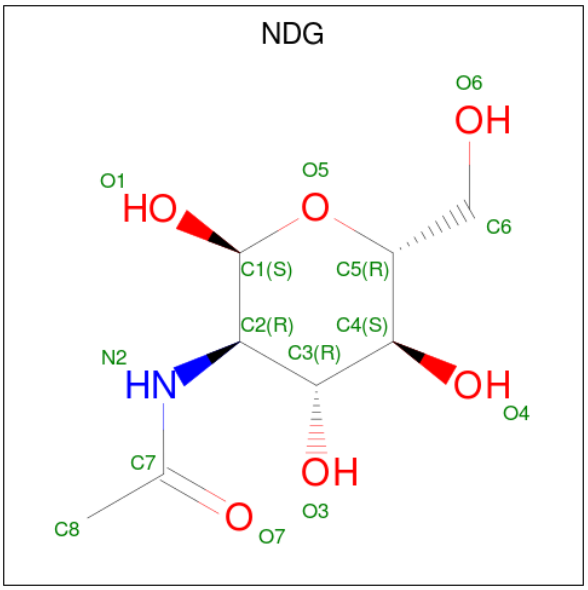
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			182	104	13	65	

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			28	16	2	10	
3	A	1	Total	C	N	O	0
			28	16	2	10	
3	B	1	Total	C	N	O	0
			28	16	2	10	
3	B	1	Total	C	N	O	0
			28	16	2	10	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

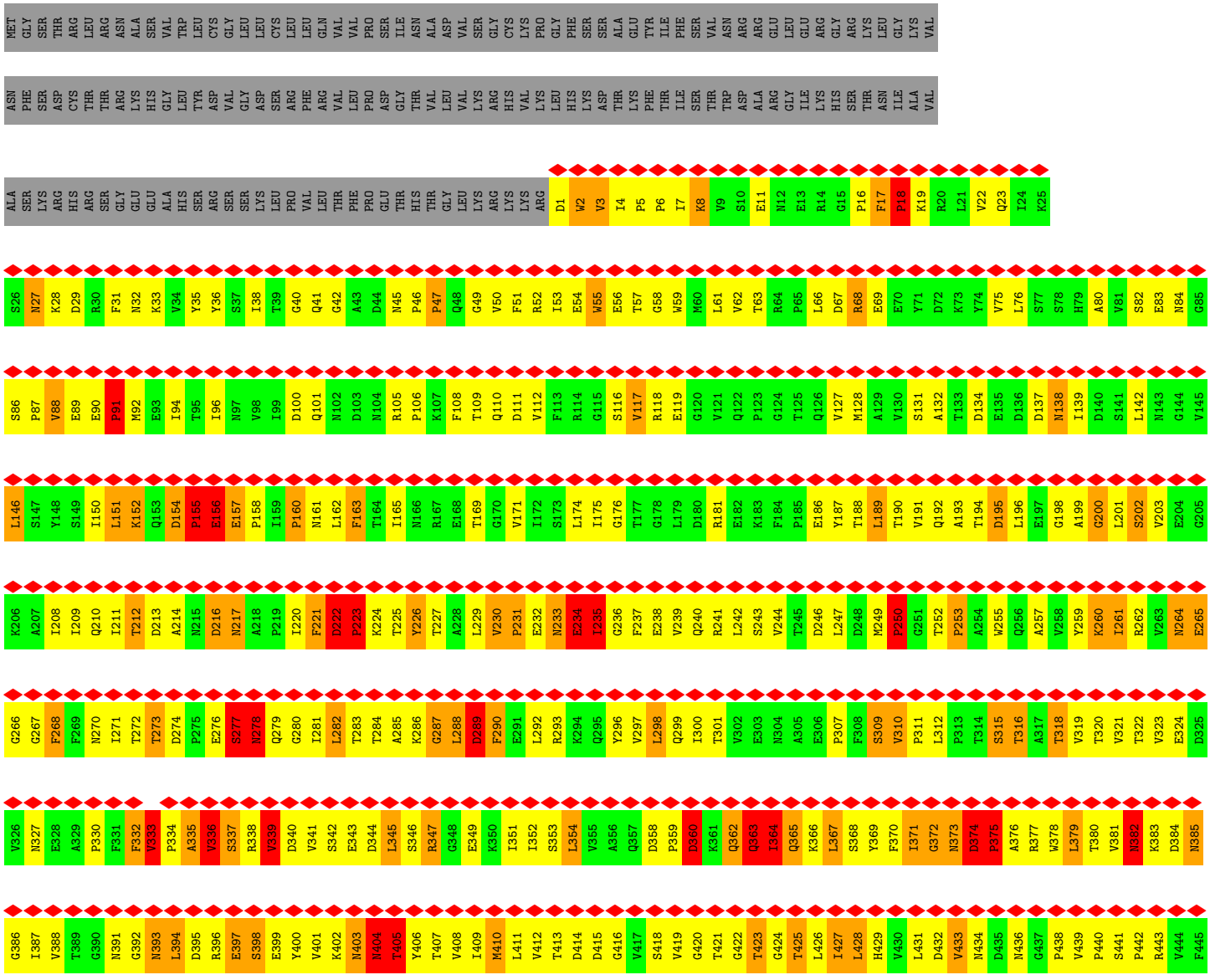
Mol	Chain	Residues	Atoms		AltConf
4	A	12	Total	Ca	0
			12	12	
4	B	12	Total	Ca	0
			12	12	

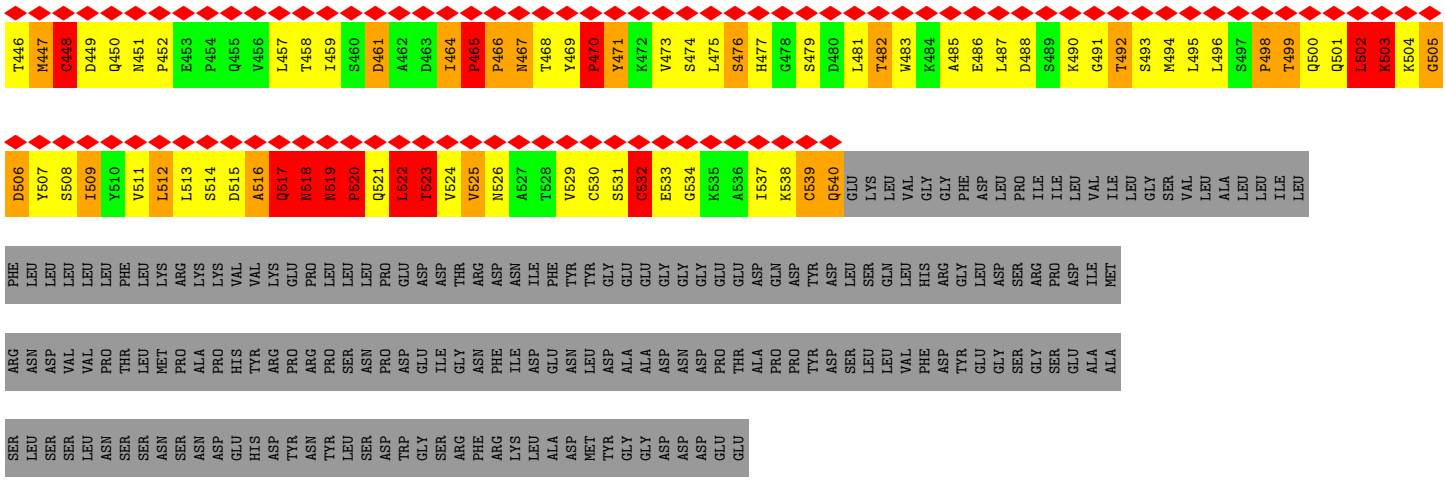
3 Residue-property plots (i)

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: EP-cadherin

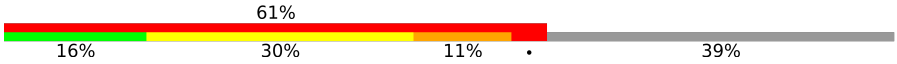
Chain A:

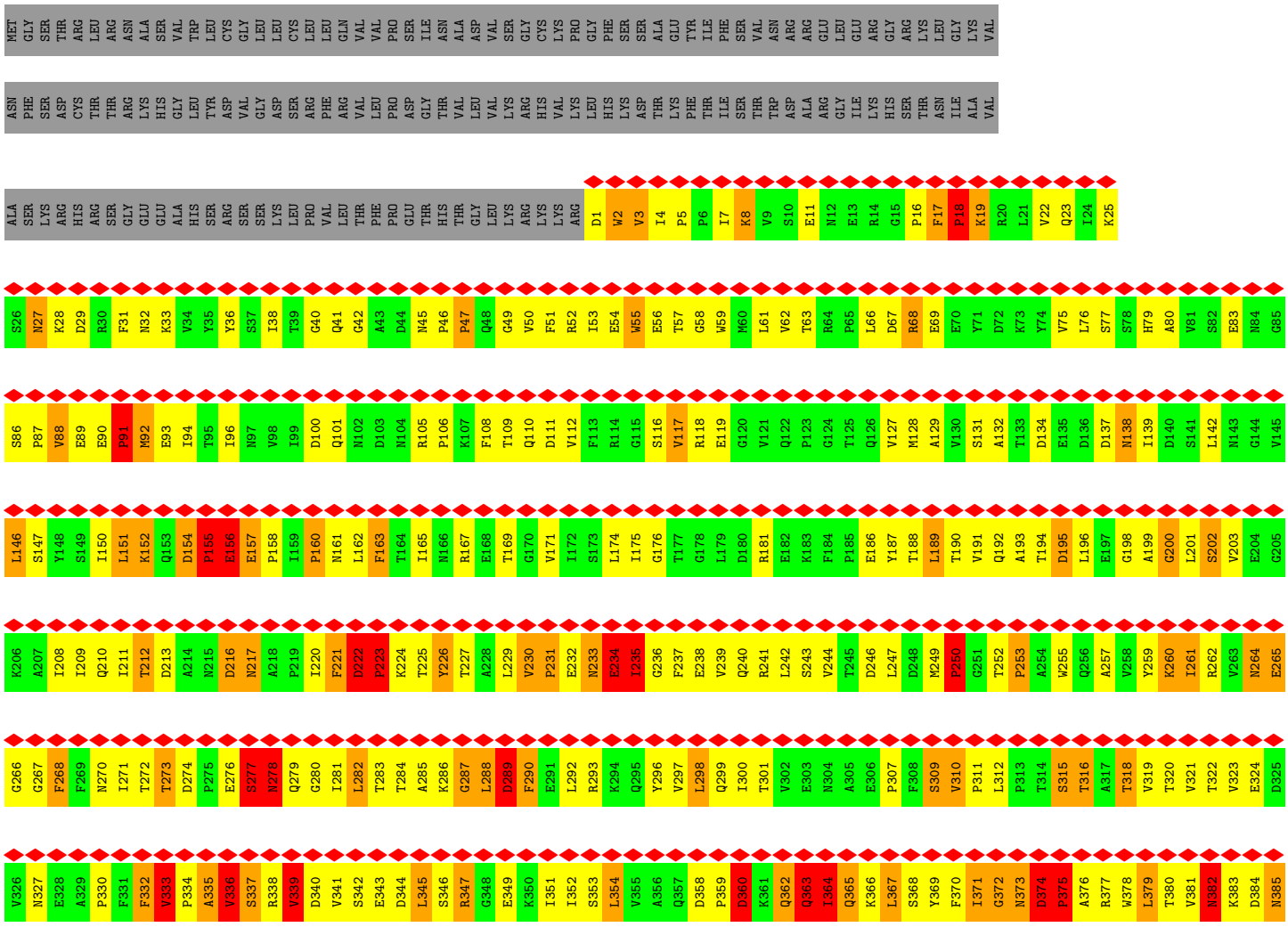


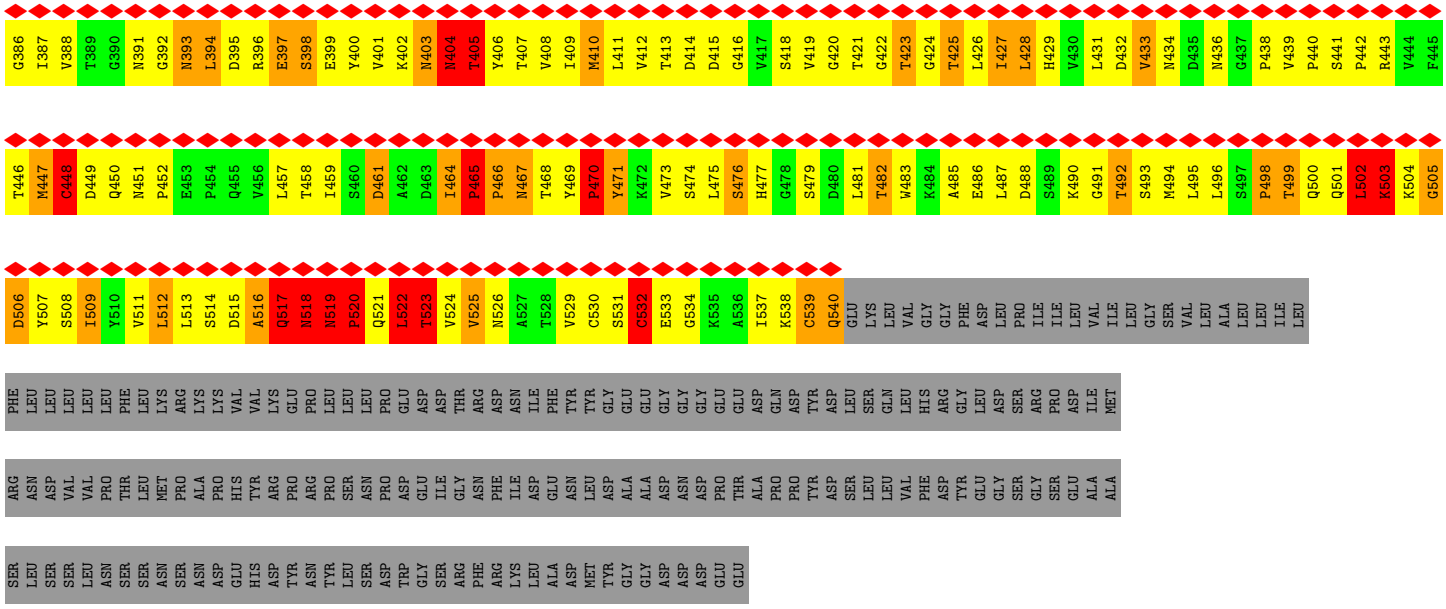


- Molecule 1: EP-cadherin

Chain B:






G386 I387 V388 T389 G390 N391 G392 N393 L394 D395 R396 E397 S398 E399 Y400 V401 K402 N403 N404 T405 Y406 T407 V408 I409 M410 L411 V412 T413 D414 D415 G416 V417 S418 V419 G420 T421 G422 T423 G424 T425 L426 I427 L428 H429 V430 L431 D432 V433 N434 D435 N436 G437 P438 V439 P440 S441 P442 R443 V444 F445
T446 M447 C448 D449 Q450 N451 P452 E453 P454 Q455 V456 L457 T458 I459 S460 D461 A462 D463 I464 P465 P466 N467 T468 Y469 P470 Y471 K472 V473 S474 L475 S476 H477 G478 S479 D480 L481 T482 W483 K484 A485 E486 L487 D488 S489 K490 G491 T492 S493 M494 L495 L496 S497 P498 T499 Q500 Q501 L502 K503 K504 G505
D506 Y507 S508 I509 Y510 V511 L512 L513 S514 D515 A516 Q517 N518 N519 P520 Q521 L522 T523 V524 V525 N526 A527 T528 V529 C530 S531 C532 E533 G534 K535 A536 I537 K538 C539 Q540 GLU LYS LEU VAL GLY GLY PHE ASP LEU PRO ILE ILE LEU VAL ILE LEU GLY SER VAL LEU ALA LEU LEU ILE LEU
PHE LEU LEU LEU LEU LEU PHE LEU LYS ARG LYS LYS VAL VAL LYS GLU PRO LEU LEU LEU PRO GLU ASP ASP THR ARG ASP ASN ILE PHE TYR TYR GLY GLU GLU GLY GLY GLY GLU GLU ASP GLN ASP TYR ASP LEU SER GLN LEU HIS ARG GLY LEU ASP SER ARG PRO ASP ILE MET
ARG ASN ASP VAL VAL PRO THR LEU MET PRO ALA PRO HIS TYR ARG PRO ARG PRO SER ASN PRO ASP GLU ILE GLY ASN PHE ILE ASP GLU ASN LEU ASP ALA ALA ASP ASN ASP PRO THR ALA PRO PRO TYR ASP SER LEU LEU VAL PHE ASP TYR GLU GLY SER GLY SER GLU ALA ALA
SER LEU SER SER LEU ASN SER SER SER ASN SER ASN ASP GLU HIS ASP TYR ASN TYR LEU SER ASP TRP GLY SER ARG PHE ARG LYS LEU ALA ASP MET TYR GLY GLY ASP ASP ASP GLU GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	no CTF correction. Imaging at underfocus 0.4 micron with CM200FEG microscope at 50,000 magnification	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1200	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum voxel value	2603.000	Depositor
Minimum voxel value	-1866.000	Depositor
Average voxel value	1323.980	Depositor
Voxel value standard deviation	218.755	Depositor
Recommended contour level	1760.0	Depositor
Tomogram size (Å)	3720.19, 3720.19, 617.61	wwPDB
Tomogram dimensions	512, 512, 85	wwPDB
Tomogram angles (°)	90, 90, 90	wwPDB
Grid spacing (Å)	7.266, 7.266, 7.266	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, NDG

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	0.70	8/4276 (0.2%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
All	All	0.70	16/8552 (0.2%)	1.42	160/11678 (1.4%)

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	1	4
1	B	0	4
All	All	1	8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.37	1.34	1.52
1	B	335	ALA	CA-CB	-8.33	1.34	1.52
1	A	539	CYS	CB-SG	8.17	1.96	1.82
1	B	539	CYS	CB-SG	8.15	1.96	1.82
1	B	223	PRO	CG-CD	7.02	1.73	1.50
1	A	223	PRO	CG-CD	7.00	1.73	1.50
1	A	523	THR	N-CA	-6.26	1.33	1.46
1	B	523	THR	N-CA	-6.24	1.33	1.46
1	A	522	LEU	N-CA	-5.98	1.34	1.46
1	A	18	PRO	N-CD	5.97	1.56	1.47
1	B	522	LEU	N-CA	-5.97	1.34	1.46
1	B	18	PRO	N-CD	5.91	1.56	1.47
1	A	530	CYS	CB-SG	5.53	1.91	1.82
1	B	530	CYS	CB-SG	5.46	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	THR	CA-CB	5.05	1.66	1.53
1	B	499	THR	CA-CB	5.02	1.66	1.53

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	490	LYS	N-CA-CB	-28.44	59.41	110.60
1	A	520	PRO	CA-C-N	-13.30	87.95	117.20
1	B	520	PRO	CA-C-N	-13.28	87.99	117.20
1	B	290	PHE	N-CA-C	12.73	145.38	111.00
1	A	235	ILE	N-CA-C	12.72	145.34	111.00
1	B	235	ILE	N-CA-C	12.72	145.34	111.00
1	A	290	PHE	N-CA-C	12.71	145.32	111.00
1	B	374	ASP	N-CA-C	11.61	142.35	111.00
1	A	374	ASP	N-CA-C	11.61	142.34	111.00
1	A	17	PHE	C-N-CD	-11.55	95.19	120.60
1	B	17	PHE	C-N-CD	-11.54	95.22	120.60
1	B	398	SER	N-CA-C	11.37	141.70	111.00
1	A	398	SER	N-CA-C	11.36	141.68	111.00
1	B	465	PRO	C-N-CD	-11.04	96.31	120.60
1	A	465	PRO	C-N-CD	-11.03	96.33	120.60
1	B	222	ASP	CB-CG-OD2	10.06	127.35	118.30
1	A	222	ASP	CB-CG-OD2	10.03	127.33	118.30
1	A	236	GLY	N-CA-C	-9.99	88.11	113.10
1	B	236	GLY	N-CA-C	-9.98	88.15	113.10
1	A	230	VAL	C-N-CD	-9.94	98.73	120.60
1	B	230	VAL	C-N-CD	-9.92	98.77	120.60
1	A	374	ASP	CB-CA-C	-9.67	91.05	110.40
1	B	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	B	376	ALA	N-CA-C	9.65	137.04	111.00
1	A	376	ALA	N-CA-C	9.64	137.04	111.00
1	B	522	LEU	CA-CB-CG	-9.38	93.74	115.30
1	A	522	LEU	CA-CB-CG	-9.36	93.77	115.30
1	B	223	PRO	N-CA-C	-9.30	87.91	112.10
1	B	520	PRO	N-CA-C	9.30	136.28	112.10
1	A	221	PHE	C-N-CA	-9.30	98.46	121.70
1	B	221	PHE	C-N-CA	-9.29	98.46	121.70
1	A	223	PRO	N-CA-C	-9.29	87.94	112.10
1	A	520	PRO	N-CA-C	9.29	136.25	112.10
1	B	481	LEU	N-CA-C	-9.29	85.92	111.00
1	A	481	LEU	N-CA-C	-9.27	85.97	111.00
1	B	481	LEU	CA-CB-CG	-8.76	95.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	481	LEU	CA-CB-CG	-8.75	95.17	115.30
1	A	289	ASP	C-N-CA	-8.43	100.62	121.70
1	B	289	ASP	C-N-CA	-8.42	100.66	121.70
1	A	516	ALA	N-CA-C	-8.35	88.47	111.00
1	B	516	ALA	N-CA-C	-8.35	88.46	111.00
1	B	222	ASP	C-N-CD	-8.21	102.54	120.60
1	A	290	PHE	CA-C-N	-8.20	99.16	117.20
1	B	290	PHE	CA-C-N	-8.19	99.18	117.20
1	A	222	ASP	C-N-CD	-8.19	102.59	120.60
1	A	46	PRO	C-N-CD	-8.05	102.89	120.60
1	B	46	PRO	C-N-CD	-8.03	102.93	120.60
1	B	233	ASN	N-CA-C	7.88	132.28	111.00
1	A	233	ASN	N-CA-C	7.86	132.22	111.00
1	A	336	VAL	N-CA-C	7.82	132.10	111.00
1	B	336	VAL	N-CA-C	7.81	132.09	111.00
1	B	522	LEU	C-N-CA	-7.79	102.21	121.70
1	A	522	LEU	C-N-CA	-7.78	102.25	121.70
1	B	362	GLN	N-CA-C	-7.71	90.18	111.00
1	A	362	GLN	N-CA-C	-7.71	90.20	111.00
1	A	234	GLU	N-CA-C	-7.59	90.51	111.00
1	B	234	GLU	N-CA-C	-7.58	90.52	111.00
1	A	234	GLU	C-N-CA	7.42	140.24	121.70
1	B	234	GLU	C-N-CA	7.41	140.22	121.70
1	A	521	GLN	C-N-CA	-7.38	103.25	121.70
1	B	521	GLN	C-N-CA	-7.38	103.26	121.70
1	A	490	LYS	CB-CA-C	7.32	125.04	110.40
1	B	277	SER	N-CA-C	-7.21	91.54	111.00
1	A	277	SER	N-CA-C	-7.20	91.56	111.00
1	A	337	SER	N-CA-C	-7.19	91.59	111.00
1	B	337	SER	N-CA-C	-7.16	91.67	111.00
1	B	503	LYS	N-CA-C	7.01	129.94	111.00
1	A	503	LYS	N-CA-C	7.00	129.91	111.00
1	B	523	THR	N-CA-CB	-6.95	97.10	110.30
1	A	523	THR	N-CA-CB	-6.93	97.13	110.30
1	A	492	THR	N-CA-C	6.78	129.30	111.00
1	B	492	THR	N-CA-C	6.75	129.23	111.00
1	B	448	CYS	CA-CB-SG	-6.70	101.95	114.00
1	A	448	CYS	CA-CB-SG	-6.68	101.98	114.00
1	A	398	SER	C-N-CA	-6.57	105.29	121.70
1	B	476	SER	N-CA-C	6.57	128.72	111.00
1	A	476	SER	N-CA-C	6.56	128.72	111.00
1	B	491	GLY	N-CA-C	6.55	129.47	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	398	SER	C-N-CA	-6.55	105.33	121.70
1	A	491	GLY	N-CA-C	6.53	129.43	113.10
1	B	525	VAL	N-CA-C	-6.50	93.46	111.00
1	A	525	VAL	N-CA-C	-6.48	93.50	111.00
1	A	335	ALA	N-CA-C	-6.32	93.95	111.00
1	B	335	ALA	N-CA-C	-6.31	93.96	111.00
1	B	532	CYS	N-CA-C	6.30	128.01	111.00
1	A	532	CYS	N-CA-C	6.30	128.00	111.00
1	B	234	GLU	CA-C-N	-6.28	103.38	117.20
1	A	234	GLU	CA-C-N	-6.28	103.39	117.20
1	A	222	ASP	N-CA-C	6.17	127.64	111.00
1	B	222	ASP	N-CA-C	6.15	127.61	111.00
1	A	235	ILE	CA-C-N	-6.14	103.91	116.20
1	A	397	GLU	C-N-CA	-6.14	106.35	121.70
1	B	235	ILE	CA-C-N	-6.13	103.94	116.20
1	B	397	GLU	C-N-CA	-6.12	106.40	121.70
1	A	18	PRO	CA-N-CD	-6.11	102.94	111.50
1	B	503	LYS	CB-CA-C	-6.09	98.21	110.40
1	A	503	LYS	CB-CA-C	-6.07	98.25	110.40
1	B	18	PRO	CA-N-CD	-6.07	103.00	111.50
1	B	502	LEU	N-CA-C	6.07	127.40	111.00
1	A	502	LEU	N-CA-C	6.04	127.31	111.00
1	A	2	TRP	N-CA-C	-6.03	94.72	111.00
1	B	2	TRP	N-CA-C	-6.01	94.77	111.00
1	B	374	ASP	C-N-CD	5.97	140.95	128.40
1	B	222	ASP	N-CA-CB	5.96	121.32	110.60
1	A	374	ASP	C-N-CD	5.95	140.90	128.40
1	A	222	ASP	N-CA-CB	5.95	121.31	110.60
1	A	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	376	ALA	CA-C-N	-5.85	104.33	117.20
1	A	376	ALA	CA-C-N	-5.83	104.36	117.20
1	A	382	ASN	N-CA-C	-5.83	95.27	111.00
1	B	382	ASN	N-CA-C	-5.81	95.31	111.00
1	B	471	TYR	N-CA-C	5.74	126.51	111.00
1	A	471	TYR	N-CA-C	5.73	126.46	111.00
1	A	481	LEU	CA-C-N	-5.67	104.72	117.20
1	B	481	LEU	CA-C-N	-5.67	104.72	117.20
1	A	374	ASP	C-N-CA	-5.67	98.20	122.00
1	B	374	ASP	C-N-CA	-5.67	98.20	122.00
1	B	403	ASN	N-CA-C	-5.63	95.81	111.00
1	A	403	ASN	N-CA-C	-5.62	95.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	221	PHE	CA-C-N	5.58	129.48	117.20
1	A	221	PHE	CA-C-N	5.57	129.46	117.20
1	A	505	GLY	N-CA-C	5.57	127.02	113.10
1	B	505	GLY	N-CA-C	5.54	126.96	113.10
1	B	502	LEU	CB-CA-C	-5.54	99.67	110.20
1	A	502	LEU	CB-CA-C	-5.52	99.71	110.20
1	A	157	GLU	C-N-CD	-5.48	108.54	120.60
1	B	157	GLU	C-N-CD	-5.47	108.57	120.60
1	B	519	ASN	N-CA-C	5.35	125.45	111.00
1	A	519	ASN	N-CA-C	5.35	125.44	111.00
1	A	405	THR	N-CA-C	5.33	125.40	111.00
1	B	405	THR	N-CA-C	5.32	125.35	111.00
1	A	367	LEU	CA-CB-CG	-5.31	103.08	115.30
1	B	367	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	521	GLN	N-CA-C	-5.21	96.93	111.00
1	B	521	GLN	N-CA-C	-5.21	96.94	111.00
1	A	290	PHE	O-C-N	5.19	131.01	122.70
1	A	532	CYS	N-CA-CB	-5.16	101.31	110.60
1	B	290	PHE	O-C-N	5.16	130.96	122.70
1	B	520	PRO	C-N-CA	5.15	134.58	121.70
1	B	532	CYS	N-CA-CB	-5.14	101.35	110.60
1	A	520	PRO	C-N-CA	5.13	134.54	121.70
1	A	18	PRO	CA-CB-CG	-5.13	94.25	104.00
1	B	522	LEU	N-CA-C	-5.12	97.17	111.00
1	A	522	LEU	N-CA-C	-5.11	97.19	111.00
1	B	18	PRO	CA-CB-CG	-5.11	94.28	104.00
1	A	339	VAL	N-CA-C	5.11	124.80	111.00
1	B	339	VAL	N-CA-C	5.10	124.77	111.00
1	B	16	PRO	C-N-CA	-5.09	108.98	121.70
1	A	16	PRO	C-N-CA	-5.07	109.02	121.70
1	A	332	PHE	N-CA-C	-5.04	97.39	111.00
1	B	234	GLU	O-C-N	5.03	130.75	122.70
1	B	332	PHE	N-CA-C	-5.03	97.43	111.00
1	A	470	PRO	N-CA-C	5.02	125.16	112.10
1	B	221	PHE	N-CA-C	5.02	124.56	111.00
1	A	539	CYS	N-CA-C	5.01	124.53	111.00
1	B	470	PRO	N-CA-C	5.01	125.13	112.10
1	B	539	CYS	N-CA-C	5.01	124.53	111.00
1	A	221	PHE	N-CA-C	5.01	124.52	111.00
1	A	234	GLU	O-C-N	5.00	130.71	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	490	LYS	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain
1	B	17	PHE	Sidechain
1	B	18	PRO	Mainchain
1	B	222	ASP	Mainchain
1	B	520	PRO	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	4191	0	4085	708	0
1	B	4191	0	4090	720	0
2	A	182	0	169	93	0
2	B	182	0	169	92	0
3	A	28	0	24	9	0
3	B	28	0	24	9	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
All	All	8826	0	8561	1393	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 80.

All (1393) 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:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.58
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.55
1:A:87:PRO:CG	1:B:89:GLU:HB3	1.16	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.41
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.37
1:A:87:PRO:CG	1:B:89:GLU:CB	2.03	1.36
1:A:82:SER:O	1:B:91:PRO:HD2	1.18	1.32
1:A:82:SER:OG	1:B:91:PRO:CB	1.79	1.28
1:A:31:PHE:HB2	1:B:93:GLU:OE2	1.08	1.25
1:A:82:SER:OG	1:B:91:PRO:HB2	1.12	1.23
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.20
1:A:87:PRO:HG3	1:B:89:GLU:CB	1.66	1.19
1:A:540:GLN:CD	1:A:540:GLN:O	1.79	1.19
1:A:31:PHE:CB	1:B:93:GLU:OE2	1.90	1.18
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.18
1:A:84:ASN:HB2	1:B:79:HIS:CE1	1.77	1.17
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.16
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.81	1.16
1:B:482:THR:HG23	1:B:499:THR:CG2	1.74	1.16
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.15
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.44	1.15
1:A:8:LYS:H	1:A:8:LYS:HD2	1.04	1.15
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.15
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.14
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.13
1:B:8:LYS:H	1:B:8:LYS:HD2	1.04	1.13
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.12
1:B:403:ASN:HB2	2:B:902:NAG:H83	1.30	1.12
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.12
1:A:89:GLU:OE1	1:B:1:ASP:C	1.88	1.11
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.11
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.10
1:B:222:ASP:OD1	1:B:222:ASP:O	1.69	1.10
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.10
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.10
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.09
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.09
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.09
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.09
1:A:90:GLU:O	1:B:1:ASP:OD1	1.70	1.08
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.26	1.07
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:A:485:ALA:O	1:A:486:GLU:HG2	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASN:HD21	1:B:83:GLU:HB2	0.98	1.07
1:B:450:GLN:CG	1:B:532:CYS:O	2.02	1.07
1:A:450:GLN:CG	1:A:532:CYS:O	2.03	1.07
1:B:485:ALA:O	1:B:486:GLU:HG2	1.54	1.07
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:A:403:ASN:HB2	2:A:902:NAG:H83	1.30	1.06
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.06
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.06
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.06
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.55	1.06
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:A:90:GLU:HB2	1:B:2:TRP:HB2	1.35	1.05
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.05
1:A:87:PRO:CD	1:B:89:GLU:HB3	1.86	1.05
1:B:290:PHE:HB2	1:B:292:LEU:H	0.89	1.05
1:A:84:ASN:CB	1:B:79:HIS:HE1	1.70	1.04
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.92	1.04
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.91	1.03
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.03
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.03
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.03
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.03
1:A:84:ASN:HB2	1:B:79:HIS:HE1	0.91	1.03
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.02
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.02
1:B:403:ASN:HB2	2:B:902:NAG:C8	1.90	1.02
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.02
1:A:403:ASN:HB2	2:A:902:NAG:C8	1.90	1.01
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	1.01
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.01
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	1.01
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	1.01
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	1.00
1:A:82:SER:HG	1:B:91:PRO:CB	1.61	1.00
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	0.99
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.99
1:A:523:THR:HG23	1:A:524:VAL:H	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.99
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.99
1:B:482:THR:HG21	1:B:499:THR:H	1.23	0.99
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.98
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:A:82:SER:O	1:B:91:PRO:CD	2.12	0.97
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.97
1:A:8:LYS:H	1:A:8:LYS:CD	1.74	0.97
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.96
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.96
1:B:32:ASN:HD21	1:B:83:GLU:CB	1.79	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.96
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.95
1:A:82:SER:OG	1:B:91:PRO:CA	2.14	0.94
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.94
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.94
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.94
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.93
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.93
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.93
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.93
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.93
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.93
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.93
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.92
1:A:87:PRO:HG2	1:B:89:GLU:CB	2.00	0.92
1:A:87:PRO:HG2	1:B:89:GLU:HB3	1.49	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.92
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.92
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.92
1:B:446:THR:HG23	1:B:539:CYS:SG	2.09	0.92
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.92
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.92
1:B:403:ASN:HB2	2:B:902:NAG:C7	2.00	0.92
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.92
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.91
1:B:32:ASN:ND2	1:B:83:GLU:HB2	1.84	0.91
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.91
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.91
1:A:403:ASN:HB2	2:A:902:NAG:C7	2.00	0.91
1:A:404:ASN:O	1:A:404:ASN:ND2	2.03	0.91
2:B:805:NAG:H62	2:B:806:NAG:C7	1.99	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.91
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.91
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.91
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.91
1:A:90:GLU:HB2	1:B:2:TRP:CB	2.00	0.90
1:B:404:ASN:O	1:B:404:ASN:ND2	2.03	0.90
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.90
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.90
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.90
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.90
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.90
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.89
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.89
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.89
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.89
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.89
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.89
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.89
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.89
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.89
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.88
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.88
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.88
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.88
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.88
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.88
1:A:87:PRO:CD	1:B:89:GLU:CB	2.46	0.87
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.87
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.87
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.87
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.87
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.87
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.87
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.87
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.87
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.87
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.86
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.86
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.86
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.86
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.86
1:A:82:SER:HG	1:B:91:PRO:HB2	0.90	0.86
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.86
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.86
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.86
1:A:90:GLU:CB	1:B:2:TRP:HB2	2.06	0.86
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.86
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.86
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.85
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.85
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.85
1:A:464:ILE:HD12	1:A:465:PRO:N	1.91	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.85
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.85
1:A:87:PRO:HG2	1:B:89:GLU:CG	2.06	0.84
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.84
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.84
1:A:89:GLU:OE2	1:B:3:VAL:HG13	1.76	0.84
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.58	0.84
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.84
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.83
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.83
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.83
1:B:147:SER:OG	1:B:167:ARG:HD2	1.78	0.83
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.83
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.83
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.83
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:A:89:GLU:OE1	1:B:1:ASP:CA	2.09	0.83
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.83
1:A:289:ASP:O	1:A:289:ASP:OD2	1.97	0.83
1:B:289:ASP:O	1:B:289:ASP:OD2	1.97	0.83
1:B:396:ARG:NE	1:B:432:ASP:HB2	1.93	0.83
1:A:87:PRO:HD3	1:B:89:GLU:HB2	1.61	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.83
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.82
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.82
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.82
1:B:32:ASN:ND2	1:B:83:GLU:H	1.77	0.82
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.82
1:A:540:GLN:O	1:A:540:GLN:OE1	1.97	0.82
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.45	0.82
1:A:87:PRO:HD3	1:B:89:GLU:CB	2.10	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.59	0.82
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.44	0.82
1:B:482:THR:HG21	1:B:500:GLN:N	1.94	0.82
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.81
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.63	0.81
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.81
1:A:482:THR:HG21	1:A:500:GLN:N	1.94	0.81
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.81
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.81
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.81
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.81
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.81
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.80
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:B:540:GLN:O	1:B:540:GLN:OE1	1.97	0.80
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.80
1:A:84:ASN:CG	1:B:77:SER:OG	2.19	0.80
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.80
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.80
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.80
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.80
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.80
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.80
1:A:82:SER:C	1:B:91:PRO:HD2	2.01	0.79
1:B:396:ARG:HD3	1:B:431:LEU:C	2.02	0.79
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.79
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.79
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.79
1:B:540:GLN:O	1:B:540:GLN:CG	2.31	0.79
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.79
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.79
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.79
1:B:27:ASN:HD22	1:B:27:ASN:C	1.85	0.79
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.79
2:B:904:NAG:O7	2:B:904:NAG:H3	1.82	0.79
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.30	0.79
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.79
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.79
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.79
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLN:O	1:B:365:GLN:HG3	1.82	0.79
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.79
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.79
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.78
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:A:396:ARG:HD3	1:A:431:LEU:C	2.03	0.78
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.78
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.78
1:B:155:PRO:C	1:B:157:GLU:H	1.86	0.78
1:B:147:SER:OG	1:B:167:ARG:CG	2.32	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.30	0.78
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	0.78
1:B:147:SER:OG	1:B:167:ARG:CD	2.32	0.78
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.78
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.78
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.78
1:A:89:GLU:OE1	1:B:2:TRP:N	2.18	0.77
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.31	0.77
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.77
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.77
1:A:540:GLN:O	1:A:540:GLN:CG	2.30	0.77
1:B:501:GLN:HG2	1:B:501:GLN:O	1.84	0.77
1:A:89:GLU:CD	1:B:1:ASP:H3	1.86	0.77
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.77
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.77
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.77
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.77
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.77
1:B:222:ASP:OD1	1:B:222:ASP:C	2.20	0.77
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:B:194:THR:HB	1:B:198:GLY:HA2	1.66	0.77
1:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.77
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.76
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.76
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.76
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.76
1:A:272:THR:HG22	1:A:273:THR:H	1.51	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.76
1:A:194:THR:HB	1:A:198:GLY:HA2	1.66	0.76
1:A:501:GLN:O	1:A:501:GLN:HG2	1.84	0.76
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.76
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.76
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.76
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.75
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.75
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.75
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.75
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.68	0.75
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.75
1:A:90:GLU:HB3	1:B:2:TRP:HD1	1.52	0.75
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.75
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.75
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.75
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.75
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.33	0.75
1:A:87:PRO:HG3	1:B:89:GLU:HB3	0.75	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:A:84:ASN:HD22	1:B:79:HIS:CE1	2.04	0.75
1:A:90:GLU:C	1:B:1:ASP:OD1	2.26	0.75
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.75
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.75
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.87	0.74
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.74
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.74
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.27	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:B:364:ILE:O	1:B:364:ILE:HG13	1.87	0.74
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.99	0.74
1:A:364:ILE:HG13	1:A:364:ILE:O	1.86	0.74
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.74
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:N	1:B:298:LEU:HD23	2.03	0.74
1:A:87:PRO:HG2	1:B:89:GLU:HG3	1.67	0.73
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.73
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.73
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.73
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.73
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.73
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.73
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.72
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.72
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.98	0.72
1:A:35:TYR:HB3	1:B:90:GLU:OE1	1.89	0.72
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.72
1:A:298:LEU:N	1:A:298:LEU:HD23	2.03	0.72
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:A:87:PRO:CG	1:B:89:GLU:CG	2.67	0.72
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.72
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.72
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.72
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.72
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.72
1:B:394:LEU:HD12	1:B:394:LEU:N	2.05	0.72
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.72
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.72
1:A:28:LYS:NZ	1:B:4:ILE:H	1.87	0.71
1:A:90:GLU:HB3	1:B:2:TRP:CD1	2.25	0.71
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.71
1:A:364:ILE:O	1:A:364:ILE:CG1	2.37	0.71
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.71
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.71
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.02	0.71
1:A:394:LEU:N	1:A:394:LEU:HD12	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ILE:O	1:B:364:ILE:CG1	2.37	0.71
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.71
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.71
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.71
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.71
1:A:290:PHE:CD2	1:A:293:ARG:N	2.55	0.71
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.71
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.71
1:A:368:SER:HG	1:A:370:PHE:HE1	1.39	0.71
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.71
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.70
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.70
1:B:403:ASN:CB	2:B:902:NAG:N2	2.54	0.70
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.90	0.70
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.70
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.70
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.70
1:A:403:ASN:CB	2:A:902:NAG:N2	2.54	0.70
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.02	0.70
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.70
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.70
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.70
1:A:289:ASP:O	1:A:289:ASP:CG	2.29	0.69
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.69
1:A:485:ALA:C	1:A:486:GLU:HG2	2.11	0.69
1:B:27:ASN:C	1:B:27:ASN:ND2	2.46	0.69
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.69
1:B:289:ASP:O	1:B:289:ASP:CG	2.30	0.69
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.69
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.69
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.69
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.69
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.69
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.69
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.69
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HD3	1:B:431:LEU:O	1.93	0.69
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.68
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.68
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.77	0.68
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.68
1:A:282:LEU:HD23	1:A:283:THR:H	1.59	0.68
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.68
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.67
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.67
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.67
1:A:482:THR:HG21	1:A:500:GLN:H	1.58	0.67
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.67
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.67
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.67
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.67
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.67
2:A:902:NAG:O7	2:A:902:NAG:H3	1.95	0.67
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.67
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.67
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.67
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.67
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.67
1:A:403:ASN:HB2	2:A:902:NAG:N2	2.10	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.67
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.67
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.67
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.67
1:B:403:ASN:HB2	2:B:902:NAG:N2	2.10	0.67
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.67
1:A:396:ARG:HD3	1:A:431:LEU:O	1.94	0.67
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.66
1:A:222:ASP:O	1:A:222:ASP:CG	2.32	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.66
1:B:482:THR:HG21	1:B:500:GLN:H	1.58	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
2:B:902:NAG:O7	2:B:902:NAG:H3	1.95	0.66
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.66
1:B:282:LEU:HD23	1:B:283:THR:H	1.58	0.66
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.96	0.66
1:A:88:VAL:HA	1:B:92:MET:HG2	1.76	0.66
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.66
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.66
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.66
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:A:32:ASN:CG	1:A:33:LYS:H	1.98	0.66
1:A:82:SER:OG	1:B:91:PRO:C	2.33	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.66
1:B:32:ASN:CG	1:B:33:LYS:H	1.98	0.66
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.66
1:A:482:THR:OG1	1:A:500:GLN:CG	2.44	0.66
1:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.66
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.66
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.65
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.65
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.77	0.65
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.77	0.65
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.65
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.65
1:A:28:LYS:NZ	1:B:4:ILE:N	2.38	0.65
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.65
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.65
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.65
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.65
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.65
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.65
1:A:364:ILE:O	1:A:364:ILE:HD12	1.97	0.64
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:B:364:ILE:O	1:B:364:ILE:HD12	1.98	0.64
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.64
1:B:446:THR:CG2	1:B:537:ILE:O	2.44	0.64
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.64
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.64
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.64
2:B:904:NAG:O7	2:B:904:NAG:C3	2.45	0.64
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.64
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.64
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.64
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.64
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.64
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.64
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.64
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.63
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.63
1:B:364:ILE:O	1:B:364:ILE:CD1	2.46	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.63
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.63
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.63
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.63
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.63
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.63
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.63
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.63
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.63
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.63
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.63
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.63
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.63
1:B:403:ASN:CB	2:B:902:NAG:C7	2.76	0.63
1:A:87:PRO:CD	1:B:89:GLU:HB2	2.22	0.63
1:A:364:ILE:O	1:A:364:ILE:CD1	2.46	0.63
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.63
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.62
1:A:504:LYS:NZ	1:A:531:SER:OG	2.31	0.62
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.62
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.80	0.62
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.81	0.62
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.62
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.62
1:A:31:PHE:CG	1:B:93:GLU:OE2	2.52	0.62
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.62
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.62
1:B:368:SER:HG	1:B:370:PHE:HE1	1.47	0.62
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.62
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.62
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.62
1:B:147:SER:OG	1:B:167:ARG:HG3	1.99	0.62
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.62
1:B:517:GLN:C	1:B:519:ASN:N	2.47	0.62
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.62
1:B:486:GLU:O	1:B:495:LEU:N	2.32	0.62
1:B:508:SER:HB3	1:B:526:ASN:OD1	2.00	0.62
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.61
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.61
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.61
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.61
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.61
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.61
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.61
1:A:89:GLU:CD	1:B:3:VAL:HG13	2.20	0.61
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.61
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.61
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.61
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.61
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.61
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.61
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.60
1:A:379:LEU:HD23	1:A:379:LEU:H	1.66	0.60
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.60
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.60
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.60
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.60
1:A:403:ASN:CB	2:A:902:NAG:C7	2.76	0.60
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.60
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.60
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.60
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.60
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.60
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.60
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.60
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.60
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.60
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.59
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.59
1:A:189:LEU:N	1:A:189:LEU:HD23	2.17	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.59
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.59
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.85	0.59
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.59
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.59
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	0.59
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.59
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.59
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.59
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.58
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.58
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.58
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.58
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.58
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.58
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.58
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.58
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.58
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.58
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:B:443:ARG:HG3	1:B:443:ARG:HH11	1.67	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.58
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.58
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.58
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ALA:HB1	3:A:811:NDG:H6	1.69	0.57
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.57
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.67	0.57
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.57
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.57
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.57
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.57
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.57
1:B:505:GLY:HA2	1:B:529:VAL:H	1.70	0.57
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.57
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.57
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.57
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.57
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.57
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.56
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.56
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.56
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.56
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.56
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.56
1:B:32:ASN:CG	1:B:33:LYS:N	2.59	0.56
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.56
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.56
1:B:394:LEU:N	1:B:394:LEU:CD1	2.69	0.56
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.56
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.56
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.56
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.56
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.56
1:B:32:ASN:HD22	1:B:83:GLU:H	1.51	0.56
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.56
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.56
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.56
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.56
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.56
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.56
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.55
1:B:365:GLN:O	1:B:365:GLN:CG	2.54	0.55
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.55
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.37	0.55
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.55
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.55
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.55
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.87	0.55
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.55
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.55
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.55
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.55
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.55
1:B:278:ASN:HD22	1:B:278:ASN:N	2.05	0.55
1:B:403:ASN:CB	2:B:902:NAG:H83	2.21	0.55
1:A:272:THR:CG2	1:A:273:THR:H	2.19	0.55
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.55
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.55
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.55
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.55
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.55
1:B:75:VAL:O	1:B:76:LEU:HD23	2.07	0.55
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.55
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.55
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.54
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.54
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.54
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.54
1:A:367:LEU:C	1:A:367:LEU:HD12	2.28	0.54
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.54
1:A:84:ASN:ND2	1:B:77:SER:OG	2.41	0.54
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.54
1:B:363:GLN:C	1:B:364:ILE:CG2	2.75	0.54
1:A:75:VAL:O	1:A:76:LEU:HD23	2.08	0.54
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.54
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.54
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.54
1:B:367:LEU:HD12	1:B:367:LEU:C	2.28	0.54
1:A:363:GLN:C	1:A:364:ILE:CG2	2.76	0.54
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.54
1:A:82:SER:OG	1:B:91:PRO:N	2.40	0.54
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.54
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	0.54
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.54
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.54
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.54
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.54
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.54
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.54
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:A:84:ASN:ND2	1:B:79:HIS:CE1	2.76	0.53
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.53
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.53
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.08	0.53
1:B:268:PHE:CD2	1:B:268:PHE:N	2.75	0.53
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.53
1:B:458:THR:HG22	1:B:493:SER:HB3	1.90	0.53
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.53
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.53
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	0.53
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.53
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.53
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.53
1:A:533:GLU:HA	1:A:533:GLU:OE2	2.09	0.53
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.53
1:A:88:VAL:HA	1:B:92:MET:CG	2.39	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.53
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.53
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.53
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.53
1:A:84:ASN:CG	1:B:77:SER:HG	2.12	0.53
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.53
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.53
1:A:512:LEU:HD11	1:A:519:ASN:HD21	1.74	0.53
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.33	0.53
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.53
1:B:482:THR:HG22	1:B:482:THR:O	2.09	0.53
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.74	0.53
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.52
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.52
1:B:426:LEU:HD13	1:B:426:LEU:O	2.10	0.52
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.52
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.52
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:A:82:SER:O	1:B:90:GLU:OE2	2.25	0.52
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.52
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.52
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.52
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.52
1:A:90:GLU:CB	1:B:2:TRP:CD1	2.92	0.52
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.91	0.52
1:A:379:LEU:H	1:A:379:LEU:CD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.52
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.40	0.52
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.44	0.52
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.52
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.52
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.52
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.52
1:B:31:PHE:CD2	1:B:32:ASN:HB2	2.44	0.51
1:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.51
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.51
1:B:8:LYS:CD	1:B:8:LYS:N	2.51	0.51
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.51
1:A:471:TYR:CD1	1:A:471:TYR:N	2.79	0.51
1:A:428:LEU:HD23	1:A:428:LEU:O	2.11	0.51
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51
1:A:426:LEU:HD13	1:A:426:LEU:O	2.10	0.51
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.51
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.51
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.51
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.51
1:B:471:TYR:CD1	1:B:471:TYR:N	2.79	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.51
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.51
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.51
1:B:154:ASP:C	2:B:801:NAG:C8	2.62	0.51
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:B:458:THR:HG22	1:B:493:SER:CB	2.41	0.51
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.51
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.51
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.50
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.50
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.50
1:B:397:GLU:N	1:B:397:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:C	1:A:138:ASN:HD22	2.13	0.50
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.50
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.50
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.50
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.50
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.50
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.50
1:B:217:ASN:N	1:B:217:ASN:HD22	2.09	0.50
1:B:428:LEU:O	1:B:428:LEU:HD23	2.11	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.50
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.50
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.50
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.50
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.50
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.50
1:A:278:ASN:HD22	1:A:278:ASN:N	2.05	0.50
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.50
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.50
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.93	0.50
1:B:423:THR:HB	2:B:810:NAG:H83	1.94	0.50
1:A:84:ASN:CB	1:B:79:HIS:CE1	2.62	0.50
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.50
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.50
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.50
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.50
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.50
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.50
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.50
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.50
1:A:458:THR:HG22	1:A:493:SER:CB	2.42	0.50
1:B:80:ALA:O	1:B:88:VAL:HG23	2.11	0.50
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.50
1:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.89	0.50
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.50
2:B:807:NAG:O7	2:B:807:NAG:H3	2.11	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:A:217:ASN:N	1:A:217:ASN:HD22	2.10	0.50
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.50
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.24	0.50
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.49
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.49
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.49
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.49
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.49
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.49
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.94	0.49
1:B:151:LEU:HD12	1:B:151:LEU:H	1.78	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.49
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.49
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.49
1:B:273:THR:H	2:B:803:NAG:HN2	1.61	0.49
1:A:82:SER:H	1:B:90:GLU:C	2.15	0.49
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.49
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.49
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.49
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.49
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.49
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.49
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.49
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.49
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.49
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.93	0.49
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.49
1:A:482:THR:HG22	1:A:482:THR:O	2.09	0.49
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.33	0.49
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.49
2:A:807:NAG:O7	2:A:807:NAG:H3	2.11	0.49
1:B:281:ILE:HG23	1:B:281:ILE:O	2.13	0.49
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.49
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.49
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.49
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.49
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.49
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.49
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.49
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.49
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.49
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.49
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.49
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.49
1:A:397:GLU:OE1	1:A:397:GLU:N	2.45	0.49
1:A:423:THR:HB	2:A:810:NAG:H83	1.94	0.49
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.49
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.49
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.48
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.48
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.48
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.96	0.48
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.48
1:A:89:GLU:OE2	1:B:3:VAL:CG1	2.55	0.48
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.48
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.48
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.48
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.48
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.48
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.48
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.48
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.48
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.48
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.48
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.48
2:B:812:NAG:C1	2:B:812:NAG:O7	2.60	0.48
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.48
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.66	0.48
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.48
1:A:366:LYS:HG2	1:A:367:LEU:H	1.75	0.47
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.47
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.47
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.47
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.47
1:A:82:SER:C	1:B:90:GLU:HG3	2.21	0.47
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.47
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.47
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.47
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.47
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.47
1:A:514:SER:HG	1:A:519:ASN:HA	1.79	0.47
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.47
1:B:300:ILE:HD12	1:B:300:ILE:N	2.29	0.47
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.47
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.47
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.47
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.47
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.47
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.29	0.47
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.47
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
2:A:812:NAG:O7	2:A:812:NAG:C1	2.60	0.47
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.47
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.47
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.47
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.47
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.47
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.47
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.47
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.46
1:B:226:TYR:O	1:B:227:THR:HG23	2.15	0.46
1:B:379:LEU:H	1:B:379:LEU:CD2	2.22	0.46
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.81	0.46
1:A:27:ASN:ND2	1:A:28:LYS:N	2.50	0.46
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.46
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.46
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.46
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.46
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.81	0.46
1:A:374:ASP:N	1:A:374:ASP:OD1	2.49	0.46
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.46
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.92	0.46
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:B:374:ASP:N	1:B:374:ASP:OD1	2.49	0.46
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.46
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.46
1:A:403:ASN:CB	2:A:902:NAG:H83	2.21	0.46
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.46
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.46
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.46
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ILE:HD13	1:B:381:VAL:HG11	1.95	0.46
1:B:415:ASP:CG	1:B:416:GLY:H	2.17	0.46
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.86	0.46
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.46
1:B:271:ILE:HG23	1:B:271:ILE:O	2.15	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:A:84:ASN:O	1:B:79:HIS:CE1	2.69	0.46
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.46
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.46
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.46
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.46
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.46
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.46
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.45
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.45
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.45
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:A:363:GLN:O	1:A:364:ILE:CG2	2.64	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.45
1:B:506:ASP:OD1	1:B:506:ASP:N	2.49	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.45
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.45
1:B:252:THR:HA	1:B:253:PRO:HD3	1.81	0.45
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.45
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.45
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.45
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.45
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.16	0.45
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.45
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.45
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.45
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.45
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.45
1:B:408:VAL:O	1:B:426:LEU:N	2.49	0.45
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:B:272:THR:CG2	1:B:273:THR:N	2.76	0.45
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.45
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.45
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.45
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.44
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.44
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.44
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.44
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.44
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.44
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.44
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.44
1:B:32:ASN:ND2	1:B:83:GLU:CB	2.62	0.44
1:B:299:GLN:CG	1:B:318:THR:HG23	2.42	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.44
1:B:232:GLU:HA	1:B:288:LEU:HD12	1.99	0.44
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.44
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.44
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.44
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.44
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.44
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.44
1:B:519:ASN:CG	1:B:519:ASN:O	2.55	0.44
1:A:4:ILE:HA	1:A:5:PRO:HD3	1.72	0.44
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.44
1:B:86:SER:HA	1:B:87:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.44
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.44
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.44
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.44
1:B:151:LEU:HD12	1:B:151:LEU:N	2.33	0.44
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.44
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.44
1:B:396:ARG:NH2	1:B:464:ILE:HG22	2.12	0.44
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.44
1:A:426:LEU:HD13	1:A:426:LEU:C	2.38	0.44
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.44
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.44
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.44
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.43
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.43
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.43
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.43
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.43
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	0.43
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.43
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.43
1:B:366:LYS:HG2	1:B:367:LEU:H	1.75	0.43
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.43
1:B:502:LEU:HD23	1:B:502:LEU:HA	1.82	0.43
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.43
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.43
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.43
1:A:35:TYR:HB3	1:B:90:GLU:CD	2.38	0.43
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.43
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:A:82:SER:HG	1:B:91:PRO:C	2.19	0.43
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.43
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.43
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.43
1:B:4:ILE:HA	1:B:5:PRO:HD3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.43
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.43
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.43
1:A:344:ASP:O	1:A:344:ASP:CG	2.57	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:A:519:ASN:O	1:A:519:ASN:CG	2.55	0.43
1:B:1:ASP:CG	1:B:2:TRP:N	2.70	0.43
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.43
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.43
1:B:239:VAL:HG13	1:B:240:GLN:N	2.34	0.43
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.43
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.43
1:A:419:VAL:HG13	1:A:420:GLY:N	2.34	0.43
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.43
1:B:367:LEU:H	1:B:367:LEU:HG	1.41	0.43
1:B:419:VAL:HG13	1:B:420:GLY:N	2.34	0.43
2:B:810:NAG:O7	2:B:810:NAG:C1	2.67	0.43
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:A:347:ARG:HG3	1:A:392:GLY:N	2.33	0.42
1:B:522:LEU:HD23	1:B:522:LEU:HA	1.36	0.42
1:A:32:ASN:ND2	1:A:83:GLU:CB	2.62	0.42
1:A:89:GLU:CD	1:B:1:ASP:N	2.37	0.42
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.42
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.42
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.42
1:B:32:ASN:HD22	1:B:83:GLU:N	2.13	0.42
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.42
1:A:450:GLN:HG3	1:A:532:CYS:O	2.10	0.42
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.42
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.42
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.42
1:B:138:ASN:C	1:B:138:ASN:ND2	2.73	0.42
1:B:261:ILE:HD13	1:B:261:ILE:H	1.85	0.42
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.42
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:N	1:A:298:LEU:CD2	2.75	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.42
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.42
1:B:482:THR:HG22	1:B:499:THR:H	1.70	0.42
1:A:84:ASN:O	1:B:79:HIS:ND1	2.53	0.42
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.42
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.42
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.42
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.42
1:B:235:ILE:HD13	1:B:235:ILE:HG21	1.84	0.42
1:B:250:PRO:HA	1:B:255:TRP:CG	2.55	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.53	0.42
1:A:3:VAL:HB	1:A:4:ILE:H	1.51	0.42
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.42
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.42
1:A:539:CYS:HB3	1:A:540:GLN:H	1.45	0.42
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.42
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.42
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.42
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:344:ASP:CG	1:B:344:ASP:O	2.57	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.41
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.41
1:A:502:LEU:HD22	1:A:503:LYS:H	1.85	0.41
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.41
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.41
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.41
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.41
1:B:514:SER:HG	1:B:519:ASN:HA	1.85	0.41
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.41
1:A:250:PRO:HA	1:A:255:TRP:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:810:NAG:O7	2:A:810:NAG:C1	2.67	0.41
1:B:127:VAL:HG13	1:B:128:MET:N	2.25	0.41
1:B:231:PRO:O	1:B:235:ILE:HD13	2.21	0.41
1:B:347:ARG:HG3	1:B:392:GLY:N	2.33	0.41
1:A:86:SER:HB3	1:B:92:MET:HB2	1.39	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.41
1:B:154:ASP:HB3	2:B:801:NAG:C7	2.48	0.41
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.41
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.41
1:B:449:ASP:N	1:B:532:CYS:HB3	2.19	0.41
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.41
1:B:502:LEU:HD22	1:B:503:LYS:H	1.85	0.41
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.41
1:A:230:VAL:HG23	1:A:323:VAL:HA	2.03	0.41
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.53	0.41
1:B:19:LYS:HB3	1:B:62:VAL:HG12	2.03	0.41
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.41
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.41
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.41
1:B:474:SER:N	1:B:512:LEU:O	2.53	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:82:SER:OG	1:B:91:PRO:CD	2.68	0.41
1:A:261:ILE:HD13	1:A:261:ILE:H	1.85	0.41
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:62:VAL:O	1:A:62:VAL:HG13	2.21	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:138:ASN:HD22	1:A:138:ASN:N	2.19	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HG21	1.84	0.41
1:A:290:PHE:CG	1:A:292:LEU:HB2	2.56	0.41
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.41
1:A:345:LEU:HD22	1:A:349:GLU:HB2	2.03	0.41
1:B:25:LYS:NZ	1:B:29:ASP:OD2	2.39	0.41
1:B:33:LYS:NZ	1:B:56:GLU:OE1	2.43	0.41
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:CYS:C	1:B:452:PRO:HG3	2.40	0.41
1:B:449:ASP:HB2	1:B:531:SER:HA	2.03	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:B:193:ALA:O	1:B:202:SER:HA	2.21	0.41
1:B:319:VAL:CG1	1:B:320:THR:N	2.84	0.41
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.40
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.40
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.40
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.40
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:A:409:ILE:HD13	3:A:811:NDG:C8	2.51	0.40
1:B:316:THR:OG1	2:B:806:NAG:H83	2.21	0.40
1:B:540:GLN:O	1:B:540:GLN:NE2	2.47	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:A:373:ASN:CG	1:A:374:ASP:N	2.75	0.40
1:A:466:PRO:O	1:A:469:TYR:N	2.46	0.40
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.40
1:B:239:VAL:HG11	1:B:282:LEU:HD22	2.02	0.40
1:B:272:THR:O	1:B:281:ILE:HG22	2.21	0.40
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.40
1:A:28:LYS:NZ	1:B:4:ILE:HG22	2.37	0.40
1:A:249:MET:HA	1:A:250:PRO:HD3	1.85	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:A:371:ILE:HD12	1:A:371:ILE:HA	1.65	0.40
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.40
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.40
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.40
1:B:298:LEU:N	1:B:298:LEU:CD2	2.75	0.40
1:B:396:ARG:HH21	1:B:432:ASP:CG	2.25	0.40
1:B:423:THR:CG2	2:B:810:NAG:N2	2.84	0.40
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.40
1:B:409:ILE:HD13	3:B:811:NDG:C8	2.51	0.40
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	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	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1 12
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1 12
All	All	1076/1760 (61%)	802 (74%)	184 (17%)	90 (8%)	2 12

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN
1	A	364	ILE
1	A	374	ASP
1	A	404	ASN
1	A	467	ASN
1	A	476	SER
1	A	502	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	B	91	PRO
1	B	155	PRO
1	B	235	ILE
1	B	347	ARG
1	B	363	GLN
1	B	364	ILE
1	B	374	ASP
1	B	404	ASN
1	B	467	ASN
1	B	476	SER
1	B	502	LEU

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Mol	Chain	Res	Type
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	A	3	VAL
1	A	156	GLU
1	A	260	LYS
1	A	287	GLY
1	A	470	PRO
1	A	503	LYS
1	B	3	VAL
1	B	156	GLU
1	B	260	LYS
1	B	287	GLY
1	B	470	PRO
1	B	503	LYS
1	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP
1	A	372	GLY
1	A	377	ARG
1	A	506	ASP
1	B	55	TRP
1	B	212	THR
1	B	250	PRO
1	B	333	VAL
1	B	360	ASP
1	B	372	GLY
1	B	377	ARG
1	B	506	ASP
1	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	B	152	LYS
1	B	223	PRO
1	B	359	PRO
1	B	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN

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Mol	Chain	Res	Type
1	A	289	ASP
1	A	482	THR
1	B	160	PRO
1	B	265	GLU
1	B	278	ASN
1	B	289	ASP
1	B	482	THR
1	A	498	PRO
1	A	523	THR
1	B	498	PRO
1	B	523	THR
1	A	154	ASP
1	A	307	PRO
1	B	154	ASP
1	B	307	PRO
1	A	222	ASP
1	B	222	ASP
1	A	200	GLY
1	B	200	GLY
1	A	47	PRO
1	A	158	PRO
1	B	47	PRO
1	B	158	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	480/779 (62%)	381 (79%)	99 (21%)	1 7
1	B	480/779 (62%)	381 (79%)	99 (21%)	1 7
All	All	960/1558 (62%)	762 (79%)	198 (21%)	3 7

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO
1	A	19	LYS
1	A	27	ASN
1	A	52	ARG
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET
1	A	117	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	156	GLU
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	202	SER
1	A	216	ASP
1	A	217	ASN
1	A	223	PRO
1	A	226	TYR
1	A	231	PRO
1	A	233	ASN
1	A	234	GLU
1	A	235	ILE
1	A	237	PHE
1	A	250	PRO
1	A	253	PRO
1	A	261	ILE
1	A	264	ASN
1	A	268	PHE
1	A	273	THR
1	A	277	SER
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	309	SER
1	A	310	VAL
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	345	LEU
1	A	353	SER
1	A	354	LEU
1	A	360	ASP
1	A	363	GLN
1	A	364	ILE
1	A	365	GLN
1	A	371	ILE
1	A	373	ASN
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	385	ASN
1	A	393	ASN
1	A	394	LEU
1	A	395	ASP
1	A	398	SER
1	A	399	GLU
1	A	404	ASN
1	A	405	THR
1	A	407	THR
1	A	410	MET
1	A	423	THR
1	A	425	THR
1	A	427	ILE
1	A	428	LEU
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	461	ASP
1	A	464	ILE
1	A	465	PRO

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Mol	Chain	Res	Type
1	A	466	PRO
1	A	470	PRO
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	512	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	520	PRO
1	A	522	LEU
1	A	523	THR
1	A	532	CYS
1	A	540	GLN
1	B	8	LYS
1	B	18	PRO
1	B	19	LYS
1	B	27	ASN
1	B	52	ARG
1	B	61	LEU
1	B	66	LEU
1	B	68	ARG
1	B	88	VAL
1	B	91	PRO
1	B	92	MET
1	B	117	VAL
1	B	138	ASN
1	B	146	LEU
1	B	151	LEU
1	B	155	PRO
1	B	156	GLU
1	B	161	ASN
1	B	163	PHE
1	B	189	LEU
1	B	195	ASP
1	B	202	SER
1	B	216	ASP
1	B	217	ASN
1	B	223	PRO
1	B	226	TYR
1	B	231	PRO
1	B	233	ASN

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Mol	Chain	Res	Type
1	B	234	GLU
1	B	235	ILE
1	B	237	PHE
1	B	250	PRO
1	B	253	PRO
1	B	261	ILE
1	B	264	ASN
1	B	268	PHE
1	B	273	THR
1	B	277	SER
1	B	278	ASN
1	B	282	LEU
1	B	284	THR
1	B	288	LEU
1	B	298	LEU
1	B	309	SER
1	B	310	VAL
1	B	315	SER
1	B	316	THR
1	B	318	THR
1	B	333	VAL
1	B	336	VAL
1	B	339	VAL
1	B	345	LEU
1	B	353	SER
1	B	354	LEU
1	B	360	ASP
1	B	363	GLN
1	B	364	ILE
1	B	365	GLN
1	B	371	ILE
1	B	373	ASN
1	B	375	PRO
1	B	379	LEU
1	B	382	ASN
1	B	384	ASP
1	B	385	ASN
1	B	393	ASN
1	B	394	LEU
1	B	395	ASP
1	B	398	SER
1	B	399	GLU

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Mol	Chain	Res	Type
1	B	404	ASN
1	B	405	THR
1	B	407	THR
1	B	410	MET
1	B	423	THR
1	B	425	THR
1	B	427	ILE
1	B	428	LEU
1	B	433	VAL
1	B	436	ASN
1	B	447	MET
1	B	448	CYS
1	B	461	ASP
1	B	464	ILE
1	B	465	PRO
1	B	466	PRO
1	B	470	PRO
1	B	477	HIS
1	B	492	THR
1	B	509	ILE
1	B	512	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	B	520	PRO
1	B	522	LEU
1	B	523	THR
1	B	532	CYS
1	B	540	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	ASN
1	A	32	ASN
1	A	45	ASN
1	A	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
1	A	217	ASN

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	240	GLN
1	A	264	ASN
1	A	278	ASN
1	A	299	GLN
1	A	373	ASN
1	A	385	ASN
1	A	391	ASN
1	A	393	ASN
1	A	404	ASN
1	A	455	GLN
1	A	467	ASN
1	A	517	GLN
1	A	519	ASN
1	B	12	ASN
1	B	27	ASN
1	B	32	ASN
1	B	45	ASN
1	B	79	HIS
1	B	104	ASN
1	B	110	GLN
1	B	122	GLN
1	B	138	ASN
1	B	217	ASN
1	B	233	ASN
1	B	240	GLN
1	B	264	ASN
1	B	278	ASN
1	B	299	GLN
1	B	373	ASN
1	B	385	ASN
1	B	391	ASN
1	B	393	ASN
1	B	404	ASN
1	B	455	GLN
1	B	467	ASN
1	B	517	GLN
1	B	519	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 24 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	802	1	14,14,15	0.73	0	17,19,21	0.82	0
3	NDG	A	811	1	14,14,15	0.86	0	17,19,21	1.86	1 (5%)
3	NDG	B	804	1	14,14,15	0.63	0	17,19,21	0.78	0
2	NAG	A	904	1	14,14,15	0.72	1 (7%)	17,19,21	0.68	0
2	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.34	2 (11%)
2	NAG	B	812	1	14,14,15	0.81	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	B	801	1	14,14,15	0.68	0	17,19,21	0.95	1 (5%)
2	NAG	B	803	1	14,14,15	0.96	1 (7%)	17,19,21	1.12	2 (11%)
2	NAG	A	805	1	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
2	NAG	A	810	1	14,14,15	0.66	0	17,19,21	1.34	4 (23%)
2	NAG	B	902	1	14,14,15	1.06	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.34	2 (11%)
2	NAG	A	801	1	14,14,15	0.68	0	17,19,21	0.94	1 (5%)
2	NAG	B	807	1	14,14,15	0.63	0	17,19,21	1.15	2 (11%)
2	NAG	A	903	1	14,14,15	0.53	0	17,19,21	0.76	0
2	NAG	B	808	1	14,14,15	0.66	0	17,19,21	0.69	0
2	NAG	B	904	1	14,14,15	0.72	1 (7%)	17,19,21	0.68	0
2	NAG	B	802	1	14,14,15	0.73	0	17,19,21	0.82	0
3	NDG	A	804	1	14,14,15	0.64	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	903	1	14,14,15	0.53	0	17,19,21	0.77	0
2	NAG	A	812	1	14,14,15	0.80	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.15	2 (11%)
2	NAG	A	803	1	14,14,15	0.96	1 (7%)	17,19,21	1.12	2 (11%)
2	NAG	B	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	B	809	1	14,14,15	0.74	0	17,19,21	0.93	0
2	NAG	A	809	1	14,14,15	0.72	0	17,19,21	0.92	0
3	NDG	B	811	1	14,14,15	0.85	0	17,19,21	1.87	1 (5%)
2	NAG	B	810	1	14,14,15	0.65	0	17,19,21	1.34	4 (23%)
2	NAG	A	808	1	14,14,15	0.64	0	17,19,21	0.69	0
2	NAG	A	902	1	14,14,15	1.07	1 (7%)	17,19,21	1.08	2 (11%)

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	NAG	A	802	1	-	2/6/23/26	0/1/1/1
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	812	1	-	4/6/23/26	0/1/1/1
2	NAG	B	801	1	-	3/6/23/26	0/1/1/1
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1
2	NAG	B	902	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	801	1	-	3/6/23/26	0/1/1/1
2	NAG	B	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	808	1	-	3/6/23/26	0/1/1/1
2	NAG	B	904	1	-	3/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1
2	NAG	B	809	1	-	2/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
3	NDG	B	811	1	-	2/6/23/26	0/1/1/1
2	NAG	B	810	1	-	3/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	1/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.09	1.57	1.52
2	B	902	NAG	C1-C2	3.02	1.56	1.52
2	B	803	NAG	O5-C5	2.51	1.48	1.43
2	A	803	NAG	O5-C5	2.51	1.48	1.43
2	B	904	NAG	C1-C2	-2.19	1.49	1.52
2	A	904	NAG	C1-C2	-2.17	1.49	1.52
2	B	812	NAG	C1-C2	-2.13	1.49	1.52
2	A	812	NAG	C1-C2	-2.12	1.49	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	811	NDG	C2-N2-C7	-7.01	112.92	122.90
3	A	811	NDG	C2-N2-C7	-6.99	112.95	122.90
2	A	806	NAG	C2-N2-C7	-3.42	118.04	122.90
2	B	806	NAG	C2-N2-C7	-3.41	118.05	122.90
2	B	805	NAG	C2-N2-C7	-3.01	118.61	122.90
2	A	805	NAG	C2-N2-C7	-2.98	118.66	122.90
2	B	807	NAG	C2-N2-C7	-2.87	118.81	122.90
2	A	807	NAG	C2-N2-C7	-2.87	118.82	122.90
2	A	803	NAG	C2-N2-C7	-2.79	118.93	122.90
2	B	803	NAG	C2-N2-C7	-2.79	118.94	122.90
2	B	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	A	810	NAG	C4-C3-C2	-2.45	107.42	111.02
2	A	806	NAG	C4-C3-C2	-2.45	107.43	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	806	NAG	C4-C3-C2	-2.44	107.44	111.02
2	B	803	NAG	C1-O5-C5	2.41	115.45	112.19
2	A	803	NAG	C1-O5-C5	2.40	115.44	112.19
2	A	810	NAG	O5-C1-C2	-2.33	107.60	111.29
2	B	810	NAG	O5-C1-C2	-2.33	107.61	111.29
2	A	810	NAG	C1-C2-N2	2.30	114.41	110.49
2	B	810	NAG	C1-C2-N2	2.28	114.38	110.49
2	B	810	NAG	C1-O5-C5	-2.23	109.17	112.19
2	A	810	NAG	C1-O5-C5	-2.21	109.19	112.19
2	B	902	NAG	O5-C1-C2	2.13	114.65	111.29
2	A	902	NAG	O5-C1-C2	2.12	114.63	111.29
2	B	807	NAG	O5-C1-C2	-2.04	108.06	111.29
2	A	812	NAG	C2-N2-C7	-2.03	120.01	122.90
2	A	807	NAG	O5-C1-C2	-2.03	108.08	111.29
2	B	812	NAG	C2-N2-C7	-2.01	120.04	122.90
2	A	902	NAG	C1-O5-C5	2.01	114.92	112.19
2	A	801	NAG	C1-C2-N2	-2.00	107.07	110.49
2	B	801	NAG	C1-C2-N2	-2.00	107.07	110.49

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	805	NAG	C1
2	A	806	NAG	C1
2	A	902	NAG	C1
2	A	903	NAG	C1
2	B	805	NAG	C1
2	B	806	NAG	C1
2	B	902	NAG	C1
2	B	903	NAG	C1

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7
2	A	904	NAG	C3-C2-N2-C7
2	B	807	NAG	C3-C2-N2-C7
2	B	902	NAG	C3-C2-N2-C7
2	B	904	NAG	C3-C2-N2-C7
2	A	807	NAG	C4-C5-C6-O6
2	B	807	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	811	NDG	C4-C5-C6-O6
3	B	811	NDG	C4-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6
2	B	802	NAG	C4-C5-C6-O6
3	A	811	NDG	O5-C5-C6-O6
3	B	811	NDG	O5-C5-C6-O6
2	A	809	NAG	O5-C5-C6-O6
2	B	809	NAG	O5-C5-C6-O6
2	A	810	NAG	C1-C2-N2-C7
2	B	810	NAG	C1-C2-N2-C7
2	A	807	NAG	C8-C7-N2-C2
2	B	807	NAG	C8-C7-N2-C2
2	A	809	NAG	C4-C5-C6-O6
2	B	809	NAG	C4-C5-C6-O6
2	A	807	NAG	O5-C5-C6-O6
2	B	807	NAG	O5-C5-C6-O6
2	A	805	NAG	O5-C5-C6-O6
2	B	805	NAG	O5-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6
2	B	904	NAG	C4-C5-C6-O6
2	A	812	NAG	C1-C2-N2-C7
2	B	812	NAG	C1-C2-N2-C7
2	B	802	NAG	O5-C5-C6-O6
2	A	802	NAG	O5-C5-C6-O6
2	A	810	NAG	C4-C5-C6-O6
2	B	810	NAG	C4-C5-C6-O6
2	A	805	NAG	C4-C5-C6-O6
2	B	805	NAG	C4-C5-C6-O6
2	A	807	NAG	O7-C7-N2-C2
2	B	807	NAG	O7-C7-N2-C2
2	A	812	NAG	O5-C5-C6-O6
2	B	812	NAG	O5-C5-C6-O6
2	A	803	NAG	C4-C5-C6-O6
2	B	803	NAG	C4-C5-C6-O6
2	A	810	NAG	O5-C5-C6-O6
2	B	810	NAG	O5-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	B	904	NAG	O5-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	A	803	NAG	O5-C5-C6-O6
2	B	803	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	903	NAG	C4-C5-C6-O6
2	A	903	NAG	C4-C5-C6-O6
2	A	808	NAG	C1-C2-N2-C7
2	B	808	NAG	C1-C2-N2-C7
2	A	808	NAG	C4-C5-C6-O6
2	B	808	NAG	C4-C5-C6-O6
2	B	806	NAG	C4-C5-C6-O6
2	A	806	NAG	C4-C5-C6-O6
2	A	801	NAG	O5-C5-C6-O6
2	B	801	NAG	O5-C5-C6-O6
2	A	801	NAG	C3-C2-N2-C7
2	A	903	NAG	C3-C2-N2-C7
2	B	801	NAG	C3-C2-N2-C7
2	B	903	NAG	C3-C2-N2-C7
2	B	806	NAG	O5-C5-C6-O6
2	A	806	NAG	O5-C5-C6-O6
2	B	812	NAG	C4-C5-C6-O6
2	A	812	NAG	C4-C5-C6-O6
2	A	808	NAG	C3-C2-N2-C7
2	A	812	NAG	C3-C2-N2-C7
2	B	808	NAG	C3-C2-N2-C7
2	B	812	NAG	C3-C2-N2-C7

There are no ring outliers.

26 monomers are involved in 203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	811	NDG	7	0
3	B	804	NDG	2	0
2	A	904	NAG	8	0
2	A	806	NAG	12	0
2	B	812	NAG	3	0
2	B	801	NAG	21	0
2	B	803	NAG	4	0
2	A	805	NAG	7	0
2	A	810	NAG	13	0
2	B	902	NAG	8	0
2	B	806	NAG	12	0
2	A	801	NAG	21	0
2	B	807	NAG	16	0
2	B	808	NAG	2	0
2	B	904	NAG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	NDG	2	0
2	A	812	NAG	3	0
2	A	807	NAG	17	0
2	A	803	NAG	4	0
2	B	805	NAG	7	0
2	B	809	NAG	8	0
2	A	809	NAG	8	0
3	B	811	NDG	7	0
2	B	810	NAG	13	0
2	A	808	NAG	2	0
2	A	902	NAG	8	0

5.7 Other polymers

There are no such residues in this entry.

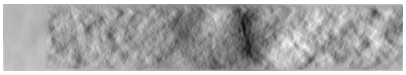
5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Tomogram visualisation

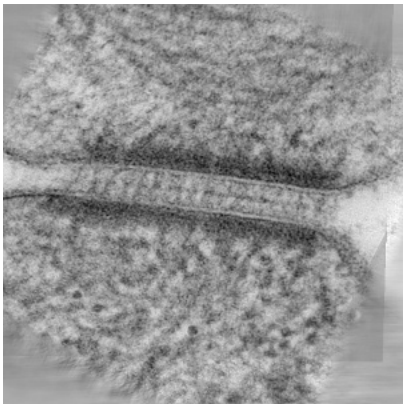
This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections



X

Y

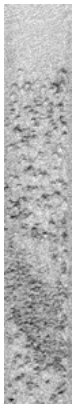


Z

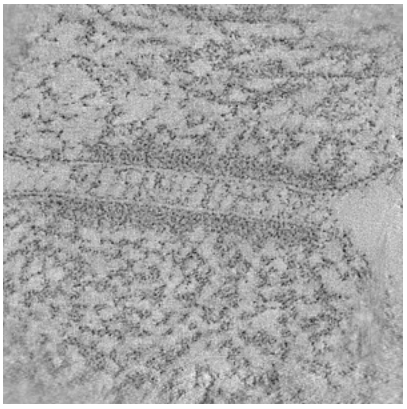
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices

X Index: 256



Y Index: 256

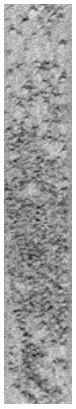


Z Index: 42

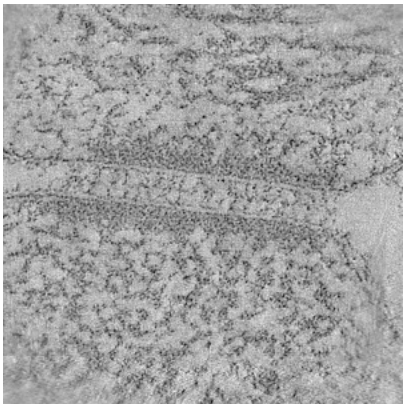
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices (i)

X Index: 243



Y Index: 315



Z Index: 39

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

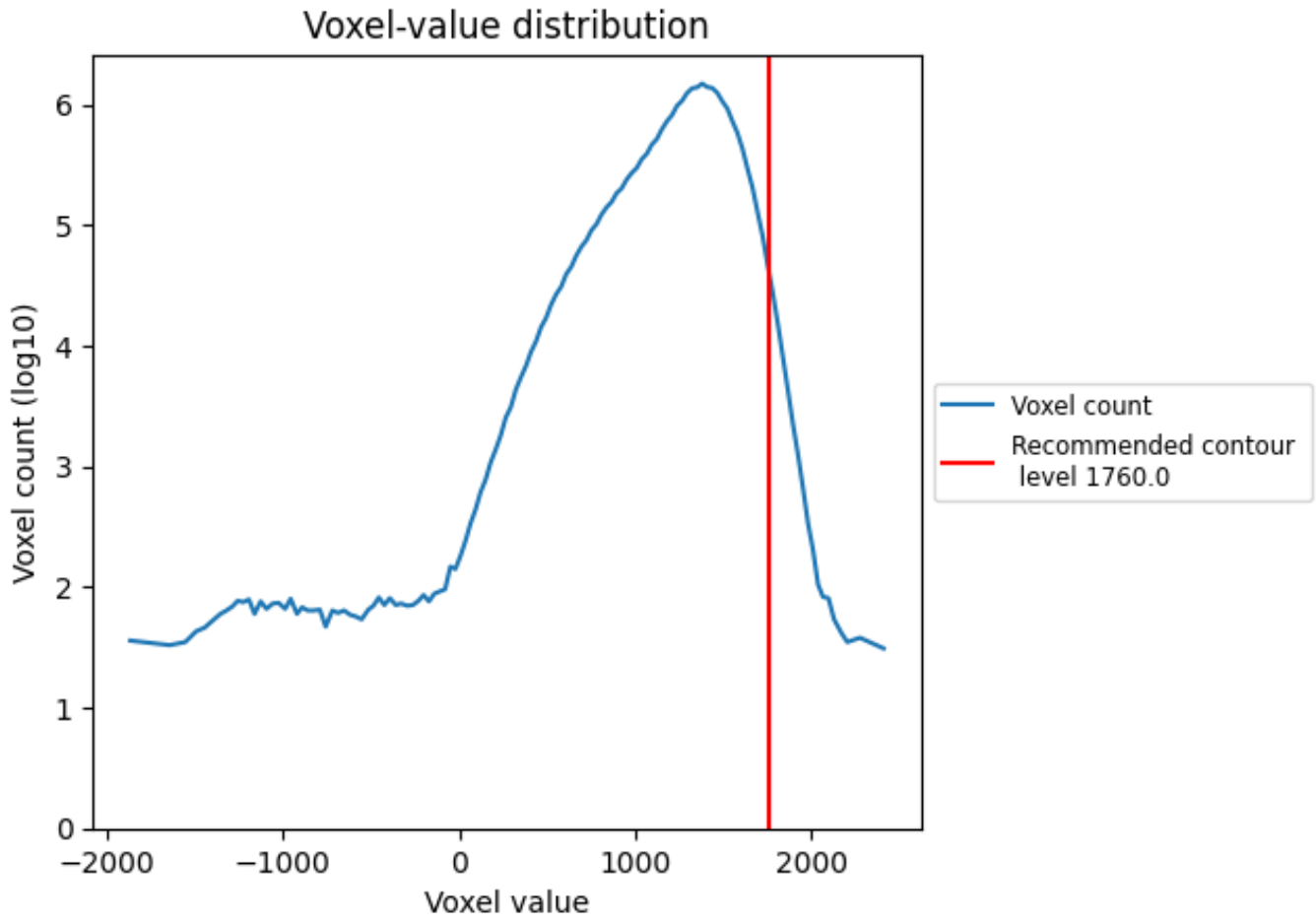
6.4 Mask visualisation (i)

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

7 Tomogram analysis (i)

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

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1052 and PDB model 1Q5A. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay

This section was not generated.

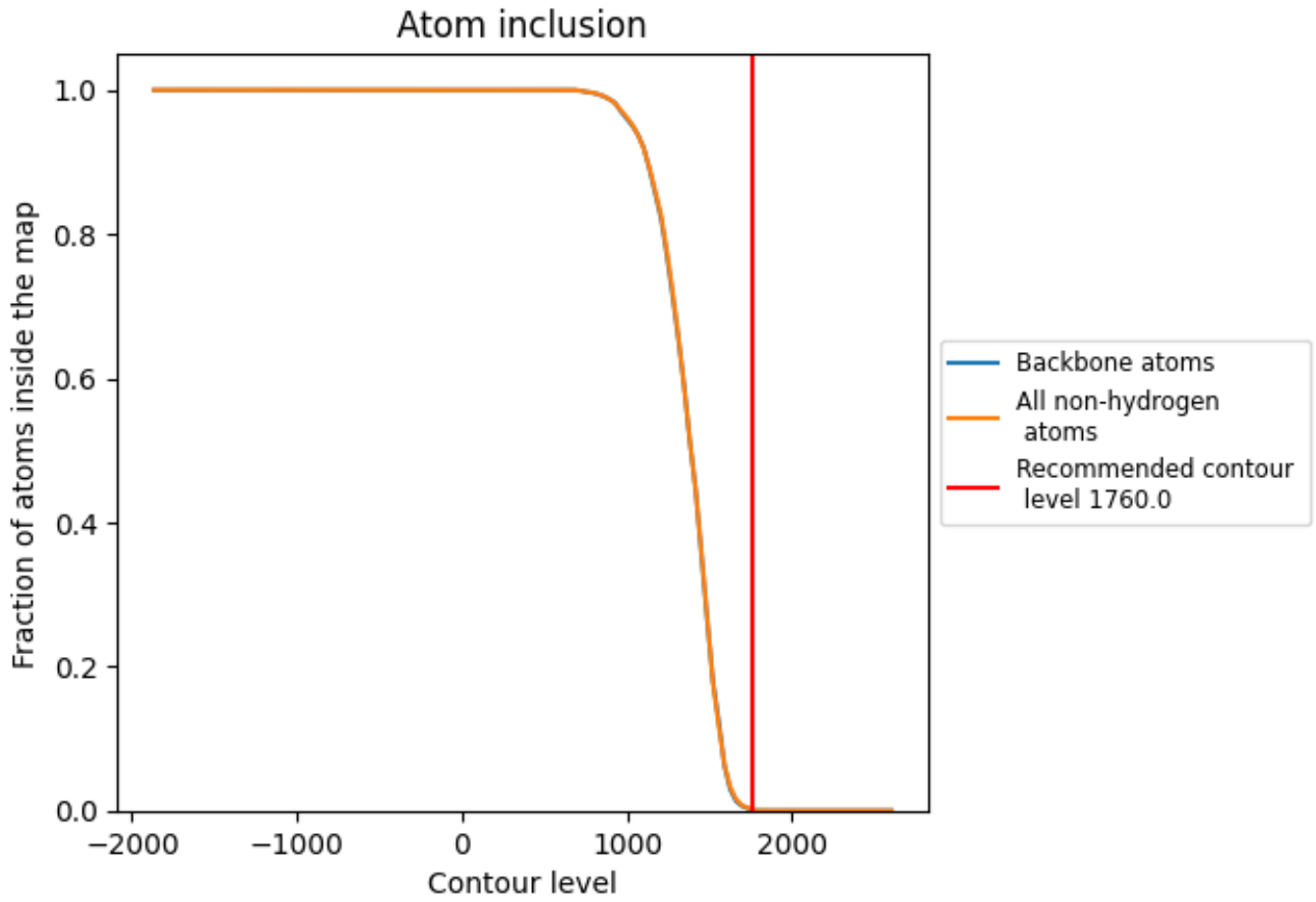
8.2 Q-score mapped to coordinate model

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.

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1760.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0008	0.0060
A	0.0016	0.0080
B	0.0000	0.0030