



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:57 AM UTC

PDB ID : 7WTC / pdb_00007wtc
EMDB ID : EMD-32778
Title : Cryo-EM structure of human pyruvate carboxylase with acetyl-CoA in the ground state
Authors : Chai, P.; Lan, P.; Wu, J.; Lei, M.
Deposited on : 2022-02-04
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

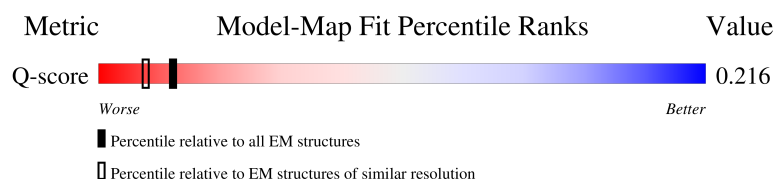
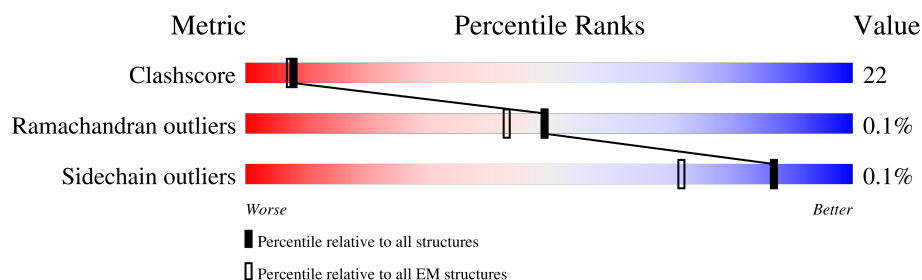
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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 $\leq 5\%$. 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	1178	15% 56% 41% .
1	B	1178	17% 57% 41% .
1	C	1178	11% 31% 27% 42%
1	D	1178	13% 34% 24% 42%

2 Entry composition [i](#)

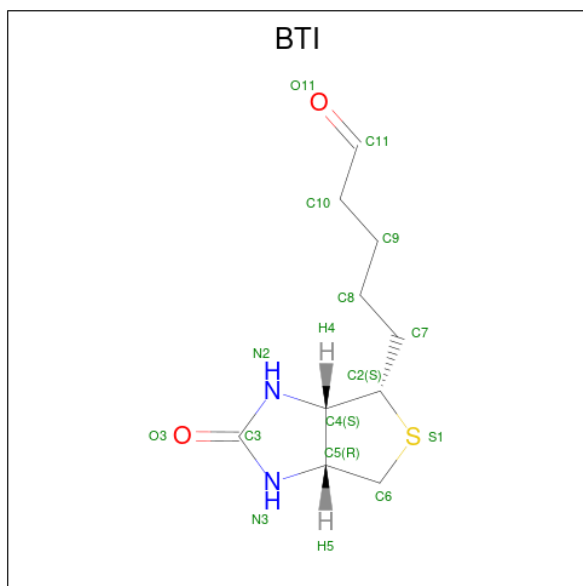
There are 3 unique types of molecules in this entry. The entry contains 28418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1146	Total	C	N	O	S	0	0
			8869	5612	1559	1651	47		
1	B	1147	Total	C	N	O	S	0	0
			8877	5618	1560	1652	47		
1	C	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		
1	D	684	Total	C	N	O	S	0	0
			5255	3339	902	978	36		

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



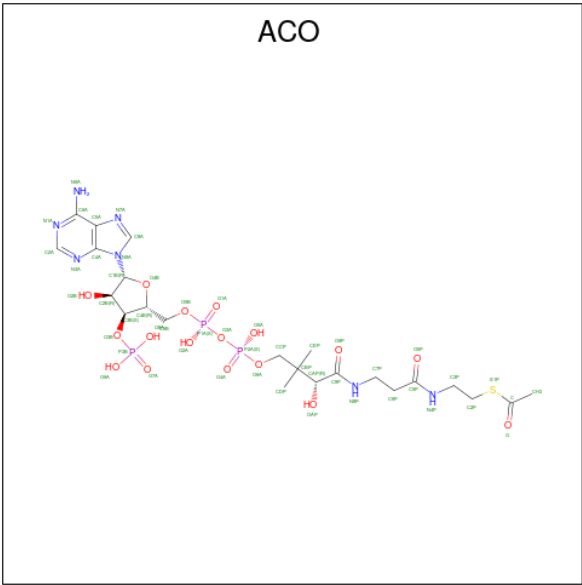
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	B	1	Total	C	N	O	S	0
			15	10	2	2	1	

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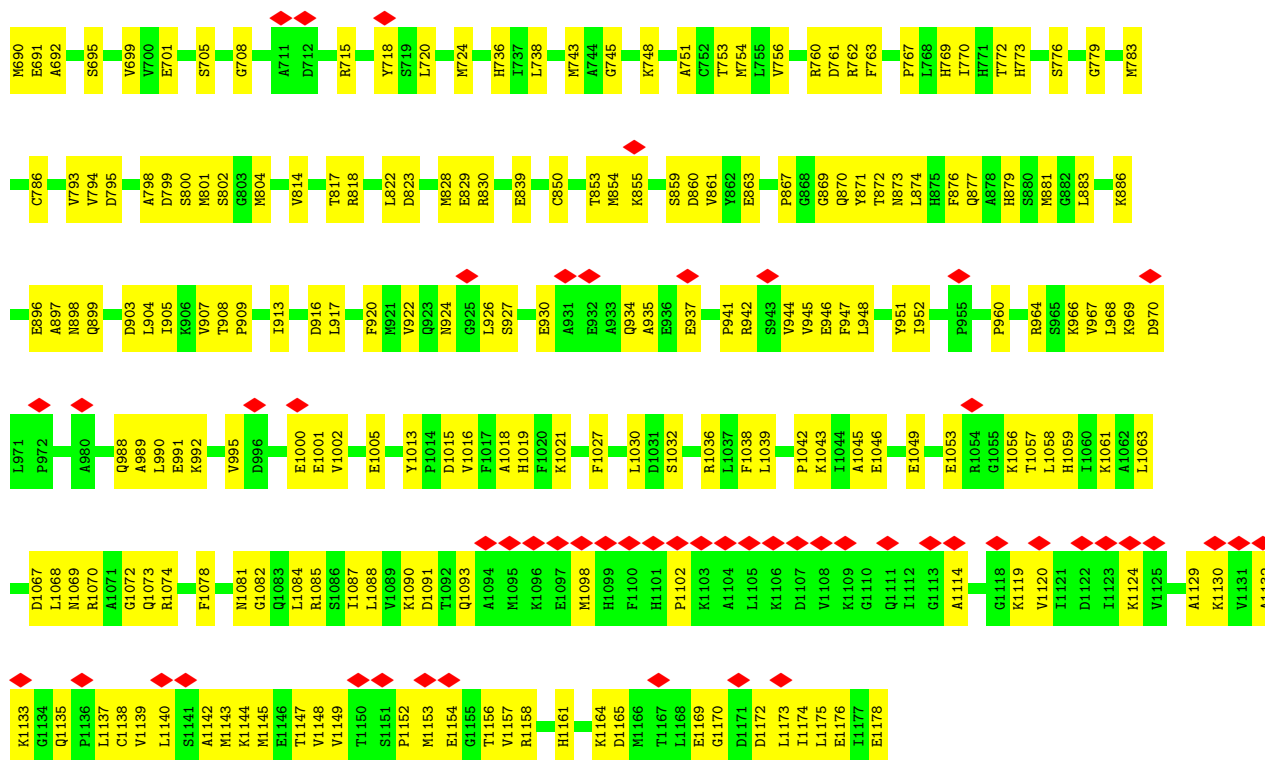
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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	D	1	Total	C	N	O	S	0
			15	10	2	2	1	

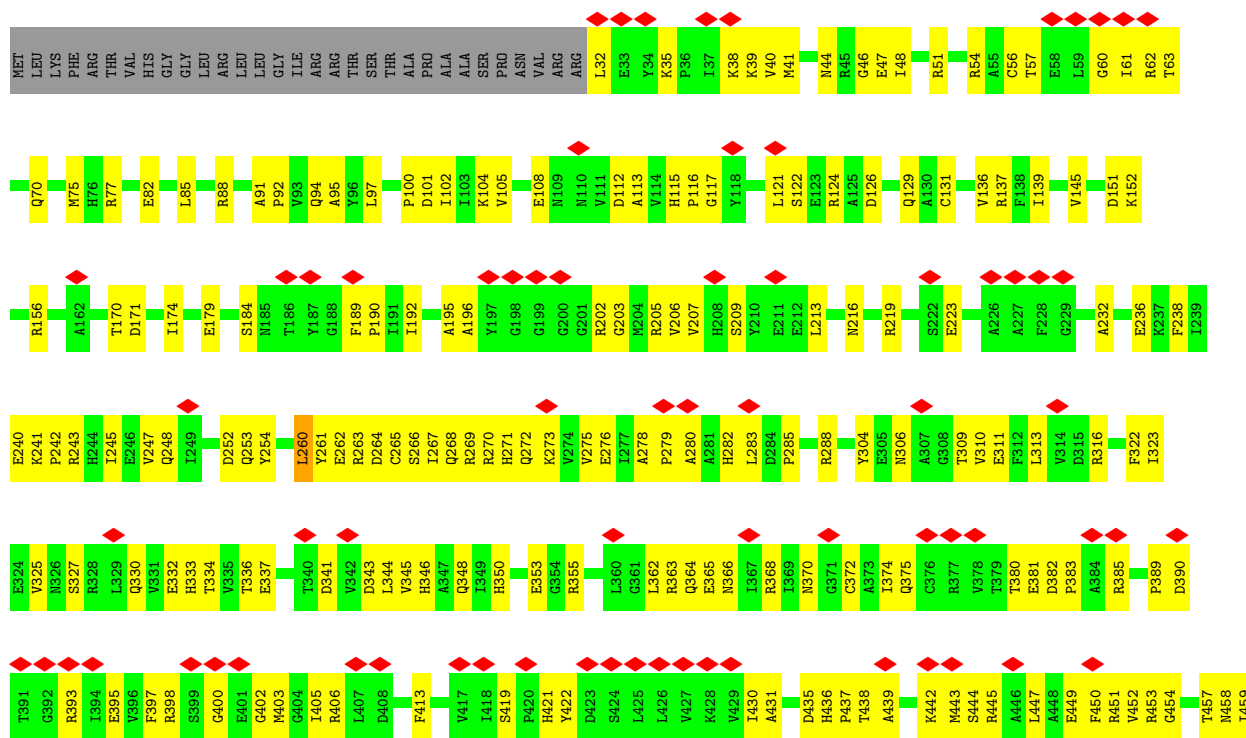
- Molecule 3 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).

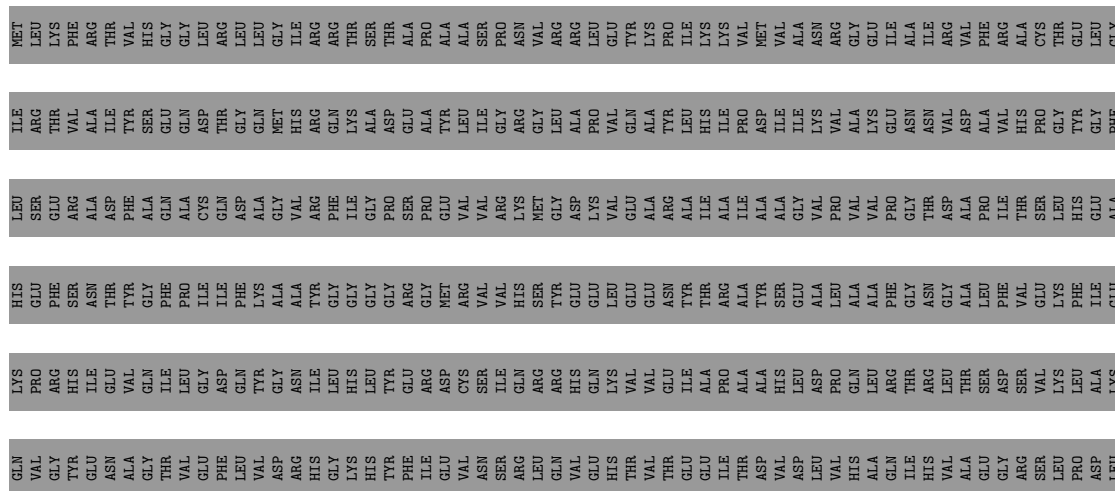
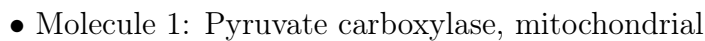


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
3	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	



• Molecule 1: Pyruvate carboxylase, mitochondrial









T1167	L1168	E1169	G1170	D1171	D1172	L1173	I1174	L1175	E1176	I1177	E1178
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.19	0/9060	0.43	0/12277
1	B	0.21	0/9068	0.46	4/12288 (0.0%)
1	C	0.23	1/5373 (0.0%)	0.49	3/7284 (0.0%)
1	D	0.18	0/5373	0.45	1/7284 (0.0%)
All	All	0.20	1/28874 (0.0%)	0.45	8/39133 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	536	PRO	CG-CD	-7.58	1.25	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	536	PRO	N-CD-CG	-11.05	86.62	103.20
1	C	536	PRO	CA-N-CD	-6.92	102.32	112.00
1	C	536	PRO	CA-CB-CG	-6.38	92.39	104.50
1	B	260	LEU	CA-C-N	5.85	132.72	121.54
1	B	260	LEU	C-N-CA	5.85	132.72	121.54
1	D	1065	VAL	N-CA-C	-5.66	107.47	112.90
1	B	851	THR	CB-CA-C	-5.47	108.67	115.89
1	B	46	GLY	N-CA-C	5.06	116.67	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8869	0	8829	409	0
1	B	8877	0	8840	391	0
1	C	5255	0	5248	273	0
1	D	5255	0	5248	230	0
2	A	15	0	15	1	0
2	B	15	0	15	2	0
2	C	15	0	15	4	0
2	D	15	0	15	5	0
3	A	51	0	34	7	0
3	B	51	0	34	10	0
All	All	28418	0	28293	1271	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 22.

All (1271) 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:C:574:HIS:HB3	1:C:580:THR:HA	1.47	0.95
1:D:586:ASP:HA	1:D:589:LYS:HD3	1.49	0.93
1:A:542:ARG:NH1	1:A:634:ILE:O	2.06	0.89
1:A:381:GLU:HA	1:A:389:PRO:HA	1.56	0.87
1:A:465:VAL:HG22	1:A:487:LEU:HD23	1.55	0.87
1:A:398:ARG:HH21	1:A:451:ARG:HD2	1.39	0.86
1:B:1047:GLU:HB2	1:B:1061:LYS:HG3	1.59	0.85
1:D:658:VAL:HB	1:D:985:LEU:HD21	1.59	0.84
1:C:647:ASN:HB3	1:C:653:ASN:HA	1.59	0.84
1:B:343:ASP:OD2	1:B:346:HIS:ND1	2.10	0.84
1:C:571:ARG:HD2	1:C:575:GLN:HE22	1.42	0.84
1:B:465:VAL:HG22	1:B:487:LEU:HD21	1.60	0.83
1:D:523:SER:O	1:D:1036:ARG:NH1	2.12	0.83
1:A:495:ASN:N	3:A:1202:ACO:O5A	2.10	0.82
1:A:402:GLY:H	1:A:405:ILE:HB	1.45	0.82
1:A:170:THR:HG22	1:A:171:ASP:H	1.45	0.82
1:C:597:ASN:O	1:C:830:ARG:NH1	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:VAL:HB	1:A:453:ARG:HB2	1.62	0.81
1:B:959:PHE:HE2	1:B:964:ARG:HD2	1.45	0.81
1:A:406:ARG:NH1	1:B:405:ILE:O	2.12	0.81
1:B:190:PRO:HA	1:B:207:VAL:O	1.79	0.81
1:B:1068:LEU:HD23	1:B:1072:GLY:HA2	1.64	0.80
1:C:581:ARG:HH22	1:C:619:LEU:HB2	1.44	0.80
1:A:116:PRO:HB2	1:A:122:SER:HA	1.62	0.80
1:A:524:PRO:HA	1:A:1036:ARG:HH12	1.49	0.78
1:B:890:VAL:HG22	1:B:922:VAL:HG11	1.65	0.78
1:B:32:LEU:N	1:B:254:TYR:HH	1.81	0.78
1:C:641:MET:HE1	1:C:643:LEU:HB2	1.63	0.78
1:A:239:ILE:HD12	1:A:242:PRO:HA	1.64	0.78
1:A:447:LEU:HB3	1:A:459:ILE:HG23	1.63	0.78
1:D:609:GLY:HA3	1:D:644:ARG:HH12	1.49	0.77
1:C:890:VAL:HG22	1:C:922:VAL:HG21	1.66	0.77
1:D:631:ARG:NH1	1:D:672:ASP:OD2	2.18	0.77
1:A:148:LYS:NZ	1:A:302:VAL:O	2.18	0.77
1:A:1057:THR:OG1	1:B:77:ARG:NH2	2.18	0.77
1:A:330:GLN:O	1:A:333:HIS:ND1	2.18	0.76
1:C:930:GLU:OE1	1:C:934:GLN:NE2	2.18	0.76
1:B:1127:ALA:HB2	1:B:1160:VAL:HG13	1.66	0.76
1:A:558:ARG:HB2	1:A:767:PRO:HG3	1.68	0.76
1:A:265:CYS:O	1:A:268:GLN:NE2	2.19	0.76
1:B:760:ARG:NH2	1:B:790:GLY:O	2.19	0.76
1:A:276:GLU:HB2	1:A:375:GLN:HB3	1.69	0.75
1:B:752:CYS:SG	1:B:786:CYS:N	2.60	0.75
1:A:1139:VAL:HG22	1:A:1148:VAL:HG22	1.68	0.75
1:C:1056:LYS:HG3	1:C:1058:LEU:HG	1.69	0.75
1:A:42:VAL:HG12	1:A:115:HIS:HB2	1.68	0.74
1:C:500:LEU:HD11	1:C:1052:LEU:HD13	1.68	0.74
1:A:269:ARG:HG3	1:A:270:ARG:HD3	1.69	0.74
1:B:241:LYS:HB3	1:B:316:ARG:HD2	1.69	0.74
1:C:924:ASN:HB2	1:C:926:LEU:HD22	1.68	0.74
1:D:558:ARG:HB2	1:D:767:PRO:HG3	1.70	0.74
1:C:661:LYS:HD3	1:C:1008:LEU:HD21	1.69	0.74
1:D:978:PRO:HA	1:D:981:SER:HB3	1.69	0.74
1:B:285:PRO:HA	1:B:288:ARG:HG2	1.70	0.74
1:B:935:ALA:HB3	1:B:966:LYS:HE3	1.70	0.73
1:A:58:GLU:OE1	1:A:346:HIS:NE2	2.21	0.73
1:A:609:GLY:HA3	1:A:644:ARG:HH12	1.54	0.73
1:B:365:GLU:O	1:B:368:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:ARG:NH1	1:B:670:GLY:O	2.20	0.73
1:A:1102:PRO:HB2	1:A:1173:LEU:HB2	1.69	0.73
1:D:592:PRO:O	1:D:596:HIS:ND1	2.21	0.73
1:A:42:VAL:HG11	1:A:52:VAL:HG21	1.71	0.73
1:B:586:ASP:OD2	1:B:845:TYR:OH	2.07	0.72
1:A:244:HIS:NE2	1:A:311:GLU:OE1	2.21	0.72
1:B:1080:LEU:HB3	1:B:1083:GLN:HG2	1.72	0.72
1:B:895:VAL:HG22	1:B:899:GLN:HE22	1.55	0.72
1:D:537:PRO:HB2	1:D:636:ASN:HD21	1.55	0.72
1:A:624:TRP:O	1:A:628:GLN:NE2	2.23	0.72
1:C:760:ARG:NH2	1:C:792:ASP:OD2	2.22	0.72
1:A:54:ARG:HH22	1:B:403:MET:H	1.35	0.72
1:B:1156:THR:O	1:B:1158:ARG:NH1	2.23	0.72
1:A:920:PHE:O	1:A:924:ASN:ND2	2.23	0.71
1:C:566:MET:HB3	1:C:795:ASP:HA	1.72	0.71
1:D:907:VAL:HG12	1:D:908:THR:H	1.55	0.71
1:A:850:CYS:HB2	1:A:872:THR:HG22	1.73	0.71
1:C:583:ARG:HD3	1:C:1035:THR:HG23	1.72	0.71
1:D:800:SER:OG	1:D:801:MET:SD	2.48	0.71
1:B:263:ARG:NH1	1:B:336:THR:OG1	2.24	0.70
1:B:908:THR:OG1	1:B:912:LYS:NZ	2.23	0.70
1:C:787:ALA:HA	1:C:791:ALA:HB3	1.72	0.70
1:D:571:ARG:NH1	1:D:575:GLN:OE1	2.24	0.70
1:A:35:LYS:NZ	1:A:36:PRO:O	2.24	0.70
1:B:330:GLN:O	1:B:333:HIS:ND1	2.25	0.70
1:B:1101:HIS:NE2	1:B:1173:LEU:O	2.23	0.70
1:B:112:ASP:OD1	1:B:137:ARG:NH1	2.24	0.70
1:B:1132:ALA:HA	1:B:1154:GLU:HG2	1.72	0.70
1:B:334:THR:O	1:B:337:GLU:HB3	1.91	0.70
1:C:644:ARG:HH22	1:C:651:TYR:HA	1.57	0.70
1:C:655:PRO:HB3	1:C:984:PRO:HA	1.71	0.70
1:C:655:PRO:HG2	1:C:985:LEU:HG	1.73	0.70
1:D:798:ALA:HA	1:D:810:MET:HE2	1.73	0.70
1:D:1090:LYS:NZ	1:D:1091:ASP:O	2.23	0.70
1:A:948:LEU:HG	1:A:967:VAL:HG11	1.74	0.70
1:C:797:ALA:HB2	1:C:807:GLN:HB2	1.71	0.70
1:B:895:VAL:O	1:B:899:GLN:NE2	2.25	0.70
1:B:655:PRO:HB3	1:B:984:PRO:HA	1.73	0.70
1:A:406:ARG:NH1	1:B:402:GLY:O	2.25	0.69
1:A:504:LEU:HD22	1:A:1042:PRO:HD3	1.73	0.69
1:D:622:CYS:H	1:D:625:ARG:HH21	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1058:LEU:HD12	1:D:1060:ILE:HD11	1.73	0.69
1:A:604:MET:O	1:A:640:GLN:N	2.26	0.69
1:A:434:LYS:HD2	1:B:341:ASP:HB3	1.74	0.69
1:A:1068:LEU:HD22	1:A:1072:GLY:HA2	1.75	0.69
1:C:851:THR:HA	1:C:854:MET:HB3	1.75	0.69
1:A:1119:LYS:NZ	1:A:1120:VAL:O	2.25	0.69
1:B:552:GLY:HA2	1:B:555:ARG:HE	1.55	0.69
1:B:599:SER:HA	1:B:637:ILE:HD11	1.74	0.69
1:C:662:PHE:CE1	1:C:1008:LEU:HB3	2.27	0.69
1:C:1132:ALA:O	1:C:1151:SER:OG	2.11	0.69
1:B:496:ARG:HA	1:B:499:LYS:HD2	1.75	0.69
1:C:907:VAL:N	1:C:910:SER:OG	2.26	0.68
1:C:510:ASN:OD1	1:C:1093:GLN:NE2	2.25	0.68
1:C:679:SER:HB3	1:C:909:PRO:HD2	1.75	0.68
1:A:97:LEU:HA	1:A:121:LEU:HD21	1.76	0.68
1:A:156:ARG:HD3	1:A:172:ALA:HA	1.75	0.68
1:D:640:GLN:HG2	1:D:675:ARG:HH21	1.58	0.68
1:B:243:ARG:NH1	1:B:266:SER:OG	2.27	0.68
1:D:752:CYS:SG	1:D:786:CYS:N	2.66	0.68
1:A:1018:ALA:HA	1:A:1021:LYS:HE3	1.75	0.67
1:B:240:GLU:OE1	1:B:316:ARG:NH2	2.25	0.67
1:C:555:ARG:O	1:C:559:ASN:ND2	2.27	0.67
1:B:205:ARG:NH2	1:B:223:GLU:OE1	2.26	0.67
1:A:498:GLN:OE1	1:A:1085:ARG:NH1	2.27	0.67
1:B:242:PRO:O	1:B:478:THR:OG1	2.13	0.67
1:D:576:SER:HA	1:D:869:GLY:HA2	1.76	0.67
1:A:570:PHE:O	1:A:574:HIS:NE2	2.25	0.67
1:B:470:GLN:HG3	1:B:476:VAL:HG22	1.76	0.67
1:A:571:ARG:NH1	1:A:575:GLN:OE1	2.28	0.67
1:B:598:PHE:HB3	1:B:601:LEU:HD13	1.77	0.67
1:C:1029:PRO:HG2	1:C:1052:LEU:HD11	1.75	0.67
1:B:248:GLN:HB3	1:B:260:LEU:HB2	1.77	0.66
1:A:1015:ASP:O	1:A:1019:HIS:ND1	2.28	0.66
1:B:787:ALA:HA	1:B:791:ALA:HB3	1.78	0.66
1:A:273:LYS:O	1:A:377:ARG:NH2	2.28	0.66
1:A:496:ARG:NH2	3:A:1202:ACO:O1A	2.28	0.66
1:A:653:ASN:ND2	1:A:951:TYR:O	2.29	0.66
1:B:243:ARG:HG2	1:B:245:ILE:HD11	1.76	0.66
1:A:310:VAL:HG22	1:A:325:VAL:HG22	1.77	0.66
1:C:615:ALA:HA	1:C:619:LEU:HB3	1.78	0.66
1:C:907:VAL:HG23	1:C:908:THR:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:ARG:O	1:D:558:ARG:NH1	2.28	0.65
1:B:595:ALA:O	1:B:636:ASN:ND2	2.28	0.65
1:D:550:PRO:HB3	1:D:699:VAL:HG22	1.77	0.65
1:A:184:SER:HB2	1:A:191:ILE:HD13	1.78	0.65
1:A:551:GLU:OE2	1:A:555:ARG:NH1	2.29	0.65
1:A:917:LEU:HB3	1:A:944:VAL:HG21	1.78	0.65
1:B:912:LYS:HD2	2:D:1900:BTI:HN2	1.61	0.65
1:C:1065:VAL:HG22	1:C:1076:VAL:HG13	1.79	0.65
1:A:1085:ARG:NH2	3:A:1202:ACO:O8A	2.29	0.65
1:B:1063:LEU:HD12	1:B:1077:PHE:HB3	1.79	0.65
1:B:760:ARG:NH2	1:B:792:ASP:OD1	2.30	0.65
1:A:610:ALA:HB2	2:C:1900:BTI:H62	1.79	0.65
1:A:947:PHE:CE1	1:A:952:ILE:HB	2.32	0.65
1:C:570:PHE:HD1	1:C:604:MET:HE2	1.62	0.65
1:C:625:ARG:NE	1:C:628:GLN:OE1	2.30	0.65
1:D:508:MET:HE2	1:D:1042:PRO:O	1.97	0.64
1:A:607:TRP:HE1	1:A:627:LEU:HD13	1.62	0.64
1:B:586:ASP:HA	1:B:589:LYS:HD3	1.79	0.64
1:D:498:GLN:HG2	1:D:1085:ARG:NH1	2.12	0.64
1:B:121:LEU:HD13	1:B:124:ARG:HG3	1.78	0.64
1:C:959:PHE:HE2	1:C:964:ARG:HH11	1.46	0.64
1:C:1061:LYS:HB3	1:C:1079:GLU:HB3	1.78	0.64
1:D:502:HIS:HA	1:D:1087:ILE:HD13	1.79	0.64
1:D:1015:ASP:O	1:D:1019:HIS:ND1	2.30	0.64
1:B:62:ARG:NH1	1:B:63:THR:O	2.30	0.64
2:B:2002:BTI:O11	1:D:617:ARG:NH1	2.31	0.64
1:C:564:LEU:HD12	1:C:602:PHE:HB2	1.80	0.64
1:B:306:ASN:OD1	1:B:348:GLN:NE2	2.29	0.64
1:B:447:LEU:HD22	1:B:459:ILE:HG23	1.80	0.64
1:C:570:PHE:CD1	1:C:604:MET:HE2	2.33	0.64
1:D:495:ASN:OD1	1:D:498:GLN:NE2	2.31	0.64
1:D:500:LEU:HD11	1:D:1033:LEU:HD21	1.80	0.64
1:A:1073:GLN:HG2	1:A:1088:LEU:HD12	1.79	0.64
1:D:499:LYS:HZ3	1:D:1029:PRO:HD2	1.62	0.64
1:A:343:ASP:OD2	1:A:346:HIS:ND1	2.22	0.64
1:B:445:ARG:NH1	1:B:449:GLU:OE1	2.28	0.64
1:C:600:LYS:NZ	1:C:825:GLU:O	2.24	0.64
1:C:1043:LYS:HZ2	1:C:1046:GLU:HB3	1.63	0.64
1:B:624:TRP:O	1:B:627:LEU:HG	1.98	0.63
1:B:1065:VAL:HG22	1:B:1076:VAL:HG23	1.79	0.63
1:A:382:ASP:OD2	1:A:385:ARG:NE	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1158:ARG:HE	1:C:1178:GLU:HG3	1.63	0.63
1:A:94:GLN:HA	1:A:97:LEU:HD12	1.80	0.63
1:A:405:ILE:HG13	1:A:445:ARG:HH12	1.63	0.63
1:B:995:VAL:HA	1:B:999:GLY:HA3	1.81	0.63
1:D:653:ASN:ND2	1:D:951:TYR:O	2.31	0.63
1:D:706:TYR:HB2	1:D:740:ILE:HD11	1.79	0.63
1:A:496:ARG:NE	3:A:1202:ACO:O2A	2.27	0.63
1:B:56:CYS:HB3	1:B:61:ILE:HB	1.81	0.63
1:B:964:ARG:O	1:B:968:LEU:HB2	1.97	0.63
1:A:641:MET:HB2	1:A:671:MET:HE2	1.81	0.63
1:D:624:TRP:O	1:D:628:GLN:NE2	2.32	0.63
1:A:145:VAL:HA	1:A:148:LYS:HE2	1.80	0.63
1:D:615:ALA:HA	1:D:619:LEU:HB2	1.81	0.63
1:C:677:PHE:HA	1:C:686:MET:HE1	1.81	0.62
1:B:894:TYR:HE2	1:B:906:LYS:HE3	1.64	0.62
1:D:520:ALA:HB3	1:D:847:ALA:HA	1.80	0.62
1:A:50:ILE:O	1:A:79:LYS:NZ	2.32	0.62
1:A:270:ARG:O	1:A:271:HIS:ND1	2.33	0.62
1:C:752:CYS:SG	1:C:786:CYS:N	2.72	0.62
1:C:1134:GLY:N	1:C:1151:SER:O	2.29	0.62
1:A:770:ILE:HG23	1:A:783:MET:HE1	1.80	0.62
1:B:41:MET:HE1	1:B:102:ILE:HG13	1.81	0.62
1:D:690:MET:HE3	1:D:733:ALA:HB1	1.80	0.62
1:B:584:THR:OG1	1:B:621:GLU:OE1	2.17	0.62
1:A:1069:ASN:OD1	1:A:1070:ARG:N	2.32	0.62
1:C:616:MET:HE1	1:C:1017:PHE:HD1	1.63	0.62
1:C:997:ARG:HH22	1:C:1018:ALA:HB1	1.64	0.62
1:D:724:MET:HE3	1:D:724:MET:HA	1.82	0.62
1:D:810:MET:HE3	1:D:831:VAL:HG13	1.81	0.62
1:A:761:ASP:OD1	1:A:762:ARG:N	2.32	0.62
1:C:908:THR:HB	1:C:909:PRO:HD3	1.81	0.62
1:A:614:VAL:HG13	1:A:618:PHE:HD2	1.65	0.62
1:A:555:ARG:HH22	1:A:767:PRO:HD3	1.65	0.61
1:B:209:SER:O	1:B:213:LEU:N	2.32	0.61
1:C:681:ASN:ND2	1:C:722:TYR:OH	2.24	0.61
1:C:581:ARG:NH2	1:C:619:LEU:HB2	2.16	0.61
1:A:508:MET:HE3	1:A:1042:PRO:HD2	1.81	0.61
1:A:563:LEU:HB2	1:A:822:LEU:HG	1.82	0.61
1:B:381:GLU:HA	1:B:389:PRO:HA	1.81	0.61
1:A:253:GLN:NE2	1:A:354:GLY:O	2.33	0.61
1:A:445:ARG:HH11	1:B:54:ARG:HH11	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1052:LEU:HB3	1:B:1056:LYS:HB2	1.82	0.61
1:D:583:ARG:NH2	1:D:1033:LEU:O	2.34	0.61
1:A:1043:LYS:HB2	1:A:1046:GLU:CD	2.25	0.61
1:B:869:GLY:O	2:D:1900:BTI:H5	2.00	0.61
1:D:1162:VAL:HG23	1:D:1166:MET:HE2	1.83	0.61
1:A:54:ARG:NH2	1:B:403:MET:H	1.97	0.61
1:B:91:ALA:HB3	1:B:94:GLN:HG2	1.83	0.61
1:B:276:GLU:HB3	1:B:375:GLN:HB2	1.82	0.61
1:B:1085:ARG:NH2	3:B:2001:ACO:O8A	2.34	0.61
1:C:571:ARG:HD2	1:C:575:GLN:NE2	2.14	0.61
1:C:603:SER:OG	1:C:640:GLN:OE1	2.19	0.61
1:D:854:MET:SD	1:D:871:TYR:OH	2.59	0.61
1:A:44:ASN:ND2	1:A:118:TYR:O	2.34	0.61
1:B:592:PRO:HD3	1:B:633:LEU:HD12	1.83	0.61
1:C:1059:HIS:N	1:C:1081:ASN:OD1	2.28	0.61
1:A:174:ILE:HB	1:A:233:LEU:HB2	1.82	0.61
1:A:406:ARG:HH12	1:B:405:ILE:C	2.07	0.60
1:A:631:ARG:HD3	1:A:670:GLY:HA3	1.82	0.60
1:A:908:THR:OG1	2:C:1900:BTI:N3	2.34	0.60
1:C:595:ALA:HB2	1:C:634:ILE:HG13	1.83	0.60
2:A:1201:BTI:H4	1:C:873:ASN:OD1	2.01	0.60
1:B:1114:ALA:O	1:B:1171:ASP:N	2.30	0.60
1:A:35:LYS:HB3	1:A:137:ARG:HH22	1.66	0.60
1:C:1139:VAL:HG22	1:C:1148:VAL:HG22	1.83	0.60
1:D:978:PRO:O	1:D:982:LEU:N	2.34	0.60
1:A:484:ASN:HB3	1:A:487:LEU:HD13	1.82	0.60
1:B:508:MET:HE1	1:B:1041:GLY:HA3	1.83	0.60
1:D:930:GLU:O	1:D:934:GLN:HG2	2.01	0.60
1:D:1096:LYS:HB2	1:D:1098:MET:HE3	1.82	0.60
1:D:1049:GLU:HG2	1:D:1059:HIS:HB3	1.84	0.60
1:A:1124:LYS:HB2	1:A:1137:LEU:HA	1.82	0.60
1:B:398:ARG:NH2	3:B:2001:ACO:O9A	2.35	0.60
1:C:1090:LYS:NZ	1:C:1091:ASP:O	2.34	0.60
1:A:294:ASP:HA	1:A:297:LYS:HE3	1.84	0.60
1:B:35:LYS:HB2	1:B:137:ARG:HH21	1.66	0.60
1:C:538:PRO:HG2	1:C:599:SER:HB2	1.83	0.60
1:C:576:SER:O	1:C:805:THR:OG1	2.20	0.60
1:C:991:GLU:HG2	1:C:1007:VAL:HG21	1.84	0.60
1:B:778:ALA:HB2	1:C:812:ALA:HB1	1.84	0.59
1:A:651:TYR:OH	2:C:1900:BTI:S1	2.55	0.59
1:B:375:GLN:HE22	1:B:430:ILE:HG13	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:GLU:H	1:A:1056:LYS:HB2	1.67	0.59
1:C:739:CYS:HB2	1:C:769:HIS:HB3	1.82	0.59
1:B:1080:LEU:HG	1:B:1081:ASN:H	1.67	0.59
1:A:400:GLY:H	1:A:450:PHE:HE1	1.47	0.59
1:A:624:TRP:CD2	1:A:1005:GLU:HB2	2.37	0.59
1:B:1000:GLU:HG2	1:B:1001:GLU:OE1	2.01	0.59
1:A:783:MET:HE3	1:A:794:VAL:HG22	1.84	0.59
1:B:85:LEU:O	1:B:88:ARG:NH1	2.36	0.59
1:B:304:TYR:OH	1:B:327:SER:O	2.19	0.59
1:B:444:SER:O	1:B:463:GLN:NE2	2.35	0.59
1:D:985:LEU:H	1:D:985:LEU:HD23	1.68	0.59
1:C:783:MET:HE2	1:C:794:VAL:HG13	1.84	0.59
1:C:599:SER:HA	1:C:637:ILE:HD11	1.84	0.59
1:A:91:ALA:HB3	1:A:94:GLN:HB3	1.84	0.59
1:C:1142:ALA:HB3	1:C:1145:MET:HB3	1.85	0.59
1:B:310:VAL:HG22	1:B:325:VAL:HG22	1.84	0.59
1:B:451:ARG:NH1	3:B:2001:ACO:O7A	2.35	0.59
1:B:930:GLU:HG2	1:B:934:GLN:HE22	1.68	0.59
2:B:2002:BTI:N3	1:D:908:THR:OG1	2.36	0.59
1:C:542:ARG:NH1	1:C:672:ASP:OD1	2.36	0.59
1:C:644:ARG:NH2	1:C:650:GLY:O	2.36	0.59
1:D:1140:LEU:HD21	1:D:1168:LEU:HD12	1.85	0.58
1:A:1144:LYS:HG2	1:C:617:ARG:HH12	1.68	0.58
1:B:644:ARG:NE	1:B:908:THR:HG21	2.18	0.58
1:C:597:ASN:HB3	1:C:830:ARG:HD2	1.85	0.58
1:D:624:TRP:CZ3	1:D:1009:SER:HB2	2.37	0.58
1:D:780:VAL:HG12	1:D:808:PRO:HB3	1.83	0.58
1:D:574:HIS:HE1	1:D:838:TRP:HZ3	1.51	0.58
1:A:241:LYS:HA	1:A:479:GLN:NE2	2.18	0.58
1:B:624:TRP:CD2	1:B:1005:GLU:HB3	2.37	0.58
1:B:742:ASP:OD2	1:B:746:LEU:N	2.29	0.58
1:D:496:ARG:NH2	1:D:1053:GLU:OE1	2.36	0.58
1:C:581:ARG:HH12	1:C:619:LEU:HB2	1.69	0.58
1:C:702:ALA:O	1:C:739:CYS:N	2.31	0.58
1:C:728:GLU:OE1	1:C:762:ARG:NH1	2.37	0.58
1:A:496:ARG:HE	3:A:1202:ACO:P1A	2.27	0.58
1:A:557:VAL:HG13	1:A:564:LEU:HD12	1.86	0.58
1:C:827:PRO:HD2	1:C:830:ARG:NH2	2.19	0.58
1:A:177:LEU:HD21	1:A:214:GLU:HG3	1.86	0.57
1:B:494:GLN:N	3:B:2001:ACO:O5A	2.35	0.57
1:C:1083:GLN:HG2	1:C:1085:ARG:CZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HH22	1:A:276:GLU:HB3	1.69	0.57
1:B:616:MET:HE2	1:B:1017:PHE:HA	1.86	0.57
1:D:1072:GLY:HA3	1:D:1090:LYS:NZ	2.19	0.57
1:A:1133:LYS:NZ	1:A:1152:PRO:O	2.32	0.57
1:B:350:HIS:HA	1:B:355:ARG:HH21	1.68	0.57
1:B:1105:LEU:HD12	1:B:1111:GLN:HE22	1.68	0.57
1:C:900:MET:HE3	1:C:928:ARG:HG3	1.86	0.57
1:D:501:LEU:HD11	1:D:1060:ILE:HG21	1.87	0.57
1:B:381:GLU:OE2	1:B:458:ASN:ND2	2.25	0.57
1:C:516:ILE:HG23	1:C:847:ALA:HB1	1.87	0.57
1:A:1142:ALA:HB3	1:A:1145:MET:HB2	1.87	0.57
1:A:115:HIS:CE1	1:A:139:ILE:HG13	2.40	0.57
1:B:380:THR:O	1:B:390:ASP:N	2.24	0.57
1:C:739:CYS:SG	1:C:740:ILE:N	2.77	0.57
1:B:174:ILE:HG23	1:B:179:GLU:HB2	1.86	0.57
1:D:748:LYS:HG2	1:D:749:PRO:HD2	1.87	0.57
1:D:761:ASP:OD1	1:D:762:ARG:N	2.37	0.57
1:A:523:SER:O	1:A:1036:ARG:NH1	2.38	0.56
1:B:263:ARG:NH1	1:B:336:THR:HG1	2.03	0.56
1:A:494:GLN:HE22	1:A:496:ARG:HD2	1.71	0.56
1:B:39:LYS:HE2	1:B:62:ARG:HD2	1.87	0.56
1:D:622:CYS:H	1:D:625:ARG:NH2	2.02	0.56
1:A:679:SER:HA	1:A:907:VAL:HB	1.86	0.56
1:A:743:MET:HG3	1:A:867:PRO:HB3	1.87	0.56
1:B:778:ALA:HA	1:C:780:VAL:HG11	1.86	0.56
1:C:578:LEU:HD23	1:C:848:PHE:HE2	1.70	0.56
1:C:997:ARG:HG3	1:C:998:HIS:N	2.20	0.56
1:D:613:ASP:CG	1:D:617:ARG:HH12	2.11	0.56
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.86	0.56
1:A:38:LYS:C	1:A:61:ILE:HG23	2.30	0.56
1:A:87:GLY:HA2	1:A:90:LEU:HD13	1.87	0.56
1:A:542:ARG:HE	1:A:638:PRO:HA	1.70	0.56
1:C:863:GLU:N	1:C:863:GLU:OE1	2.38	0.56
1:C:935:ALA:HB3	1:C:966:LYS:HE3	1.88	0.56
1:A:876:PHE:HE2	1:C:1143:MET:HE1	1.69	0.56
1:B:812:ALA:HB1	1:C:778:ALA:HB2	1.86	0.56
1:B:437:PRO:HB3	1:B:472:LEU:HD23	1.87	0.56
1:B:912:LYS:HD2	2:D:1900:BTI:H73	1.88	0.56
1:C:650:GLY:H	1:C:1012:MET:HE3	1.71	0.56
1:C:739:CYS:HG	1:C:769:HIS:HD1	0.66	0.56
1:C:581:ARG:NH2	1:C:619:LEU:HD13	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1038:PHE:HD2	1:D:1039:LEU:HD12	1.71	0.56
1:A:66:ILE:HD11	1:A:86:ILE:HG12	1.88	0.56
1:A:804:MET:HE1	1:A:854:MET:HB2	1.87	0.56
1:B:278:ALA:HB3	1:B:279:PRO:HD3	1.88	0.56
1:C:827:PRO:HD2	1:C:830:ARG:HH21	1.71	0.56
1:D:501:LEU:HD13	1:D:504:LEU:HD12	1.88	0.56
1:A:680:LEU:HD21	1:A:904:LEU:HD12	1.86	0.56
1:A:1038:PHE:HD2	1:A:1039:LEU:HD12	1.70	0.56
1:B:195:ALA:HB3	1:B:202:ARG:HH12	1.70	0.56
1:C:604:MET:O	1:C:640:GLN:N	2.35	0.56
1:A:239:ILE:HD11	1:A:315:ASP:HA	1.88	0.55
1:A:937:GLU:OE1	1:A:937:GLU:N	2.34	0.55
1:B:94:GLN:HA	1:B:97:LEU:HD12	1.87	0.55
1:D:631:ARG:NH2	1:D:634:ILE:O	2.27	0.55
1:D:724:MET:HE1	1:D:759:LEU:HD22	1.87	0.55
1:A:54:ARG:HH22	1:B:403:MET:HG3	1.70	0.55
1:A:604:MET:HE1	1:A:606:ASN:HD22	1.72	0.55
1:C:571:ARG:O	1:C:575:GLN:NE2	2.39	0.55
1:A:449:GLU:HG2	1:B:54:ARG:HH12	1.71	0.55
1:A:776:SER:HA	1:A:861:VAL:HG21	1.88	0.55
1:B:1158:ARG:NH2	1:B:1178:GLU:H	2.05	0.55
1:D:584:THR:HA	1:D:587:LEU:HD12	1.87	0.55
1:A:576:SER:HA	1:A:869:GLY:HA2	1.88	0.55
1:B:267:ILE:HG21	1:B:275:VAL:HG22	1.87	0.55
1:B:494:GLN:HB3	1:B:496:ARG:CD	2.36	0.55
1:A:535:GLY:O	1:A:596:HIS:NE2	2.37	0.55
1:A:886:LYS:HE3	1:A:922:VAL:HG22	1.89	0.55
1:A:896:GLU:HA	1:A:899:GLN:HG2	1.88	0.55
1:A:91:ALA:O	1:A:95:ALA:N	2.34	0.55
1:D:574:HIS:ND1	1:D:582:VAL:HG21	2.22	0.55
1:A:385:ARG:HG3	1:A:386:SER:H	1.71	0.55
1:C:1033:LEU:HD11	1:C:1038:PHE:HB2	1.88	0.55
1:D:733:ALA:HB3	1:D:735:THR:HG23	1.87	0.55
1:B:677:PHE:HZ	1:B:705:SER:HB3	1.72	0.55
1:C:997:ARG:HH12	1:C:1018:ALA:HB2	1.72	0.55
1:C:1121:ILE:HD13	1:C:1139:VAL:HG12	1.89	0.55
1:D:619:LEU:HB3	1:D:621:GLU:OE1	2.06	0.55
1:D:1156:THR:OG1	1:D:1158:ARG:NH2	2.39	0.55
1:A:818:ARG:HH21	1:A:828:MET:HE3	1.72	0.55
1:B:656:ASP:OD1	1:B:657:ASN:N	2.38	0.55
1:B:280:ALA:HB1	1:B:283:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1104:ALA:HB2	1:C:1173:LEU:HA	1.88	0.55
1:D:644:ARG:HH21	1:D:908:THR:HG21	1.72	0.55
1:A:960:PRO:O	1:A:964:ARG:N	2.32	0.54
1:B:62:ARG:HH22	1:B:82:GLU:CG	2.20	0.54
1:C:676:VAL:HG11	1:C:689:GLY:HA3	1.88	0.54
1:A:395:GLU:O	1:A:414:GLN:NE2	2.41	0.54
1:A:406:ARG:HB3	1:A:430:ILE:HG23	1.89	0.54
1:A:572:ASP:HA	1:A:575:GLN:HB3	1.89	0.54
1:B:599:SER:HB3	1:B:636:ASN:HD21	1.71	0.54
1:C:542:ARG:CZ	1:C:631:ARG:HH22	2.20	0.54
1:A:77:ARG:O	3:B:2001:ACO:N6A	2.41	0.54
1:A:445:ARG:NH1	1:B:54:ARG:HH11	2.04	0.54
1:A:653:ASN:HD21	1:A:952:ILE:HA	1.71	0.54
1:A:934:GLN:HB2	1:A:937:GLU:CD	2.33	0.54
1:B:32:LEU:N	1:B:254:TYR:OH	2.40	0.54
1:B:715:ARG:HE	1:B:716:THR:H	1.56	0.54
1:D:615:ALA:HB1	1:D:626:ARG:HH22	1.71	0.54
1:D:1063:LEU:HD11	1:D:1079:GLU:HB2	1.89	0.54
1:D:1067:ASP:O	1:D:1074:ARG:NE	2.40	0.54
1:D:1169:GLU:N	1:D:1172:ASP:OD2	2.36	0.54
1:A:1161:HIS:NE2	1:A:1176:GLU:OE1	2.40	0.54
1:B:586:ASP:OD1	1:B:587:LEU:N	2.40	0.54
1:B:887:PHE:O	1:B:891:LYS:NZ	2.39	0.54
1:B:1068:LEU:HD12	1:B:1068:LEU:H	1.72	0.54
1:C:581:ARG:HB3	1:C:848:PHE:CE2	2.43	0.54
1:C:1075:GLN:NE2	1:C:1076:VAL:O	2.40	0.54
1:A:647:ASN:ND2	1:A:650:GLY:O	2.40	0.54
1:A:927:SER:OG	1:A:930:GLU:OE1	2.18	0.54
1:A:1067:ASP:HA	1:A:1074:ARG:NH1	2.23	0.54
1:B:783:MET:SD	1:B:794:VAL:HG13	2.47	0.54
1:B:1149:VAL:HG11	1:B:1174:ILE:HD11	1.90	0.54
1:C:509:VAL:HG11	1:C:1089:VAL:HG11	1.90	0.54
1:C:571:ARG:NE	1:C:605:GLU:OE2	2.38	0.54
1:A:53:PHE:HB2	1:A:79:LYS:NZ	2.21	0.54
1:B:395:GLU:N	1:B:395:GLU:OE1	2.41	0.54
1:D:729:GLU:HA	1:D:732:ARG:HG3	1.89	0.54
1:A:312:PHE:CD1	1:A:322:PHE:HA	2.43	0.54
1:A:1053:GLU:OE1	1:A:1056:LYS:HG3	2.08	0.54
1:A:92:PRO:HG2	1:A:421:HIS:CD2	2.43	0.54
1:A:873:ASN:O	1:A:876:PHE:HB3	2.08	0.54
1:A:907:VAL:HG12	1:A:908:THR:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:964:ARG:HH12	1:B:973:ARG:HE	1.56	0.54
1:B:1036:ARG:HG3	1:B:1037:LEU:N	2.21	0.54
1:C:591:ALA:HB1	1:C:633:LEU:HB3	1.88	0.54
1:D:613:ASP:OD2	1:D:617:ARG:NH1	2.36	0.54
1:D:864:ASN:HB3	1:D:866:ILE:HG13	1.90	0.54
1:A:619:LEU:HB3	1:A:621:GLU:OE1	2.07	0.54
1:A:829:GLU:OE2	1:A:830:ARG:NH2	2.41	0.54
1:B:276:GLU:O	1:B:374:ILE:HD12	2.08	0.54
1:C:803:GLY:O	1:C:806:SER:N	2.25	0.54
1:D:588:LYS:HE2	1:D:633:LEU:HD11	1.90	0.54
1:A:90:LEU:HD21	1:A:98:HIS:CD2	2.43	0.53
1:A:437:PRO:HA	1:A:472:LEU:HD11	1.89	0.53
1:A:449:GLU:HG2	1:B:54:ARG:HH22	1.72	0.53
1:B:564:LEU:HD23	1:B:602:PHE:HB2	1.88	0.53
1:B:574:HIS:O	1:B:578:LEU:N	2.31	0.53
1:B:595:ALA:HB2	1:B:634:ILE:HA	1.90	0.53
1:B:877:GLN:HA	1:D:1143:MET:HE1	1.89	0.53
1:C:1003:THR:OG1	1:C:1006:ASP:OD2	2.19	0.53
1:D:527:PRO:HG3	1:D:841:ALA:HA	1.89	0.53
1:A:398:ARG:HB2	1:A:451:ARG:HB3	1.89	0.53
1:A:678:ASP:HB3	1:A:686:MET:HE3	1.90	0.53
1:A:817:THR:HG22	1:A:823:ASP:HA	1.89	0.53
1:A:870:GLN:O	1:A:874:LEU:N	2.19	0.53
1:C:586:ASP:OD2	1:C:845:TYR:OH	2.17	0.53
1:D:623:PRO:HA	1:D:626:ARG:HE	1.72	0.53
1:A:187:TYR:O	1:A:319:LYS:HD2	2.09	0.53
1:B:374:ILE:CG2	1:B:431:ALA:HB3	2.38	0.53
1:B:397:PHE:HD1	1:B:452:VAL:HG22	1.73	0.53
1:C:1108:VAL:HG12	1:C:1111:GLN:H	1.73	0.53
1:D:505:GLY:HA3	1:D:1087:ILE:HD11	1.90	0.53
1:A:239:ILE:HG21	1:A:316:ARG:NH1	2.23	0.53
1:A:245:ILE:HA	1:A:263:ARG:O	2.09	0.53
1:A:370:ASN:ND2	1:B:370:ASN:OD1	2.39	0.53
1:A:379:THR:OG1	1:A:458:ASN:ND2	2.39	0.53
1:A:614:VAL:HG13	1:A:618:PHE:CD2	2.43	0.53
1:A:246:GLU:HG2	1:A:263:ARG:HB2	1.90	0.53
1:B:591:ALA:HB1	1:B:634:ILE:HD11	1.91	0.53
1:B:955:PRO:HG2	1:B:958:GLY:HA2	1.90	0.53
1:C:583:ARG:HH22	1:C:1031:ASP:HA	1.73	0.53
1:A:335:VAL:HG12	1:A:430:ILE:HD13	1.91	0.53
1:A:385:ARG:HD2	1:A:388:GLN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:ALA:HB3	1:A:1135:GLN:HG2	1.91	0.53
1:B:44:ASN:HD22	1:B:117:GLY:HA3	1.74	0.53
1:B:192:ILE:HB	1:B:236:GLU:HG2	1.91	0.53
1:B:366:ASN:HA	1:B:368:ARG:HH21	1.74	0.53
1:C:774:ASP:N	1:C:806:SER:O	2.33	0.53
1:C:959:PHE:CE2	1:C:964:ARG:HD2	2.43	0.53
1:A:617:ARG:HD2	1:A:618:PHE:CE2	2.44	0.53
1:A:1061:LYS:HZ3	1:A:1063:LEU:HA	1.74	0.53
1:B:895:VAL:HG22	1:B:899:GLN:NE2	2.24	0.53
1:D:1120:VAL:HG13	1:D:1165:ASP:H	1.74	0.53
1:D:774:ASP:N	1:D:806:SER:O	2.40	0.52
1:A:90:LEU:HD21	1:A:98:HIS:HD2	1.74	0.52
1:A:1114:ALA:HB3	1:A:1170:GLY:HA2	1.89	0.52
1:B:44:ASN:ND2	1:B:116:PRO:O	2.42	0.52
1:C:688:LEU:HD12	1:C:691:GLU:OE1	2.10	0.52
1:C:1064:ALA:HB3	1:C:1077:PHE:CD2	2.44	0.52
1:B:269:ARG:NH1	1:B:270:ARG:HE	2.08	0.52
1:C:581:ARG:HH22	1:C:619:LEU:HD13	1.75	0.52
1:C:1110:GLY:O	1:C:1177:ILE:HB	2.10	0.52
1:D:769:HIS:NE2	1:D:795:ASP:OD1	2.35	0.52
1:A:324:GLU:OE1	1:A:326:ASN:ND2	2.41	0.52
1:A:375:GLN:HB2	1:A:430:ILE:HD13	1.92	0.52
1:C:1123:ILE:HD13	1:C:1162:VAL:HG21	1.92	0.52
1:C:1002:VAL:HG13	1:C:1006:ASP:HB2	1.90	0.52
1:A:1070:ARG:O	1:A:1090:LYS:NZ	2.42	0.52
1:B:353:GLU:HB3	1:B:355:ARG:HE	1.75	0.52
1:C:640:GLN:HG2	1:C:675:ARG:HD2	1.91	0.52
1:C:1080:LEU:HD12	1:C:1085:ARG:HE	1.75	0.52
1:A:563:LEU:HD21	1:A:794:VAL:HG21	1.91	0.52
1:B:717:LYS:HE3	1:B:957:GLY:HA3	1.92	0.52
1:D:501:LEU:HD21	1:D:1060:ILE:HG12	1.92	0.52
1:D:930:GLU:OE1	1:D:930:GLU:N	2.43	0.52
1:A:398:ARG:NH2	1:A:451:ARG:HD2	2.18	0.52
1:C:728:GLU:OE2	1:C:762:ARG:HD3	2.11	0.52
1:A:242:PRO:CD	1:A:479:GLN:HE22	2.23	0.51
1:C:586:ASP:HA	1:C:589:LYS:HE3	1.91	0.51
1:D:1125:VAL:HG11	1:D:1157:VAL:HG21	1.91	0.51
1:B:524:PRO:HA	1:B:1036:ARG:HH21	1.76	0.51
1:B:910:SER:HA	1:B:913:ILE:HD12	1.92	0.51
1:D:624:TRP:CH2	1:D:1009:SER:HB2	2.46	0.51
1:A:242:PRO:HD2	1:A:479:GLN:HE22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:MET:HE1	1:A:643:LEU:HB2	1.92	0.51
1:A:995:VAL:HG23	1:A:1000:GLU:HA	1.92	0.51
1:B:260:LEU:O	1:B:261:TYR:CD1	2.64	0.51
1:B:737:ILE:HG23	1:B:767:PRO:HB2	1.91	0.51
1:C:541:PHE:HB3	1:C:553:PHE:HE1	1.76	0.51
1:C:552:GLY:O	1:C:555:ARG:HD3	2.10	0.51
1:C:743:MET:HG3	1:C:907:VAL:HG12	1.91	0.51
1:D:818:ARG:NH1	1:D:823:ASP:OD1	2.43	0.51
1:A:798:ALA:O	1:A:802:SER:HB3	2.11	0.51
1:B:393:ARG:NH2	1:B:1086:SER:OG	2.34	0.51
1:C:768:LEU:O	1:C:792:ASP:HB2	2.10	0.51
1:D:787:ALA:HA	1:D:791:ALA:HB3	1.91	0.51
1:A:256:ASN:HD22	1:A:358:PRO:HD3	1.75	0.51
1:B:247:VAL:HG22	1:B:262:GLU:OE1	2.11	0.51
1:B:583:ARG:NH2	1:B:1033:LEU:H	2.08	0.51
1:C:1034:ASN:HD22	1:C:1036:ARG:NH2	2.08	0.51
1:D:866:ILE:HG21	1:D:871:TYR:HD1	1.75	0.51
1:A:799:ASP:OD2	1:D:859:SER:OG	2.24	0.51
1:B:574:HIS:HB3	1:B:580:THR:HA	1.91	0.51
1:B:1148:VAL:O	1:D:939:SER:OG	2.28	0.51
1:A:335:VAL:HG12	1:A:430:ILE:CD1	2.40	0.51
1:A:617:ARG:HH21	1:C:1144:LYS:NZ	2.09	0.51
1:A:620:TYR:HB2	1:A:1030:LEU:HD12	1.92	0.51
1:C:575:GLN:H	1:C:575:GLN:CD	2.19	0.51
1:D:508:MET:SD	1:D:508:MET:N	2.82	0.51
1:D:1073:GLN:HB3	1:D:1088:LEU:HD12	1.93	0.51
1:A:332:GLU:O	1:A:335:VAL:HG22	2.10	0.51
1:C:1040:GLN:HG3	1:C:1042:PRO:HD3	1.93	0.51
1:D:987:LEU:H	1:D:987:LEU:HD23	1.76	0.51
1:B:62:ARG:HH22	1:B:82:GLU:HG3	1.76	0.50
1:B:464:ASN:ND2	1:B:487:LEU:O	2.44	0.50
1:C:607:TRP:HB2	1:C:641:MET:HG2	1.94	0.50
1:C:1043:LYS:NZ	1:C:1046:GLU:HB3	2.26	0.50
1:A:639:PHE:HB2	1:A:671:MET:SD	2.51	0.50
1:A:715:ARG:CZ	1:A:718:TYR:HB2	2.42	0.50
1:B:363:ARG:HG3	1:B:364:GLN:H	1.76	0.50
1:B:419:SER:OG	1:B:422:TYR:HB2	2.12	0.50
1:B:818:ARG:HG3	1:B:819:GLY:H	1.76	0.50
1:B:1073:GLN:NE2	1:B:1088:LEU:HB3	2.25	0.50
1:C:1068:LEU:HD22	1:C:1072:GLY:HA2	1.93	0.50
1:D:504:LEU:O	1:D:508:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:702:ALA:HB1	1:D:730:LEU:HD12	1.93	0.50
1:D:810:MET:HE1	1:D:834:TYR:HD2	1.75	0.50
1:A:616:MET:HA	1:A:616:MET:HE2	1.93	0.50
1:C:509:VAL:HG23	1:C:1074:ARG:HH21	1.76	0.50
1:A:502:HIS:CE1	1:A:1087:ILE:HD12	2.45	0.50
1:B:375:GLN:OE1	1:B:430:ILE:HA	2.11	0.50
1:D:726:LEU:O	1:D:730:LEU:HD23	2.11	0.50
1:A:948:LEU:HB3	1:A:968:LEU:HD21	1.94	0.50
1:A:1138:CYS:O	1:A:1149:VAL:N	2.28	0.50
1:B:600:LYS:NZ	1:B:825:GLU:O	2.42	0.50
1:C:906:LYS:HA	1:C:910:SER:HB2	1.94	0.50
1:D:1142:ALA:HB3	1:D:1145:MET:SD	2.52	0.50
1:A:101:ASP:HA	1:A:104:LYS:HG2	1.92	0.50
1:A:947:PHE:HE1	1:A:952:ILE:HB	1.77	0.50
1:B:124:ARG:HB3	1:B:126:ASP:OD1	2.11	0.50
1:B:206:VAL:O	1:B:216:ASN:ND2	2.44	0.50
1:B:1125:VAL:HG11	1:B:1131:VAL:HG22	1.93	0.50
1:A:751:ALA:O	1:A:754:MET:HG3	2.11	0.50
1:A:970:ASP:OD1	1:A:970:ASP:N	2.44	0.50
1:B:486:GLU:O	1:B:489:GLN:NE2	2.29	0.50
1:B:679:SER:HB3	1:B:909:PRO:HG2	1.93	0.50
1:B:810:MET:HE3	1:B:810:MET:HA	1.93	0.50
1:B:896:GLU:O	1:B:900:MET:HG3	2.12	0.50
1:C:558:ARG:HB2	1:C:767:PRO:HG3	1.93	0.50
1:C:850:CYS:SG	1:C:854:MET:HB2	2.52	0.50
1:B:156:ARG:NH2	1:B:171:ASP:HA	2.27	0.50
1:C:926:LEU:HB2	1:C:930:GLU:OE2	2.12	0.50
1:A:1053:GLU:HB2	1:A:1056:LYS:HG3	1.93	0.49
1:B:115:HIS:HB2	1:B:139:ILE:HD12	1.94	0.49
1:B:461:PHE:O	1:B:465:VAL:HG23	2.12	0.49
1:A:41:MET:HE3	1:A:42:VAL:O	2.12	0.49
1:A:183:PHE:O	1:A:321:TYR:OH	2.19	0.49
1:A:336:THR:O	1:A:340:THR:HG22	2.11	0.49
1:A:496:ARG:NH1	1:A:1053:GLU:OE2	2.23	0.49
1:B:495:ASN:N	3:B:2001:ACO:O2A	2.45	0.49
1:B:827:PRO:HD2	1:B:830:ARG:HH21	1.77	0.49
1:B:912:LYS:HD2	2:D:1900:BTI:N2	2.27	0.49
1:B:1039:LEU:HD12	1:B:1040:GLN:N	2.27	0.49
1:B:1159:LYS:NZ	1:B:1176:GLU:OE1	2.28	0.49
1:D:566:MET:HB3	1:D:602:PHE:HD2	1.77	0.49
1:A:622:CYS:HB3	1:A:625:ARG:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HB3	1:A:322:PHE:HB2	1.93	0.49
1:A:170:THR:HB	1:A:322:PHE:HB3	1.93	0.49
1:D:607:TRP:NE1	1:D:627:LEU:HD13	2.26	0.49
1:D:642:LEU:HA	1:D:675:ARG:HG2	1.94	0.49
1:A:291:LEU:HG	1:A:312:PHE:HD2	1.77	0.49
1:A:800:SER:HB2	1:A:839:GLU:HB2	1.94	0.49
1:B:145:VAL:HG11	1:B:304:TYR:HD1	1.77	0.49
1:B:677:PHE:CE2	1:B:907:VAL:HG21	2.48	0.49
1:B:1116:MET:HE1	1:B:1142:ALA:HB2	1.93	0.49
1:A:394:ILE:CG2	1:A:416:ALA:H	2.26	0.49
1:B:866:ILE:HD12	1:B:867:PRO:HD2	1.93	0.49
1:B:1160:VAL:HG12	1:B:1175:LEU:HD21	1.95	0.49
1:C:1033:LEU:HD23	1:C:1033:LEU:H	1.76	0.49
1:B:541:PHE:HB3	1:B:553:PHE:HE1	1.78	0.49
1:D:1047:GLU:HB2	1:D:1061:LYS:HZ3	1.77	0.49
1:A:609:GLY:HA2	1:A:649:VAL:HB	1.93	0.49
1:A:942:ARG:HE	1:A:946:GLU:HG2	1.77	0.49
1:B:920:PHE:O	1:B:924:ASN:HB2	2.12	0.49
1:C:621:GLU:HG2	1:C:1031:ASP:HB3	1.94	0.49
1:C:644:ARG:NH2	1:C:651:TYR:HA	2.27	0.49
1:C:883:LEU:HA	1:C:886:LYS:NZ	2.27	0.49
1:A:640:GLN:OE1	1:A:675:ARG:NE	2.46	0.49
1:C:583:ARG:NH2	1:C:1031:ASP:HA	2.28	0.49
1:A:383:PRO:HA	1:A:387:PHE:CD1	2.48	0.49
1:B:40:VAL:HA	1:B:113:ALA:O	2.13	0.49
1:B:537:PRO:HG3	1:B:635:PRO:HD2	1.95	0.49
1:D:849:ASP:OD1	1:D:851:THR:OG1	2.29	0.49
1:A:584:THR:HG23	1:A:626:ARG:HG3	1.95	0.48
1:A:1132:ALA:HA	1:A:1154:GLU:OE1	2.13	0.48
3:A:1202:ACO:C	1:B:57:THR:HG21	2.42	0.48
1:B:677:PHE:HE2	1:B:907:VAL:HG21	1.78	0.48
1:B:913:ILE:HG12	1:B:943:SER:OG	2.13	0.48
1:C:772:THR:O	1:C:807:GLN:HG2	2.13	0.48
1:D:742:ASP:HB3	1:D:772:THR:HA	1.95	0.48
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.95	0.48
1:B:310:VAL:HG13	1:B:322:PHE:HE1	1.78	0.48
1:B:375:GLN:NE2	1:B:430:ILE:HG13	2.28	0.48
1:B:964:ARG:NH1	1:B:973:ARG:HE	2.11	0.48
1:C:595:ALA:HA	1:C:634:ILE:HG23	1.94	0.48
1:D:704:ILE:HD11	1:D:738:LEU:HD11	1.93	0.48
1:B:117:GLY:O	1:B:122:SER:OG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:HD2	1:B:272:GLN:NE2	2.27	0.48
1:B:720:LEU:HD22	1:B:754:MET:SD	2.54	0.48
3:B:2001:ACO:H51A	3:B:2001:ACO:OAP	2.13	0.48
1:C:1045:ALA:N	1:C:1062:ALA:O	2.33	0.48
1:A:989:ALA:O	1:A:992:LYS:HG3	2.12	0.48
1:A:1164:LYS:NZ	1:A:1165:ASP:OD1	2.44	0.48
1:B:38:LYS:NZ	1:B:112:ASP:HB2	2.29	0.48
1:B:192:ILE:HD11	1:B:238:PHE:CD1	2.48	0.48
1:B:571:ARG:HD2	1:B:575:GLN:HE22	1.79	0.48
1:C:650:GLY:HA3	1:C:654:TYR:HE2	1.79	0.48
1:C:889:GLU:OE1	1:C:889:GLU:N	2.38	0.48
1:D:1072:GLY:HA3	1:D:1090:LYS:HZ3	1.77	0.48
1:A:278:ALA:HB2	1:A:335:VAL:HB	1.96	0.48
1:A:753:THR:HA	1:A:786:CYS:HB3	1.95	0.48
1:C:601:LEU:HD22	1:C:637:ILE:HG21	1.96	0.48
1:D:538:PRO:HG2	1:D:599:SER:HB2	1.96	0.48
1:B:241:LYS:H	1:B:316:ARG:NH1	2.12	0.48
1:B:968:LEU:HD22	1:B:973:ARG:NH2	2.28	0.48
1:C:1101:HIS:CD2	1:C:1172:ASP:HB3	2.49	0.48
1:D:678:ASP:HB2	1:D:686:MET:HE3	1.96	0.48
1:D:854:MET:N	1:D:854:MET:HE2	2.28	0.48
1:D:1006:ASP:OD1	1:D:1007:VAL:N	2.47	0.48
1:A:201:GLY:HA3	1:A:204:MET:HE2	1.96	0.48
1:A:524:PRO:HA	1:A:1036:ARG:NH1	2.25	0.48
1:B:100:PRO:C	1:B:104:LYS:HZ3	2.22	0.48
1:B:451:ARG:HD2	1:B:453:ARG:NH2	2.28	0.48
1:D:1045:ALA:C	1:D:1061:LYS:HD2	2.38	0.48
1:A:935:ALA:HB3	1:A:966:LYS:HB3	1.95	0.48
1:B:272:GLN:N	1:B:272:GLN:OE1	2.46	0.48
1:B:850:CYS:HB3	1:B:854:MET:HB2	1.96	0.48
1:A:121:LEU:HD12	1:A:127:PHE:HB2	1.95	0.48
1:A:948:LEU:HB3	1:A:968:LEU:CD2	2.44	0.48
1:B:571:ARG:HH11	1:B:575:GLN:HE21	1.60	0.48
1:C:936:GLU:HG2	1:C:966:LYS:HB3	1.96	0.48
1:D:500:LEU:HD23	1:D:501:LEU:HD22	1.95	0.48
1:D:748:LYS:HZ2	1:D:750:THR:HG1	1.52	0.48
1:A:40:VAL:HG23	1:A:61:ILE:HG21	1.96	0.48
1:A:249:ILE:HG23	1:A:257:ILE:HG23	1.96	0.48
1:A:859:SER:N	1:D:799:ASP:OD2	2.34	0.48
1:B:1119:LYS:HG3	1:B:1167:THR:HG22	1.96	0.48
1:C:1138:CYS:O	1:C:1149:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:GLY:O	1:D:728:GLU:HB2	2.14	0.48
1:B:538:PRO:HG2	1:B:599:SER:HB3	1.94	0.47
1:B:567:ASP:HA	1:B:796:VAL:O	2.14	0.47
1:B:1036:ARG:O	1:B:1040:GLN:HG3	2.14	0.47
1:D:604:MET:HG2	1:D:606:ASN:HD21	1.79	0.47
1:D:1010:ALA:HB2	1:D:1017:PHE:CD2	2.49	0.47
1:A:907:VAL:HG12	1:A:908:THR:N	2.29	0.47
1:B:614:VAL:HG23	1:B:618:PHE:CD2	2.49	0.47
1:C:1064:ALA:H	1:C:1077:PHE:HB2	1.79	0.47
1:C:1158:ARG:CZ	1:C:1178:GLU:HA	2.44	0.47
1:B:1156:THR:HB	1:B:1158:ARG:HH11	1.79	0.47
1:C:510:ASN:HA	1:C:1093:GLN:HE22	1.79	0.47
1:C:644:ARG:NE	1:C:647:ASN:OD1	2.47	0.47
1:C:702:ALA:HB2	1:C:735:THR:HG21	1.97	0.47
1:C:706:TYR:HE1	1:C:710:VAL:HB	1.80	0.47
1:D:906:LYS:HA	1:D:910:SER:HB2	1.95	0.47
1:A:624:TRP:CE2	1:A:1005:GLU:HB2	2.50	0.47
1:B:582:VAL:HA	1:B:845:TYR:CZ	2.49	0.47
1:B:1133:LYS:HG3	1:B:1154:GLU:HB2	1.96	0.47
1:C:605:GLU:HA	1:C:640:GLN:O	2.14	0.47
1:C:1075:GLN:HE22	1:C:1077:PHE:HD1	1.62	0.47
1:D:512:PRO:HB3	1:D:1039:LEU:O	2.14	0.47
1:D:919:GLN:HA	1:D:922:VAL:HG22	1.96	0.47
1:A:243:ARG:HG3	1:A:244:HIS:N	2.29	0.47
1:A:779:GLY:O	1:A:783:MET:HB2	2.15	0.47
1:C:644:ARG:NH1	1:C:909:PRO:HG3	2.29	0.47
1:C:731:VAL:HG11	1:C:763:PHE:CZ	2.49	0.47
1:C:899:GLN:HG3	1:C:928:ARG:NH2	2.29	0.47
1:D:647:ASN:HA	1:D:654:TYR:HD2	1.79	0.47
1:A:876:PHE:CE2	1:C:1143:MET:HE1	2.49	0.47
1:B:741:LYS:HD2	1:B:771:HIS:HD2	1.79	0.47
1:C:724:MET:O	1:C:728:GLU:HG2	2.14	0.47
1:C:741:LYS:HE3	1:C:743:MET:SD	2.54	0.47
1:C:1044:ILE:HA	1:C:1062:ALA:HB3	1.96	0.47
1:A:180:ALA:HA	1:A:235:VAL:HG21	1.96	0.47
1:A:905:ILE:HG22	1:A:907:VAL:HG23	1.95	0.47
1:A:1161:HIS:N	1:A:1174:ILE:O	2.48	0.47
1:B:105:VAL:HA	1:B:108:GLU:HG2	1.95	0.47
1:B:309:THR:O	1:B:325:VAL:HA	2.15	0.47
1:B:400:GLY:H	1:B:450:PHE:HE1	1.61	0.47
1:B:665:VAL:HG12	1:B:669:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ARG:HE	1:B:716:THR:N	2.12	0.47
1:B:849:ASP:OD1	1:B:850:CYS:N	2.47	0.47
1:B:886:LYS:O	1:B:890:VAL:HG23	2.15	0.47
1:B:933:ALA:O	1:B:966:LYS:NZ	2.39	0.47
1:C:729:GLU:O	1:C:732:ARG:HG3	2.14	0.47
1:C:864:ASN:HB3	1:C:866:ILE:HG13	1.96	0.47
1:A:79:LYS:HE2	3:B:2001:ACO:HH33	1.96	0.47
1:A:908:THR:CG2	1:A:909:PRO:HD3	2.44	0.47
1:B:47:GLU:HG2	1:B:48:ILE:N	2.30	0.47
1:B:608:GLY:O	1:B:611:THR:OG1	2.20	0.47
1:C:571:ARG:HB3	1:C:605:GLU:CD	2.40	0.47
1:C:686:MET:SD	1:C:690:MET:HE3	2.55	0.47
1:C:1174:ILE:HG23	1:C:1175:LEU:HD23	1.96	0.47
1:A:992:LYS:HA	1:A:995:VAL:HG12	1.97	0.47
1:A:1130:LYS:HG3	1:A:1156:THR:HG22	1.96	0.47
1:B:464:ASN:HB3	1:B:487:LEU:HG	1.97	0.47
1:D:720:LEU:HD22	1:D:754:MET:HE1	1.97	0.47
1:D:739:CYS:HB2	1:D:769:HIS:HB3	1.96	0.47
1:A:544:ILE:HG13	1:A:547:ARG:NH2	2.29	0.47
1:A:607:TRP:HZ2	1:A:627:LEU:HB2	1.80	0.47
1:D:571:ARG:HG2	1:D:611:THR:HG21	1.97	0.47
1:D:579:ALA:HA	1:D:873:ASN:OD1	2.15	0.47
1:D:1006:ASP:HB2	1:D:1017:PHE:CZ	2.50	0.47
1:A:720:LEU:HD11	1:A:724:MET:HE2	1.96	0.46
1:A:760:ARG:NH1	1:A:763:PHE:O	2.48	0.46
1:D:907:VAL:HG12	1:D:908:THR:N	2.29	0.46
1:A:374:ILE:O	1:A:430:ILE:HD12	2.15	0.46
1:A:1073:GLN:HB2	1:A:1090:LYS:NZ	2.31	0.46
1:A:1156:THR:OG1	1:A:1158:ARG:NH2	2.39	0.46
1:B:56:CYS:O	1:B:60:GLY:N	2.48	0.46
1:B:270:ARG:C	1:B:271:HIS:HD1	2.24	0.46
1:A:898:ASN:HD21	1:A:903:ASP:HA	1.81	0.46
1:B:506:HIS:CE1	1:B:510:ASN:HD22	2.33	0.46
1:B:609:GLY:HA3	1:B:644:ARG:HH22	1.79	0.46
1:B:1069:ASN:OD1	1:B:1073:GLN:HB3	2.15	0.46
1:B:1117:PRO:HB3	1:B:1169:GLU:HA	1.97	0.46
1:C:1066:SER:O	1:C:1074:ARG:NH1	2.48	0.46
1:D:884:GLY:O	1:D:887:PHE:HB2	2.16	0.46
1:A:195:ALA:HB1	1:A:202:ARG:HH21	1.81	0.46
1:A:1001:GLU:HG2	1:A:1001:GLU:O	2.15	0.46
1:C:639:PHE:H	1:C:672:ASP:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:ALA:HA	1:D:1052:LEU:HD11	1.97	0.46
1:D:743:MET:CE	1:D:869:GLY:H	2.29	0.46
1:A:375:GLN:NE2	1:A:430:ILE:HB	2.31	0.46
1:B:545:LEU:HD11	1:B:699:VAL:HG21	1.98	0.46
1:B:614:VAL:HG23	1:B:618:PHE:HD2	1.80	0.46
1:B:1119:LYS:O	1:B:1141:SER:N	2.46	0.46
1:C:800:SER:OG	1:C:839:GLU:OE1	2.26	0.46
1:C:997:ARG:HG3	1:C:998:HIS:H	1.79	0.46
1:B:571:ARG:NE	1:B:605:GLU:OE2	2.34	0.46
1:B:681:ASN:ND2	1:B:722:TYR:OH	2.48	0.46
1:B:1052:LEU:HG	1:B:1053:GLU:HG2	1.97	0.46
1:C:644:ARG:HA	1:C:677:PHE:H	1.80	0.46
1:C:896:GLU:OE2	1:C:921:MET:HG2	2.15	0.46
1:D:671:MET:HE3	1:D:673:VAL:H	1.81	0.46
1:B:350:HIS:HA	1:B:355:ARG:NH2	2.30	0.46
1:B:783:MET:HE2	1:B:783:MET:HB2	1.74	0.46
1:D:916:ASP:HA	1:D:919:GLN:HE21	1.81	0.46
1:A:550:PRO:HB3	1:A:699:VAL:HG22	1.98	0.46
1:A:551:GLU:OE1	1:A:736:HIS:ND1	2.43	0.46
1:A:626:ARG:O	1:A:629:GLU:HG3	2.15	0.46
1:A:745:GLY:HA2	1:A:772:THR:OG1	2.16	0.46
1:A:883:LEU:HD22	1:A:886:LYS:HE2	1.97	0.46
1:B:374:ILE:HG22	1:B:431:ALA:HB3	1.97	0.46
1:B:724:MET:HE2	1:B:758:SER:HB2	1.98	0.46
1:C:806:SER:OG	1:C:807:GLN:N	2.48	0.46
1:C:1068:LEU:HD23	1:C:1074:ARG:HG2	1.98	0.46
1:D:1023:PHE:HE2	1:D:1030:LEU:HD21	1.81	0.46
1:A:44:ASN:CG	1:A:120:PHE:HB2	2.40	0.46
1:A:916:ASP:HB3	1:C:1145:MET:HE1	1.97	0.46
1:A:1169:GLU:OE2	1:A:1172:ASP:HB3	2.16	0.46
1:B:70:GLN:OE1	1:B:92:PRO:HB3	2.16	0.46
1:B:775:THR:HG22	1:B:861:VAL:HG21	1.97	0.46
1:C:578:LEU:HD23	1:C:848:PHE:CE2	2.49	0.46
1:D:1021:LYS:HD2	1:D:1021:LYS:HA	1.77	0.46
1:A:66:ILE:HD12	1:A:84:TYR:O	2.15	0.46
1:A:438:THR:HG22	1:A:442:LYS:HD2	1.98	0.46
1:A:502:HIS:HE1	1:A:1087:ILE:HD12	1.79	0.46
1:A:629:GLU:OE2	1:A:630:LEU:HG	2.15	0.46
1:B:333:HIS:CG	1:B:334:THR:N	2.84	0.46
1:B:382:ASP:OD2	1:B:385:ARG:NH2	2.49	0.46
1:C:677:PHE:CE1	1:C:704:ILE:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:ARG:HA	1:D:558:ARG:HD2	1.81	0.46
1:D:1066:SER:OG	1:D:1067:ASP:N	2.49	0.46
1:A:291:LEU:HG	1:A:312:PHE:CD2	2.51	0.45
1:A:445:ARG:HD3	1:B:54:ARG:HG3	1.96	0.45
1:A:449:GLU:HG2	1:B:54:ARG:NH1	2.31	0.45
1:A:863:GLU:N	1:A:863:GLU:OE1	2.50	0.45
1:A:1015:ASP:OD1	1:A:1016:VAL:N	2.50	0.45
1:B:648:ALA:HB2	1:B:659:VAL:HG22	1.97	0.45
1:B:824:THR:HG22	1:B:826:VAL:HG23	1.98	0.45
1:D:527:PRO:HD3	1:D:844:LEU:HD11	1.97	0.45
1:D:541:PHE:HB3	1:D:553:PHE:HE1	1.80	0.45
1:A:871:TYR:O	1:A:874:LEU:HB3	2.16	0.45
1:C:794:VAL:HG12	1:C:796:VAL:HG23	1.97	0.45
1:D:949:GLN:NE2	1:D:972:PRO:HB2	2.31	0.45
1:B:269:ARG:HB3	1:B:272:GLN:NE2	2.31	0.45
1:B:402:GLY:H	1:B:405:ILE:HB	1.81	0.45
1:B:494:GLN:H	3:B:2001:ACO:P2A	2.38	0.45
1:C:568:THR:HG21	1:C:807:GLN:HE22	1.81	0.45
1:C:701:GLU:HG3	1:C:737:ILE:HB	1.99	0.45
1:C:726:LEU:HA	1:C:729:GLU:CD	2.41	0.45
1:D:921:MET:O	1:D:925:GLY:N	2.37	0.45
1:A:237:LYS:H	1:A:313:LEU:HD23	1.81	0.45
1:A:436:HIS:HB3	1:A:437:PRO:HD3	1.98	0.45
1:B:126:ASP:O	1:B:129:GLN:NE2	2.50	0.45
1:B:365:GLU:H	1:B:365:GLU:CD	2.25	0.45
1:B:395:GLU:OE1	1:B:454:GLY:HA3	2.17	0.45
1:B:616:MET:HE3	1:B:1020:PHE:HB3	1.98	0.45
1:B:690:MET:HE2	1:B:735:THR:HG22	1.97	0.45
1:B:1162:VAL:O	1:B:1166:MET:HE2	2.16	0.45
1:C:642:LEU:HA	1:C:675:ARG:HB2	1.98	0.45
1:C:1013:TYR:HB3	1:C:1016:VAL:HG22	1.99	0.45
1:D:496:ARG:O	1:D:499:LYS:HG3	2.16	0.45
1:D:818:ARG:NH1	1:D:818:ARG:HA	2.31	0.45
1:D:842:ARG:NH2	1:D:849:ASP:OD1	2.50	0.45
1:A:114:VAL:O	1:A:139:ILE:HG12	2.17	0.45
1:A:850:CYS:SG	1:A:853:THR:HB	2.56	0.45
1:A:877:GLN:O	1:A:881:MET:N	2.46	0.45
1:A:913:ILE:HG23	1:A:944:VAL:HG22	1.98	0.45
1:C:575:GLN:HB3	1:C:580:THR:OG1	2.17	0.45
1:C:595:ALA:HB2	1:C:634:ILE:HA	1.99	0.45
1:C:1013:TYR:HB3	1:C:1016:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:GLU:O	1:D:966:LYS:NZ	2.47	0.45
1:D:1163:THR:OG1	1:D:1166:MET:HE1	2.16	0.45
1:B:406:ARG:HB3	1:B:430:ILE:HB	1.98	0.45
1:B:646:ALA:HB2	1:B:685:ASN:OD1	2.17	0.45
1:C:590:ILE:HD11	1:C:837:TYR:CG	2.52	0.45
1:C:878:ALA:O	1:C:883:LEU:N	2.43	0.45
1:D:754:MET:SD	1:D:755:LEU:HG	2.57	0.45
1:D:951:TYR:O	1:D:978:PRO:HG2	2.17	0.45
1:A:98:HIS:CE1	1:A:100:PRO:HB2	2.51	0.45
1:A:115:HIS:CG	1:A:139:ILE:HG13	2.52	0.45
1:A:123:GLU:OE2	1:A:328:ARG:HD3	2.16	0.45
1:A:383:PRO:HB2	1:A:491:ARG:NH1	2.32	0.45
1:A:897:ALA:HB1	1:A:917:LEU:HD11	1.98	0.45
1:B:311:GLU:HG2	1:B:323:ILE:HB	1.97	0.45
1:B:334:THR:OG1	1:B:406:ARG:NH2	2.50	0.45
1:B:541:PHE:CE2	1:B:602:PHE:HA	2.51	0.45
1:B:612:PHE:CE1	1:B:623:PRO:HG2	2.51	0.45
1:B:961:GLU:N	1:B:962:PRO:HD2	2.32	0.45
1:C:686:MET:O	1:C:690:MET:HG2	2.17	0.45
1:C:740:ILE:HG22	1:C:770:ILE:HA	1.98	0.45
1:C:754:MET:SD	1:C:755:LEU:N	2.89	0.45
1:D:562:GLY:HA2	1:D:822:LEU:HA	1.98	0.45
1:A:44:ASN:OD1	1:A:120:PHE:HB2	2.16	0.45
1:A:254:TYR:CD1	1:A:356:SER:HB3	2.52	0.45
1:A:499:LYS:HB3	1:A:1027:PHE:C	2.42	0.45
1:A:571:ARG:HE	1:A:605:GLU:CD	2.25	0.45
1:A:708:GLY:HA3	1:A:715:ARG:NH2	2.32	0.45
1:B:436:HIS:HB2	1:B:437:PRO:HD3	1.99	0.45
1:D:683:LEU:O	1:D:687:LEU:HG	2.17	0.45
1:D:1049:GLU:HG2	1:D:1059:HIS:CB	2.47	0.45
1:A:269:ARG:HB3	1:A:272:GLN:NE2	2.32	0.45
1:A:1091:ASP:OD1	1:A:1093:GLN:HG3	2.17	0.45
1:B:51:ARG:HH21	1:B:345:VAL:HG22	1.82	0.45
1:B:578:LEU:HG	1:B:848:PHE:O	2.17	0.45
1:C:496:ARG:HD2	1:C:1052:LEU:HD21	1.99	0.45
1:C:1120:VAL:HG13	1:C:1138:CYS:SG	2.57	0.45
1:A:353:GLU:HG2	1:A:355:ARG:NH1	2.32	0.45
1:A:574:HIS:O	1:A:578:LEU:HB3	2.17	0.45
1:A:675:ARG:HH21	1:A:769:HIS:CE1	2.35	0.45
1:B:242:PRO:HB2	1:B:313:LEU:HD11	1.99	0.45
1:B:644:ARG:HA	1:B:677:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:565:LEU:HD21	1:C:824:THR:HG23	1.99	0.45
1:C:849:ASP:CG	1:C:851:THR:HG22	2.42	0.45
1:C:1123:ILE:HD12	1:C:1137:LEU:O	2.17	0.45
1:D:624:TRP:CD2	1:D:1005:GLU:HB3	2.52	0.45
1:D:992:LYS:HA	1:D:995:VAL:HG22	1.98	0.45
1:A:53:PHE:HB2	1:A:79:LYS:HZ3	1.82	0.44
1:A:449:GLU:HG2	1:B:54:ARG:NH2	2.32	0.44
1:B:202:ARG:HH11	1:B:203:GLY:H	1.64	0.44
1:B:443:MET:HE2	1:B:466:LEU:HD11	1.99	0.44
1:B:906:LYS:HA	1:B:910:SER:OG	2.17	0.44
1:C:960:PRO:O	1:C:964:ARG:HG2	2.16	0.44
1:D:701:GLU:OE2	1:D:737:ILE:HB	2.16	0.44
1:C:537:PRO:HG3	1:C:635:PRO:HD2	1.99	0.44
1:C:870:GLN:O	1:C:870:GLN:HG2	2.17	0.44
1:D:724:MET:O	1:D:728:GLU:HG3	2.18	0.44
1:A:53:PHE:HA	1:A:56:CYS:SG	2.57	0.44
1:A:201:GLY:CA	1:A:204:MET:HE2	2.48	0.44
1:A:395:GLU:OE1	1:A:454:GLY:HA3	2.17	0.44
1:A:708:GLY:HA3	1:A:715:ARG:CZ	2.47	0.44
1:A:1049:GLU:OE2	1:A:1058:LEU:N	2.50	0.44
1:A:1140:LEU:N	1:A:1147:THR:O	2.28	0.44
1:B:282:HIS:CG	1:B:282:HIS:O	2.70	0.44
1:B:1144:LYS:HD3	1:B:1144:LYS:HA	1.25	0.44
1:C:1121:ILE:HD11	1:C:1141:SER:HB3	1.98	0.44
1:A:66:ILE:HD11	1:A:86:ILE:HG23	1.99	0.44
1:A:161:ALA:HA	1:A:162:ALA:HA	1.64	0.44
1:A:174:ILE:HG12	1:A:233:LEU:O	2.17	0.44
1:A:286:GLN:HG3	1:A:287:LEU:HD22	1.99	0.44
1:A:337:GLU:O	1:A:341:ASP:HA	2.17	0.44
1:A:532:VAL:HG12	1:A:593:TYR:HD1	1.83	0.44
1:D:564:LEU:O	1:D:794:VAL:HG22	2.17	0.44
1:D:810:MET:HE1	1:D:834:TYR:CD2	2.53	0.44
1:D:827:PRO:HB2	1:D:830:ARG:HG2	1.99	0.44
1:A:479:GLN:HG3	1:A:482:ASP:OD2	2.17	0.44
1:A:584:THR:C	1:A:588:LYS:HZ3	2.25	0.44
1:C:749:PRO:O	1:C:752:CYS:HB3	2.17	0.44
1:A:156:ARG:NH1	1:A:173:PRO:HD2	2.32	0.44
1:A:1152:PRO:HB2	1:A:1153:MET:SD	2.58	0.44
1:B:768:LEU:O	1:B:792:ASP:HB2	2.18	0.44
1:C:1076:VAL:HB	1:C:1087:ILE:HG22	2.00	0.44
1:A:1013:TYR:HB3	1:A:1016:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:GLY:HA2	1:B:413:PHE:CE1	2.52	0.44
1:C:627:LEU:HD22	1:C:669:ASN:HB3	1.99	0.44
1:D:538:PRO:O	1:D:636:ASN:ND2	2.50	0.44
1:A:988:GLN:HA	1:A:991:GLU:HG3	1.99	0.44
1:B:477:ASP:OD1	1:B:477:ASP:N	2.51	0.44
1:B:964:ARG:HH22	1:B:973:ARG:HD3	1.82	0.44
1:B:1047:GLU:OE2	1:B:1059:HIS:HB3	2.17	0.44
1:C:651:TYR:HE2	1:C:912:LYS:HD3	1.82	0.44
1:C:783:MET:CE	1:C:794:VAL:HG13	2.47	0.44
1:D:643:LEU:O	1:D:676:VAL:HA	2.18	0.44
1:D:772:THR:O	1:D:807:GLN:NE2	2.50	0.44
1:A:178:HIS:NE2	1:A:182:GLU:OE2	2.51	0.44
1:A:850:CYS:CB	1:A:872:THR:HG22	2.45	0.44
1:A:942:ARG:NH2	1:A:945:VAL:HG23	2.33	0.44
1:B:91:ALA:O	1:B:95:ALA:N	2.50	0.44
1:B:468:ASN:OD1	1:B:469:GLN:HG3	2.18	0.44
1:B:748:LYS:HD3	1:B:748:LYS:HA	1.62	0.44
1:B:930:GLU:OE2	1:B:934:GLN:NE2	2.50	0.44
1:B:955:PRO:HG3	1:B:959:PHE:HD1	1.83	0.44
1:C:883:LEU:HD23	1:C:886:LYS:HE2	1.99	0.44
1:C:1133:LYS:HB2	1:C:1154:GLU:HG2	1.99	0.44
1:D:655:PRO:O	1:D:658:VAL:HG12	2.18	0.44
1:D:666:ALA:O	1:D:669:ASN:HB2	2.18	0.44
1:A:408:ASP:HB2	1:A:428:LYS:O	2.18	0.43
1:A:601:LEU:HD23	1:A:637:ILE:HG21	2.00	0.43
1:B:279:PRO:HG2	1:B:372:CYS:HA	1.99	0.43
1:B:575:GLN:O	1:B:872:THR:OG1	2.32	0.43
1:C:918:ALA:O	1:C:922:VAL:HG22	2.18	0.43
1:D:623:PRO:HA	1:D:626:ARG:NE	2.33	0.43
1:A:162:ALA:O	1:A:301:GLN:HG3	2.17	0.43
1:A:374:ILE:HB	1:A:443:MET:SD	2.58	0.43
1:A:655:PRO:O	1:A:658:VAL:HG22	2.18	0.43
1:B:268:GLN:O	1:B:481:ILE:HD13	2.19	0.43
1:B:590:ILE:HD11	1:B:837:TYR:CD1	2.53	0.43
1:B:1069:ASN:OD1	1:B:1070:ARG:N	2.45	0.43
1:C:538:PRO:HD2	1:C:595:ALA:O	2.18	0.43
1:C:1044:ILE:HG21	1:C:1065:VAL:HG23	2.01	0.43
1:D:946:GLU:HG2	1:D:951:TYR:CD1	2.52	0.43
1:A:145:VAL:HG22	1:A:148:LYS:HE2	2.00	0.43
1:A:525:THR:N	1:A:1036:ARG:HH22	2.17	0.43
1:A:988:GLN:O	1:A:991:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:LYS:HD2	1:C:816:CYS:HA	1.99	0.43
1:C:1047:GLU:OE2	1:C:1060:ILE:N	2.51	0.43
1:D:604:MET:O	1:D:640:GLN:N	2.51	0.43
1:D:678:ASP:OD2	1:D:681:ASN:N	2.51	0.43
1:D:970:ASP:N	1:D:970:ASP:OD1	2.50	0.43
1:A:45:ARG:NH2	1:A:422:TYR:HB3	2.33	0.43
1:A:86:ILE:HB	1:A:101:ASP:HB3	2.00	0.43
1:A:599:SER:HA	1:A:637:ILE:HD11	2.00	0.43
1:A:769:HIS:CE1	1:A:793:VAL:HG11	2.54	0.43
1:B:873:ASN:OD1	2:D:1900:BTI:H4	2.19	0.43
1:C:987:LEU:HA	1:C:990:LEU:HD23	2.01	0.43
1:D:566:MET:HE2	1:D:769:HIS:NE2	2.34	0.43
1:D:680:LEU:HD13	1:D:954:VAL:C	2.43	0.43
1:A:49:ALA:HA	1:A:52:VAL:HG22	2.01	0.43
1:A:692:ALA:O	1:A:695:SER:OG	2.27	0.43
1:A:1158:ARG:HA	1:A:1158:ARG:NE	2.33	0.43
1:B:196:ALA:HB3	1:B:232:ALA:HB3	2.01	0.43
1:B:253:GLN:C	1:B:254:TYR:HD1	2.27	0.43
1:B:1128:GLY:H	1:B:1157:VAL:HG13	1.83	0.43
1:C:501:LEU:HD21	1:C:1060:ILE:HG12	2.00	0.43
1:C:508:MET:HG2	1:C:1041:GLY:O	2.18	0.43
1:C:577:LEU:HD13	1:C:842:ARG:NH2	2.34	0.43
1:C:581:ARG:NH1	1:C:619:LEU:HB2	2.33	0.43
1:C:914:VAL:HA	1:C:917:LEU:HD12	2.01	0.43
1:B:54:ARG:HA	1:B:57:THR:HG22	2.00	0.43
1:B:216:ASN:HA	1:B:219:ARG:HG2	2.01	0.43
1:B:248:GLN:HE22	1:B:344:LEU:HG	1.82	0.43
1:B:581:ARG:HG3	1:B:848:PHE:CE2	2.53	0.43
1:B:935:ALA:H	1:B:966:LYS:NZ	2.17	0.43
1:B:1049:GLU:OE2	1:B:1057:THR:HG23	2.19	0.43
1:C:590:ILE:HG21	1:C:834:TYR:CE1	2.54	0.43
1:C:1000:GLU:N	1:C:1000:GLU:OE1	2.52	0.43
1:D:796:VAL:HG13	1:D:808:PRO:O	2.18	0.43
1:D:845:TYR:CE2	1:D:1035:THR:HG21	2.53	0.43
1:A:78:GLN:HA	3:B:2001:ACO:C6A	2.49	0.43
1:A:641:MET:HE1	1:A:643:LEU:HD13	2.00	0.43
1:A:800:SER:C	1:A:801:MET:HE2	2.43	0.43
1:A:814:VAL:HG12	1:A:828:MET:HE2	2.01	0.43
1:A:942:ARG:NE	1:A:946:GLU:HG2	2.33	0.43
1:A:1161:HIS:HB2	1:A:1174:ILE:HA	2.00	0.43
1:B:801:MET:SD	1:B:842:ARG:HD2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1121:ILE:HD11	1:C:1141:SER:CB	2.49	0.43
1:D:517:PRO:HA	1:D:879:HIS:CE1	2.53	0.43
1:D:585:HIS:O	1:D:589:LYS:HG3	2.17	0.43
1:D:702:ALA:O	1:D:738:LEU:HD12	2.18	0.43
1:A:36:PRO:HA	1:A:353:GLU:OE1	2.18	0.43
1:A:45:ARG:H	1:A:45:ARG:HD3	1.84	0.43
1:A:237:LYS:HG2	1:A:321:TYR:CE2	2.53	0.43
1:A:239:ILE:C	1:A:241:LYS:H	2.27	0.43
1:B:343:ASP:OD1	1:B:344:LEU:N	2.52	0.43
1:B:443:MET:CE	1:B:466:LEU:HD11	2.49	0.43
1:B:1101:HIS:HE1	1:B:1161:HIS:HB3	1.82	0.43
1:B:1124:LYS:HG3	1:B:1136:PRO:HB2	2.01	0.43
1:C:623:PRO:HA	1:C:626:ARG:HE	1.83	0.43
1:D:576:SER:CA	1:D:869:GLY:HA2	2.46	0.43
1:D:581:ARG:O	1:D:619:LEU:HD11	2.19	0.43
1:D:612:PHE:CD2	1:D:623:PRO:HG2	2.54	0.43
1:D:647:ASN:HB3	1:D:652:THR:O	2.19	0.43
1:A:98:HIS:HE1	1:A:100:PRO:HB2	1.84	0.43
1:A:1045:ALA:HA	1:A:1061:LYS:HE2	2.01	0.43
1:A:1059:HIS:HB2	1:A:1081:ASN:OD1	2.18	0.43
1:B:541:PHE:HE2	1:B:602:PHE:HA	1.84	0.43
1:B:607:TRP:HZ2	1:B:627:LEU:HD23	1.84	0.43
1:B:877:GLN:NE2	1:B:881:MET:HE3	2.34	0.43
1:C:552:GLY:HA2	1:C:555:ARG:NE	2.34	0.43
1:C:620:TYR:C	1:C:1020:PHE:HE1	2.27	0.43
1:C:1069:ASN:OD1	1:C:1070:ARG:N	2.43	0.43
1:C:1159:LYS:HG3	1:C:1161:HIS:CE1	2.54	0.43
1:D:501:LEU:CD1	1:D:1060:ILE:HG21	2.48	0.43
1:D:604:MET:HG2	1:D:606:ASN:ND2	2.33	0.43
1:A:237:LYS:HD3	1:A:237:LYS:HA	1.89	0.43
1:A:394:ILE:HG22	1:A:416:ALA:H	1.82	0.43
1:A:517:PRO:HB3	1:A:879:HIS:CD2	2.54	0.43
1:A:647:ASN:HD22	1:A:651:TYR:HA	1.83	0.43
1:A:748:LYS:HE2	1:D:816:CYS:HA	2.01	0.43
1:A:1174:ILE:HG13	1:A:1175:LEU:N	2.34	0.43
1:B:908:THR:HG23	1:B:909:PRO:CD	2.48	0.43
1:B:1030:LEU:HD13	1:B:1030:LEU:HA	1.86	0.43
1:B:1040:GLN:NE2	1:B:1041:GLY:O	2.51	0.43
1:C:533:PRO:HG2	1:C:596:HIS:HB3	2.01	0.43
1:C:644:ARG:HH21	1:C:647:ASN:ND2	2.17	0.43
1:C:677:PHE:CG	1:C:678:ASP:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1084:LEU:C	1:D:1085:ARG:HD3	2.43	0.43
1:A:464:ASN:ND2	1:A:487:LEU:HA	2.34	0.42
1:B:543:ASP:OD1	1:B:543:ASP:N	2.52	0.42
1:B:604:MET:O	1:B:639:PHE:HA	2.19	0.42
1:C:576:SER:OG	1:C:806:SER:HA	2.18	0.42
1:C:1056:LYS:HE3	1:C:1058:LEU:HD21	2.00	0.42
1:D:881:MET:HE3	1:D:883:LEU:HD12	2.00	0.42
1:D:1094:ALA:O	1:D:1095:MET:HG3	2.19	0.42
1:A:745:GLY:HA3	1:A:773:HIS:O	2.19	0.42
1:A:966:LYS:O	1:A:969:LYS:HE3	2.19	0.42
1:B:877:GLN:HE21	1:B:881:MET:HE3	1.83	0.42
1:B:900:MET:HE2	1:B:900:MET:HB3	1.83	0.42
1:B:1112:ILE:HD12	1:B:1175:LEU:HB2	2.01	0.42
1:C:505:GLY:O	1:C:509:VAL:HG12	2.19	0.42
1:C:881:MET:HA	1:C:881:MET:HE3	2.01	0.42
1:C:974:VAL:HG11	1:C:978:PRO:HB3	2.00	0.42
2:C:1900:BTI:HN2	2:C:1900:BTI:H73	1.73	0.42
1:D:504:LEU:O	1:D:507:VAL:HG12	2.19	0.42
1:D:574:HIS:HE1	1:D:838:TRP:CZ3	2.34	0.42
1:D:686:MET:HE2	1:D:686:MET:HA	2.01	0.42
1:D:732:ARG:HD2	1:D:732:ARG:C	2.45	0.42
1:A:34:TYR:HD2	1:A:137:ARG:HH21	1.67	0.42
1:A:648:ALA:HB1	1:A:662:PHE:CE2	2.55	0.42
1:A:926:LEU:HB2	1:A:930:GLU:CB	2.50	0.42
1:D:801:MET:SD	1:D:801:MET:N	2.93	0.42
1:A:36:PRO:HG2	1:A:38:LYS:HZ1	1.85	0.42
1:A:263:ARG:NH2	1:A:277:ILE:O	2.46	0.42
1:A:756:VAL:HG21	1:A:786:CYS:HB2	2.01	0.42
1:B:470:GLN:HG2	1:B:480:PHE:CD1	2.53	0.42
1:B:558:ARG:HH21	1:B:764:PRO:C	2.27	0.42
1:B:583:ARG:HH21	1:B:1033:LEU:H	1.66	0.42
1:B:1168:LEU:HD12	1:B:1168:LEU:HA	1.91	0.42
1:C:717:LYS:NZ	1:C:957:GLY:HA3	2.34	0.42
1:C:1103:LYS:HG2	1:C:1171:ASP:O	2.19	0.42
1:D:607:TRP:CE2	1:D:627:LEU:HD13	2.54	0.42
1:A:769:HIS:HE2	1:A:795:ASP:CG	2.28	0.42
1:A:850:CYS:SG	1:A:854:MET:HG2	2.59	0.42
1:B:92:PRO:HB2	1:B:421:HIS:CD2	2.55	0.42
1:B:624:TRP:CG	1:B:1005:GLU:HB3	2.53	0.42
1:B:686:MET:SD	1:B:686:MET:N	2.92	0.42
1:B:852:ALA:O	1:B:855:LYS:NZ	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:LEU:HD12	1:B:990:LEU:HB2	2.01	0.42
1:B:1169:GLU:HG3	1:B:1172:ASP:OD2	2.20	0.42
1:C:704:ILE:HG23	1:C:740:ILE:HD12	2.01	0.42
1:C:907:VAL:HG23	1:C:908:THR:N	2.32	0.42
1:C:1107:ASP:OD1	1:C:1108:VAL:N	2.52	0.42
1:A:127:PHE:CE2	1:A:138:PHE:HE1	2.38	0.42
1:C:1158:ARG:HB3	1:C:1159:LYS:HZ2	1.85	0.42
1:D:624:TRP:O	1:D:627:LEU:HB3	2.19	0.42
1:D:642:LEU:HD11	1:D:677:PHE:CD1	2.54	0.42
1:D:896:GLU:HB3	1:D:928:ARG:HD2	2.02	0.42
1:D:1070:ARG:HD2	1:D:1071:ALA:N	2.35	0.42
1:A:501:LEU:HD12	1:A:1078:PHE:CD2	2.54	0.42
1:B:920:PHE:HD2	1:B:921:MET:HE2	1.85	0.42
1:B:964:ARG:HH12	1:B:973:ARG:NE	2.17	0.42
1:B:1131:VAL:HG11	1:B:1137:LEU:HD21	2.01	0.42
1:D:564:LEU:HD21	1:D:600:LYS:NZ	2.34	0.42
1:D:948:LEU:C	1:D:968:LEU:HD11	2.44	0.42
1:D:1095:MET:O	1:D:1096:LYS:HE2	2.20	0.42
1:A:99:ILE:HD13	1:A:99:ILE:HA	1.86	0.42
1:B:435:ASP:H	1:B:438:THR:HB	1.83	0.42
1:B:963:PHE:O	1:B:967:VAL:HG22	2.19	0.42
1:C:726:LEU:O	1:C:730:LEU:HG	2.19	0.42
1:C:1021:LYS:HD3	1:C:1021:LYS:HA	1.76	0.42
1:D:509:VAL:HB	1:D:1089:VAL:HG11	2.01	0.42
1:D:657:ASN:ND2	1:D:985:LEU:O	2.53	0.42
1:D:682:TYR:CE1	1:D:954:VAL:HG12	2.54	0.42
1:D:739:CYS:CB	1:D:769:HIS:HB3	2.50	0.42
1:A:607:TRP:CZ2	1:A:627:LEU:HB2	2.54	0.42
1:A:1030:LEU:C	1:A:1032:SER:H	2.27	0.42
1:C:888:LYS:O	1:C:892:LYS:HG2	2.19	0.42
1:D:639:PHE:C	1:D:671:MET:HE1	2.45	0.42
1:D:705:SER:HA	1:D:741:LYS:HB3	2.02	0.42
1:D:1112:ILE:HB	1:D:1175:LEU:O	2.20	0.42
1:A:855:LYS:NZ	1:D:851:THR:OG1	2.32	0.42
1:A:941:PRO:O	1:A:945:VAL:HG22	2.20	0.42
1:A:1000:GLU:O	1:A:1002:VAL:N	2.52	0.42
1:B:269:ARG:HD2	1:B:272:GLN:HE22	1.85	0.42
1:B:538:PRO:HD2	1:B:595:ALA:O	2.20	0.42
1:B:935:ALA:HB1	1:B:967:VAL:CG1	2.50	0.42
1:C:571:ARG:HG3	1:C:607:TRP:O	2.20	0.42
1:C:677:PHE:HE1	1:C:704:ILE:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:LEU:HA	1:C:729:GLU:OE1	2.19	0.42
1:C:828:MET:HE2	1:C:832:PHE:CE1	2.55	0.42
1:D:621:GLU:HG3	1:D:1031:ASP:HB2	2.01	0.42
1:D:1123:ILE:HG22	1:D:1125:VAL:H	1.85	0.42
1:A:237:LYS:NZ	1:A:321:TYR:HE2	2.18	0.41
1:A:555:ARG:NH2	1:A:767:PRO:HD3	2.31	0.41
1:A:607:TRP:CH2	1:A:623:PRO:HB3	2.54	0.41
1:A:647:ASN:OD1	1:A:647:ASN:N	2.53	0.41
1:A:1084:LEU:HD23	1:A:1085:ARG:N	2.35	0.41
1:A:1098:MET:HE3	1:A:1098:MET:HB3	1.90	0.41
1:B:285:PRO:HA	1:B:288:ARG:CG	2.46	0.41
1:B:362:LEU:HD23	1:B:362:LEU:HA	1.93	0.41
1:B:565:LEU:HD23	1:B:794:VAL:HB	2.02	0.41
1:C:1125:VAL:HG11	1:C:1157:VAL:HG11	2.02	0.41
1:A:285:PRO:O	1:A:288:ARG:HG3	2.18	0.41
1:A:461:PHE:O	1:A:465:VAL:HG23	2.20	0.41
1:B:640:GLN:NE2	1:B:673:VAL:HG21	2.35	0.41
1:B:665:VAL:O	1:B:669:ASN:ND2	2.53	0.41
1:C:646:ALA:HB2	1:C:685:ASN:CG	2.45	0.41
1:C:798:ALA:O	1:C:802:SER:HB3	2.20	0.41
1:D:647:ASN:OD1	1:D:647:ASN:N	2.53	0.41
1:A:82:GLU:OE1	1:B:1056:LYS:HG2	2.20	0.41
1:A:312:PHE:HD1	1:A:322:PHE:HA	1.85	0.41
1:A:990:LEU:HD12	1:A:990:LEU:HA	1.89	0.41
1:B:243:ARG:NH2	1:B:264:ASP:OD2	2.53	0.41
1:B:263:ARG:HH21	1:B:332:GLU:HG2	1.86	0.41
1:B:381:GLU:O	1:B:458:ASN:HB3	2.20	0.41
1:C:921:MET:HE2	1:C:921:MET:HA	2.03	0.41
1:C:921:MET:O	1:C:926:LEU:HD23	2.20	0.41
1:D:592:PRO:HG3	1:D:633:LEU:HD23	2.02	0.41
1:D:994:LEU:HD21	1:D:1010:ALA:HB3	2.02	0.41
1:D:1066:SER:HB3	1:D:1077:PHE:HE1	1.85	0.41
1:A:322:PHE:CE1	1:A:325:VAL:HG23	2.55	0.41
1:A:1073:GLN:HE21	1:A:1088:LEU:HB3	1.86	0.41
1:B:126:ASP:OD1	1:B:126:ASP:N	2.53	0.41
1:B:728:GLU:HA	1:B:731:VAL:HG12	2.02	0.41
1:D:577:LEU:HD22	1:D:842:ARG:HH22	1.85	0.41
1:A:738:LEU:O	1:A:769:HIS:N	2.53	0.41
1:A:1174:ILE:C	1:A:1175:LEU:HD12	2.45	0.41
1:B:260:LEU:HB3	1:B:336:THR:HG21	2.02	0.41
1:B:453:ARG:HD3	1:B:495:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ASN:HD22	1:B:480:PHE:HZ	1.67	0.41
1:B:1048:PHE:CZ	1:B:1060:ILE:HB	2.55	0.41
1:C:1040:GLN:HG3	1:C:1041:GLY:N	2.35	0.41
1:D:725:GLY:O	1:D:729:GLU:OE1	2.38	0.41
1:A:278:ALA:HB1	1:A:339:ILE:HG13	2.03	0.41
1:A:859:SER:O	1:A:860:ASP:HB2	2.21	0.41
1:A:903:ASP:OD1	1:A:903:ASP:N	2.48	0.41
1:A:1143:MET:HG3	1:A:1144:LYS:H	1.86	0.41
1:B:101:ASP:O	1:B:105:VAL:HG23	2.21	0.41
1:B:151:ASP:OD2	1:B:152:LYS:HG3	2.20	0.41
1:B:252:ASP:OD2	1:B:254:TYR:HB2	2.21	0.41
1:B:457:THR:OG1	1:B:458:ASN:N	2.51	0.41
1:B:801:MET:HE1	1:B:842:ARG:HG3	2.02	0.41
1:C:556:ALA:HA	1:C:559:ASN:HD21	1.85	0.41
1:C:705:SER:HA	1:C:741:LYS:HB3	2.03	0.41
1:D:624:TRP:CG	1:D:1005:GLU:HB3	2.56	0.41
1:D:906:LYS:HD3	1:D:914:VAL:HG21	2.02	0.41
1:A:56:CYS:SG	1:A:63:THR:HG22	2.60	0.41
1:A:69:GLU:HG2	1:A:70:GLN:N	2.36	0.41
1:A:156:ARG:CZ	1:A:173:PRO:HD2	2.51	0.41
1:A:193:PHE:HD2	1:A:233:LEU:HD13	1.86	0.41
1:A:263:ARG:CZ	1:A:335:VAL:HG21	2.51	0.41
1:A:381:GLU:OE1	1:A:387:PHE:HA	2.20	0.41
1:A:690:MET:SD	1:A:691:GLU:N	2.94	0.41
1:B:383:PRO:HD3	1:B:458:ASN:HA	2.02	0.41
1:B:765:ASP:OD1	1:B:766:LEU:N	2.54	0.41
1:C:1158:ARG:NE	1:C:1178:GLU:HG3	2.33	0.41
1:D:657:ASN:OD1	1:D:657:ASN:N	2.54	0.41
1:D:814:VAL:O	1:D:818:ARG:HG2	2.20	0.41
1:A:335:VAL:HG23	1:A:336:THR:N	2.36	0.41
1:A:565:LEU:HD23	1:A:565:LEU:H	1.86	0.41
1:B:44:ASN:ND2	1:B:117:GLY:HA3	2.35	0.41
1:B:170:THR:HG21	1:B:174:ILE:HD11	2.02	0.41
1:B:184:SER:OG	1:B:189:PHE:HA	2.21	0.41
1:B:202:ARG:HH11	1:B:203:GLY:N	2.19	0.41
1:B:577:LEU:HB3	1:B:842:ARG:NH2	2.36	0.41
1:B:581:ARG:HD3	1:B:614:VAL:HG21	2.03	0.41
1:B:590:ILE:HD11	1:B:837:TYR:CE1	2.56	0.41
1:B:731:VAL:HG21	1:B:763:PHE:CE1	2.56	0.41
1:B:820:THR:HG22	1:B:822:LEU:H	1.86	0.41
1:B:897:ALA:HB1	1:B:917:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:THR:O	1:B:911:SER:OG	2.25	0.41
1:B:908:THR:CG2	1:B:909:PRO:HD3	2.51	0.41
1:C:799:ASP:HB3	1:C:835:SER:OG	2.21	0.41
1:C:1063:LEU:HD11	1:C:1079:GLU:HB2	2.03	0.41
1:D:671:MET:HE3	1:D:672:ASP:H	1.85	0.41
1:D:774:ASP:HB2	1:D:808:PRO:HG3	2.03	0.41
1:D:780:VAL:CG1	1:D:808:PRO:HB3	2.50	0.41
1:D:948:LEU:HD22	1:D:964:ARG:HG3	2.01	0.41
1:D:1034:ASN:HB2	1:D:1037:LEU:HG	2.02	0.41
1:A:115:HIS:CD2	1:A:139:ILE:HG13	2.56	0.41
1:A:237:LYS:HG2	1:A:321:TYR:CD2	2.56	0.41
1:A:384:ALA:HB2	1:A:491:ARG:HH22	1.85	0.41
1:A:705:SER:HB3	1:A:905:ILE:HG21	2.02	0.41
1:B:444:SER:OG	1:B:466:LEU:HD22	2.21	0.41
1:B:476:VAL:HG12	1:B:477:ASP:O	2.21	0.41
1:C:540:GLY:N	1:C:636:ASN:OD1	2.54	0.41
1:C:760:ARG:HH11	1:C:764:PRO:HA	1.86	0.41
1:C:906:LYS:HA	1:C:910:SER:CB	2.51	0.41
1:A:49:ALA:HB1	1:A:53:PHE:CZ	2.57	0.40
1:A:162:ALA:H	1:A:301:GLN:NE2	2.18	0.40
1:A:322:PHE:CZ	1:A:325:VAL:HG23	2.56	0.40
1:A:350:HIS:O	1:A:353:GLU:HB3	2.21	0.40
1:A:542:ARG:NH1	1:A:631:ARG:NH2	2.69	0.40
1:A:653:ASN:O	1:A:951:TYR:OH	2.38	0.40
1:B:405:ILE:HD11	1:B:442:LYS:HE3	2.03	0.40
1:B:1113:GLY:HA2	1:B:1172:ASP:O	2.21	0.40
1:C:581:ARG:HH22	1:C:619:LEU:CB	2.23	0.40
1:C:765:ASP:OD1	1:C:765:ASP:N	2.55	0.40
1:C:911:SER:O	1:C:915:GLY:N	2.45	0.40
1:C:1080:LEU:HB2	1:C:1083:GLN:HB3	2.03	0.40
1:D:543:ASP:HA	1:D:546:LEU:HD12	2.03	0.40
1:A:565:LEU:HG	1:A:601:LEU:HD12	2.04	0.40
1:B:131:CYS:SG	1:B:136:VAL:HG13	2.61	0.40
1:B:267:ILE:HD13	1:B:476:VAL:HG11	2.03	0.40
1:B:538:PRO:HG2	1:B:636:ASN:HD21	1.86	0.40
1:B:1163:THR:OG1	1:B:1164:LYS:N	2.54	0.40
1:C:552:GLY:O	1:C:555:ARG:NH1	2.54	0.40
1:C:625:ARG:HH21	1:C:628:GLN:NE2	2.19	0.40
1:C:987:LEU:O	1:C:990:LEU:HB2	2.21	0.40
1:A:574:HIS:ND1	1:A:580:THR:HA	2.36	0.40
1:A:1129:ALA:H	1:A:1157:VAL:HG22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:MET:N	1:B:75:MET:SD	2.94	0.40
1:B:270:ARG:O	1:B:271:HIS:ND1	2.54	0.40
1:B:374:ILE:HG22	1:B:439:ALA:HB1	2.03	0.40
1:B:995:VAL:HA	1:B:999:GLY:CA	2.50	0.40
1:C:855:LYS:HE3	1:C:855:LYS:HB3	1.86	0.40
1:C:1138:CYS:SG	1:C:1174:ILE:HD11	2.61	0.40
1:D:702:ALA:CB	1:D:730:LEU:HD12	2.51	0.40
1:D:927:SER:HB3	1:D:930:GLU:OE1	2.22	0.40
1:A:445:ARG:NH1	1:B:54:ARG:HD3	2.36	0.40
1:A:934:GLN:HB2	1:A:937:GLU:OE2	2.20	0.40
1:B:205:ARG:NH1	1:B:219:ARG:HD3	2.37	0.40
1:B:631:ARG:HB3	1:B:632:GLU:OE1	2.21	0.40
1:B:1101:HIS:HE2	1:B:1173:LEU:C	2.22	0.40
1:C:833:ASP:OD1	1:C:834:TYR:N	2.55	0.40
1:D:842:ARG:HH22	1:D:851:THR:HG23	1.86	0.40
1:A:1057:THR:O	3:A:1202:ACO:H2A	2.22	0.40
1:A:1156:THR:O	1:A:1178:GLU:N	2.42	0.40
1:A:1174:ILE:O	1:A:1175:LEU:HD12	2.21	0.40
1:B:265:CYS:SG	1:B:273:LYS:HG3	2.62	0.40
1:B:732:ARG:HA	1:B:732:ARG:NE	2.37	0.40
1:C:644:ARG:HH21	1:C:647:ASN:CG	2.30	0.40
1:C:926:LEU:HD12	1:C:930:GLU:OE2	2.21	0.40
1:D:574:HIS:C	1:D:580:THR:HB	2.47	0.40
1:D:619:LEU:HD23	1:D:619:LEU:HA	1.90	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	1144/1178 (97%)	1041 (91%)	102 (9%)	1 (0%)	48 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1145/1178 (97%)	1050 (92%)	95 (8%)	0	100	100
1	C	682/1178 (58%)	626 (92%)	56 (8%)	0	100	100
1	D	682/1178 (58%)	642 (94%)	38 (6%)	2 (0%)	36	70
All	All	3653/4712 (78%)	3359 (92%)	291 (8%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1095	MET
1	A	495	ASN
1	D	1099	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	942/968 (97%)	942 (100%)	0	100	100
1	B	943/968 (97%)	940 (100%)	3 (0%)	86	85
1	C	564/968 (58%)	564 (100%)	0	100	100
1	D	564/968 (58%)	564 (100%)	0	100	100
All	All	3013/3872 (78%)	3010 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1143	MET
1	B	1144	LYS
1	B	1146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	479	GLN
1	A	484	ASN
1	A	628	GLN
1	A	653	ASN
1	A	771	HIS
1	A	899	GLN
1	A	1099	HIS
1	B	178	HIS
1	B	208	HIS
1	B	248	GLN
1	B	330	GLN
1	B	364	GLN
1	B	470	GLN
1	B	484	ASN
1	B	510	ASN
1	B	597	ASN
1	B	669	ASN
1	B	721	GLN
1	B	807	GLN
1	B	877	GLN
1	B	898	ASN
1	B	899	GLN
1	B	919	GLN
1	B	924	ASN
1	B	1040	GLN
1	C	559	ASN
1	C	597	ASN
1	C	898	ASN
1	C	949	GLN
1	C	1075	GLN
1	C	1161	HIS
1	D	498	GLN
1	D	773	HIS
1	D	1073	GLN
1	D	1093	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACO	B	2001	-	51,53,53	0.38	0	73,79,79	0.49	1 (1%)
2	BTI	B	2002	1	15,16,16	6.45	11 (73%)	20,21,21	2.83	9 (45%)
3	ACO	A	1202	-	51,53,53	0.47	0	73,79,79	0.52	1 (1%)
2	BTI	D	1900	1	15,16,16	6.44	11 (73%)	20,21,21	2.80	9 (45%)
2	BTI	C	1900	1	15,16,16	6.45	11 (73%)	20,21,21	2.78	8 (40%)
2	BTI	A	1201	1	15,16,16	6.43	11 (73%)	20,21,21	2.83	9 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACO	B	2001	-	-	11/51/67/67	0/3/3/3
2	BTI	B	2002	1	-	2/6/27/27	0/2/2/2
3	ACO	A	1202	-	-	23/51/67/67	0/3/3/3
2	BTI	D	1900	1	-	4/6/27/27	0/2/2/2
2	BTI	C	1900	1	-	5/6/27/27	0/2/2/2
2	BTI	A	1201	1	-	3/6/27/27	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1900	BTI	C6-S1	-13.25	1.44	1.81
2	B	2002	BTI	C6-S1	-13.17	1.44	1.81
2	A	1201	BTI	C6-S1	-13.14	1.44	1.81
2	D	1900	BTI	C6-S1	-13.13	1.44	1.81
2	A	1201	BTI	C3-N3	12.46	1.58	1.35
2	C	1900	BTI	C3-N3	12.41	1.58	1.35
2	D	1900	BTI	C3-N3	12.30	1.57	1.35
2	B	2002	BTI	C3-N3	12.28	1.57	1.35
2	B	2002	BTI	C3-N2	8.80	1.51	1.35
2	A	1201	BTI	C3-N2	8.73	1.51	1.35
2	C	1900	BTI	C3-N2	8.72	1.51	1.35
2	D	1900	BTI	C3-N2	8.70	1.51	1.35
2	D	1900	BTI	C5-N3	-8.39	1.33	1.46
2	C	1900	BTI	C5-N3	-8.36	1.33	1.46
2	B	2002	BTI	C5-N3	-8.33	1.33	1.46
2	A	1201	BTI	C5-N3	-8.16	1.34	1.46
2	D	1900	BTI	C2-S1	-7.80	1.70	1.82
2	B	2002	BTI	C2-S1	-7.78	1.70	1.82
2	C	1900	BTI	C2-S1	-7.63	1.70	1.82
2	A	1201	BTI	C2-S1	-7.57	1.70	1.82
2	A	1201	BTI	C6-C5	5.56	1.64	1.53
2	C	1900	BTI	C6-C5	5.54	1.64	1.53
2	D	1900	BTI	C6-C5	5.50	1.64	1.53
2	B	2002	BTI	C6-C5	5.42	1.64	1.53
2	D	1900	BTI	C4-N2	-4.03	1.38	1.45
2	A	1201	BTI	C4-N2	-3.95	1.38	1.45
2	B	2002	BTI	C7-C2	3.94	1.63	1.52
2	C	1900	BTI	C7-C2	3.92	1.63	1.52
2	A	1201	BTI	C7-C2	3.87	1.62	1.52
2	C	1900	BTI	C2-C4	-3.78	1.43	1.53
2	D	1900	BTI	C7-C2	3.76	1.62	1.52
2	C	1900	BTI	C4-N2	-3.74	1.38	1.45
2	B	2002	BTI	C4-N2	-3.71	1.38	1.45
2	B	2002	BTI	C2-C4	-3.71	1.43	1.53
2	D	1900	BTI	C2-C4	-3.66	1.43	1.53
2	A	1201	BTI	C2-C4	-3.65	1.43	1.53
2	B	2002	BTI	C5-C4	3.29	1.65	1.55
2	A	1201	BTI	C5-C4	3.25	1.65	1.55
2	D	1900	BTI	C5-C4	3.17	1.64	1.55
2	C	1900	BTI	C5-C4	3.17	1.64	1.55
2	B	2002	BTI	O3-C3	-2.44	1.18	1.23
2	A	1201	BTI	O3-C3	-2.27	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1900	BTI	O3-C3	-2.26	1.18	1.23
2	C	1900	BTI	O3-C3	-2.09	1.18	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	BTI	C6-S1-C2	7.08	104.70	89.98
2	C	1900	BTI	C6-S1-C2	6.94	104.42	89.98
2	D	1900	BTI	C6-S1-C2	6.39	103.27	89.98
2	B	2002	BTI	C6-S1-C2	6.19	102.85	89.98
2	D	1900	BTI	C4-C5-N3	5.52	108.56	102.43
2	B	2002	BTI	C4-C5-N3	5.28	108.29	102.43
2	A	1201	BTI	C4-C5-N3	5.11	108.11	102.43
2	A	1201	BTI	C5-C4-N2	5.03	108.36	102.68
2	C	1900	BTI	C5-C4-N2	4.98	108.31	102.68
2	C	1900	BTI	C4-C5-N3	4.91	107.89	102.43
2	B	2002	BTI	C5-C4-N2	4.76	108.05	102.68
2	D	1900	BTI	C5-C4-N2	4.57	107.84	102.68
2	B	2002	BTI	C4-N2-C3	-3.99	107.61	112.56
2	A	1201	BTI	C4-N2-C3	-3.97	107.63	112.56
2	B	2002	BTI	C6-C5-N3	-3.88	108.19	113.18
2	C	1900	BTI	C4-N2-C3	-3.85	107.78	112.56
2	D	1900	BTI	C4-N2-C3	-3.67	108.00	112.56
2	D	1900	BTI	C6-C5-N3	-3.42	108.78	113.18
2	D	1900	BTI	C5-N3-C3	-3.14	107.76	112.38
2	A	1201	BTI	C5-N3-C3	-3.05	107.90	112.38
2	B	2002	BTI	C5-N3-C3	-3.00	107.98	112.38
2	C	1900	BTI	C6-C5-N3	-2.88	109.46	113.18
2	B	2002	BTI	C2-C4-C5	-2.85	105.40	108.89
3	B	2001	ACO	P2A-O6A-CCP	-2.71	106.37	121.12
3	A	1202	ACO	P2A-O6A-CCP	-2.68	106.51	121.12
2	B	2002	BTI	C6-C5-C4	-2.68	104.83	109.06
2	D	1900	BTI	C6-C5-C4	-2.68	104.83	109.06
2	C	1900	BTI	C5-N3-C3	-2.66	108.47	112.38
2	D	1900	BTI	C2-C4-C5	-2.45	105.90	108.89
2	C	1900	BTI	C6-C5-C4	-2.38	105.30	109.06
2	A	1201	BTI	C6-C5-N3	-2.35	110.16	113.18
2	B	2002	BTI	C5-C6-S1	-2.34	102.85	106.06
2	A	1201	BTI	C2-C4-N2	-2.34	110.87	113.34
2	A	1201	BTI	C2-C4-C5	-2.22	106.17	108.89
2	A	1201	BTI	C6-C5-C4	-2.21	105.57	109.06
2	C	1900	BTI	C2-C4-C5	-2.19	106.21	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1900	BTI	C8-C7-C2	-2.08	109.27	114.04

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	BTI	C9-C10-C11-O11
2	A	1201	BTI	S1-C2-C7-C8
2	A	1201	BTI	C4-C2-C7-C8
2	B	2002	BTI	S1-C2-C7-C8
2	B	2002	BTI	C4-C2-C7-C8
2	C	1900	BTI	S1-C2-C7-C8
2	C	1900	BTI	C4-C2-C7-C8
2	D	1900	BTI	C9-C10-C11-O11
2	D	1900	BTI	S1-C2-C7-C8
2	D	1900	BTI	C4-C2-C7-C8
3	A	1202	ACO	C5B-O5B-P1A-O2A
3	A	1202	ACO	P1A-O3A-P2A-O6A
3	A	1202	ACO	CCP-O6A-P2A-O3A
3	A	1202	ACO	CCP-O6A-P2A-O4A
3	A	1202	ACO	CCP-O6A-P2A-O5A
3	A	1202	ACO	CDP-CBP-CCP-O6A
3	A	1202	ACO	CEP-CBP-CCP-O6A
3	A	1202	ACO	CAP-CBP-CCP-O6A
3	A	1202	ACO	O9P-C9P-CAP-CBP
3	A	1202	ACO	N8P-C9P-CAP-OAP
3	A	1202	ACO	C3P-C2P-S1P-C
3	B	2001	ACO	CDP-CBP-CCP-O6A
3	B	2001	ACO	CEP-CBP-CCP-O6A
3	B	2001	ACO	CAP-CBP-CCP-O6A
3	B	2001	ACO	C3P-C2P-S1P-C
3	B	2001	ACO	O-C-S1P-C2P
3	B	2001	ACO	CH3-C-S1P-C2P
3	B	2001	ACO	C3B-C4B-C5B-O5B
3	B	2001	ACO	O4B-C4B-C5B-O5B
3	A	1202	ACO	C2B-C3B-O3B-P3B
3	A	1202	ACO	C4B-C3B-O3B-P3B
3	A	1202	ACO	O9P-C9P-CAP-OAP
3	A	1202	ACO	S1P-C2P-C3P-N4P
3	A	1202	ACO	N8P-C9P-CAP-CBP
3	B	2001	ACO	P1A-O3A-P2A-O6A
3	A	1202	ACO	C9P-CAP-CBP-CEP

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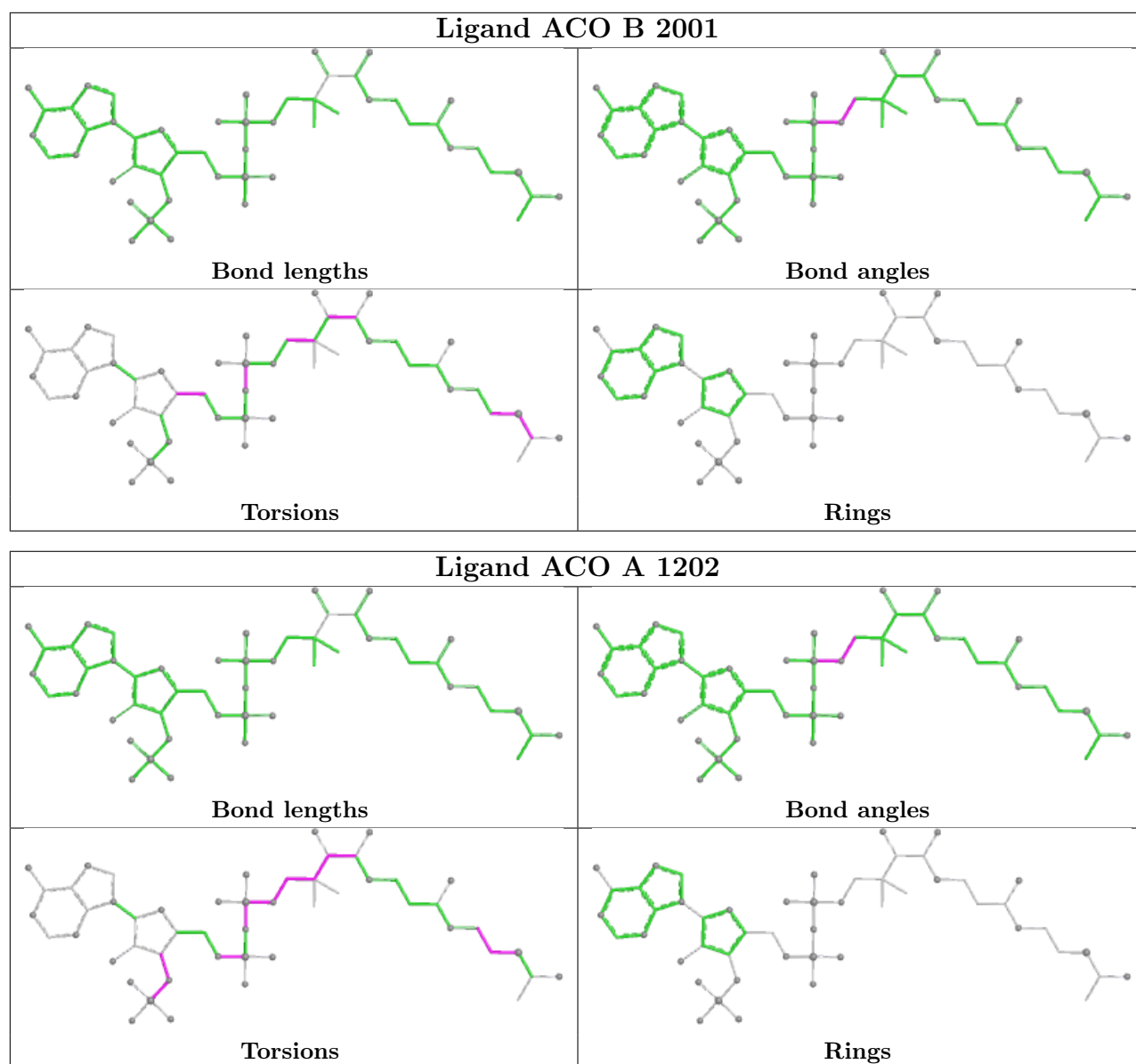
Mol	Chain	Res	Type	Atoms
2	C	1900	BTI	C11-C10-C9-C8
3	A	1202	ACO	C9P-CAP-CBP-CCP
3	A	1202	ACO	C5B-O5B-P1A-O1A
3	A	1202	ACO	C5B-O5B-P1A-O3A
2	C	1900	BTI	C2-C7-C8-C9
3	A	1202	ACO	C3B-O3B-P3B-O7A
3	A	1202	ACO	C9P-CAP-CBP-CDP
3	B	2001	ACO	P1A-O3A-P2A-O4A
2	D	1900	BTI	C7-C8-C9-C10
3	A	1202	ACO	CBP-CCP-O6A-P2A
2	C	1900	BTI	C7-C8-C9-C10
3	B	2001	ACO	N8P-C9P-CAP-OAP

There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	ACO	10	0
2	B	2002	BTI	2	0
3	A	1202	ACO	7	0
2	D	1900	BTI	5	0
2	C	1900	BTI	4	0
2	A	1201	BTI	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

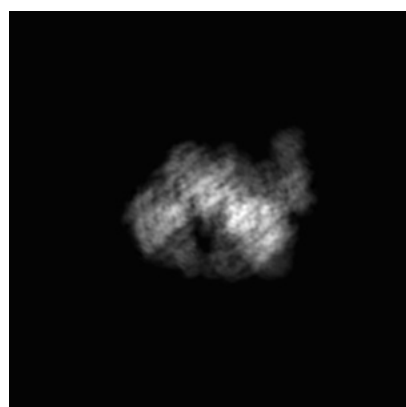
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32778. These allow visual inspection of the internal detail of the map and identification of artifacts.

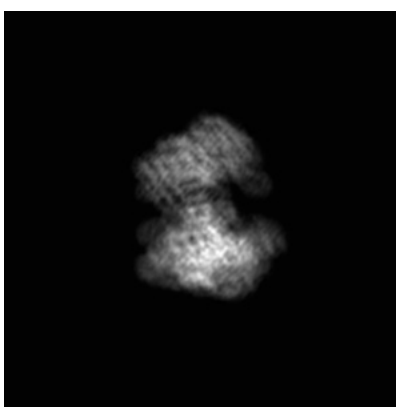
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

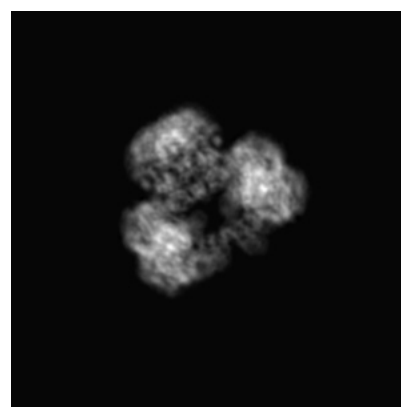
6.1.1 Primary map



X



Y



Z

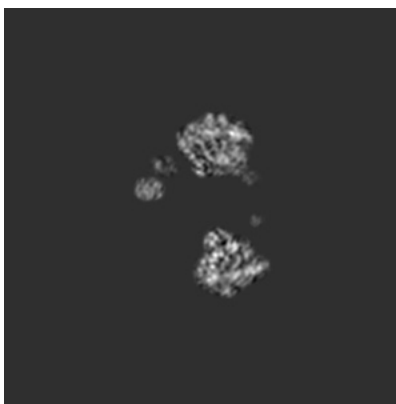
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

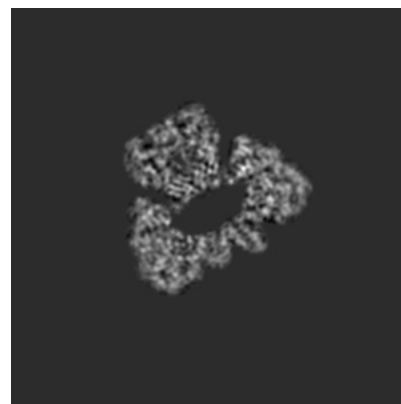
6.2.1 Primary map



X Index: 144



Y Index: 144

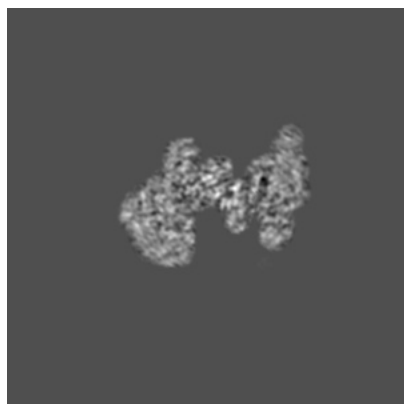


Z Index: 144

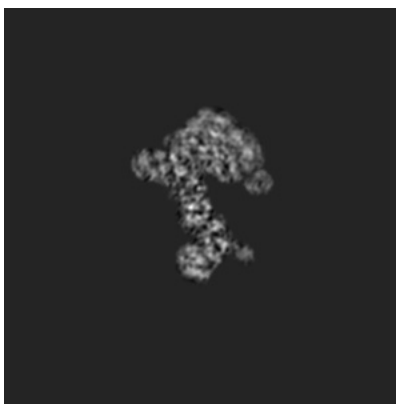
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

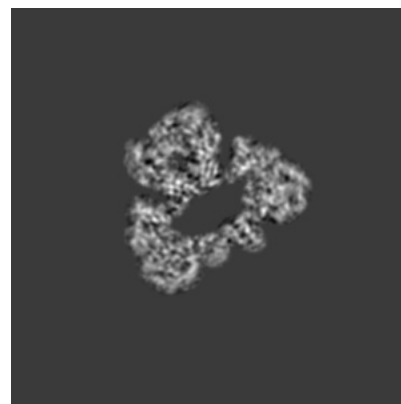
6.3.1 Primary map



X Index: 114



Y Index: 161

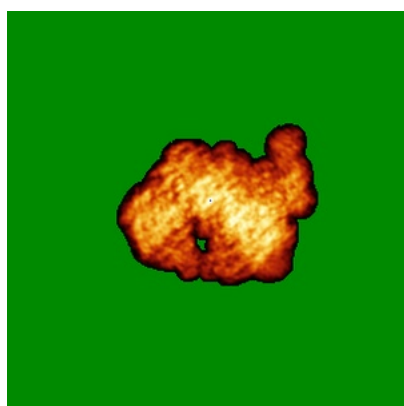


Z Index: 146

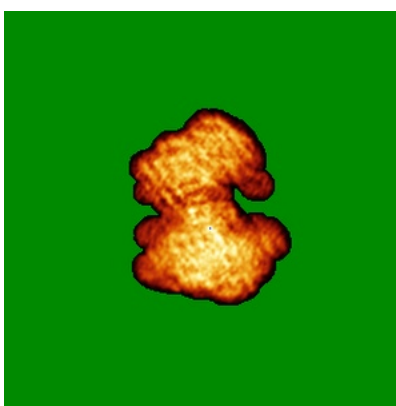
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

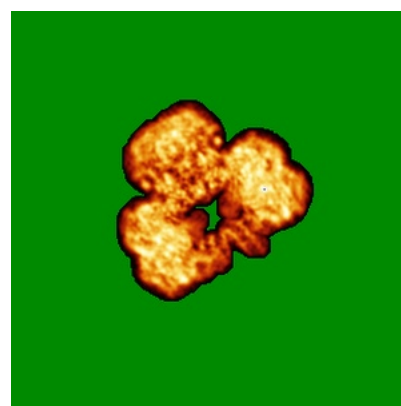
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

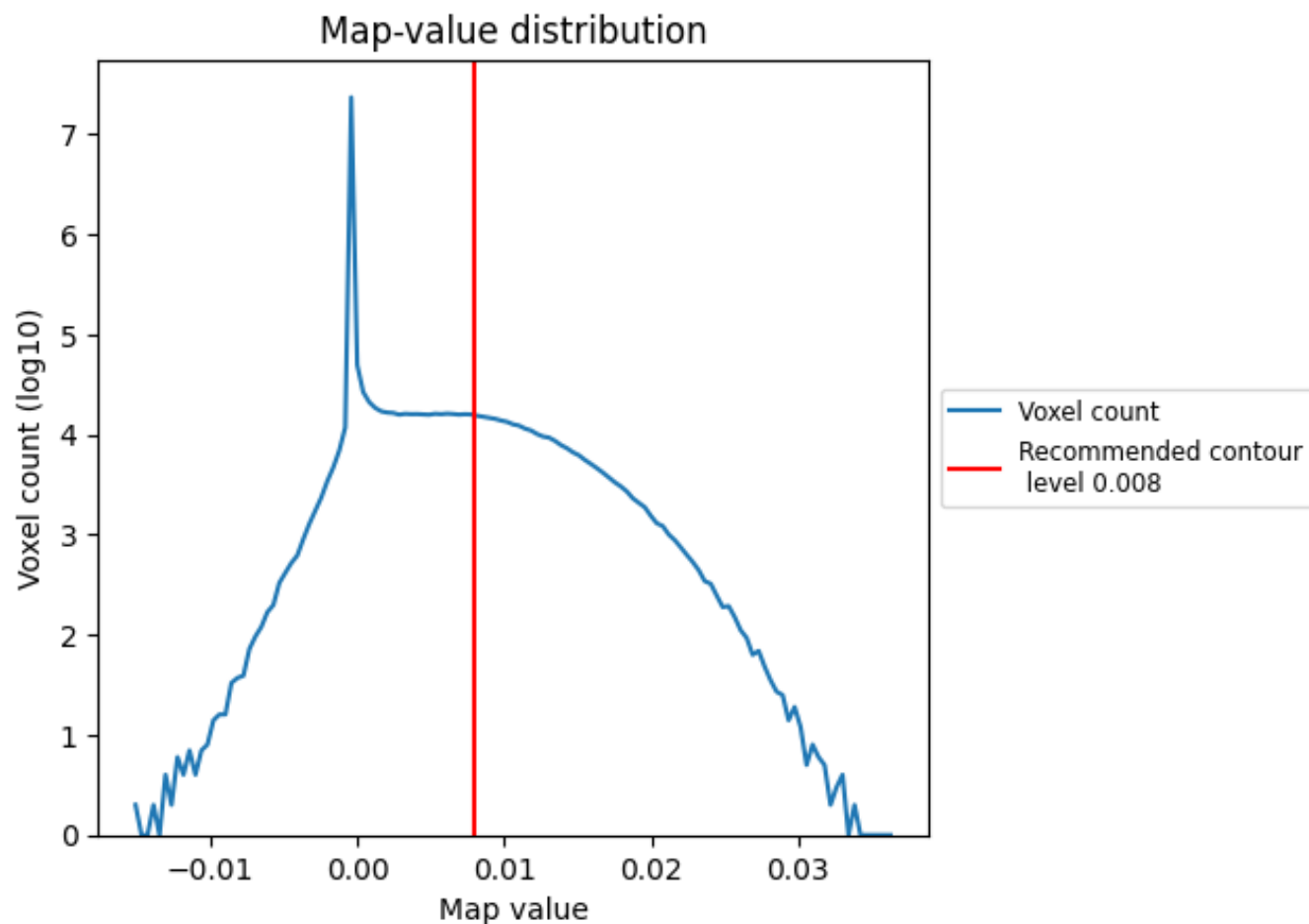
6.6 Mask visualisation

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

7 Map analysis [i](#)

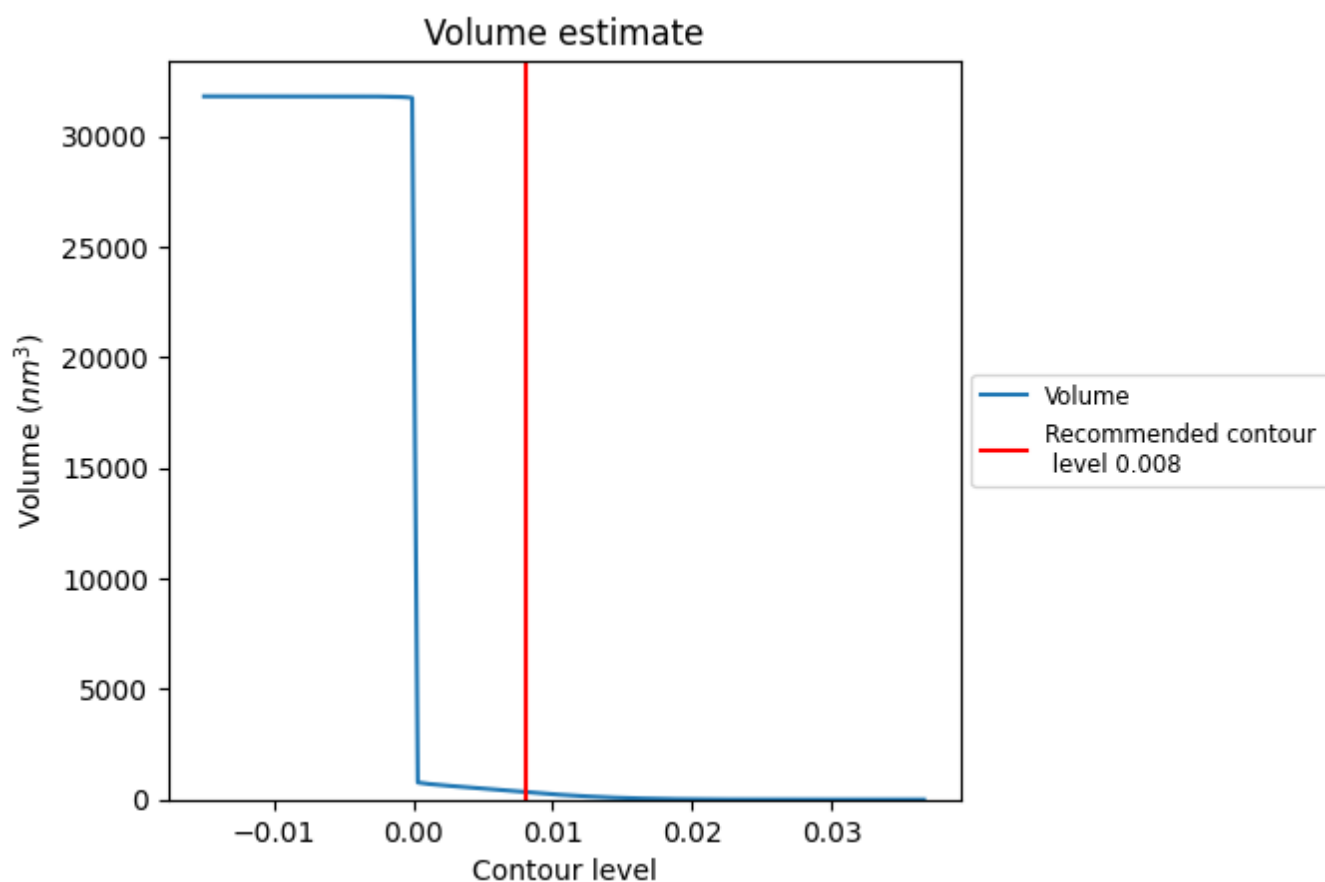
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

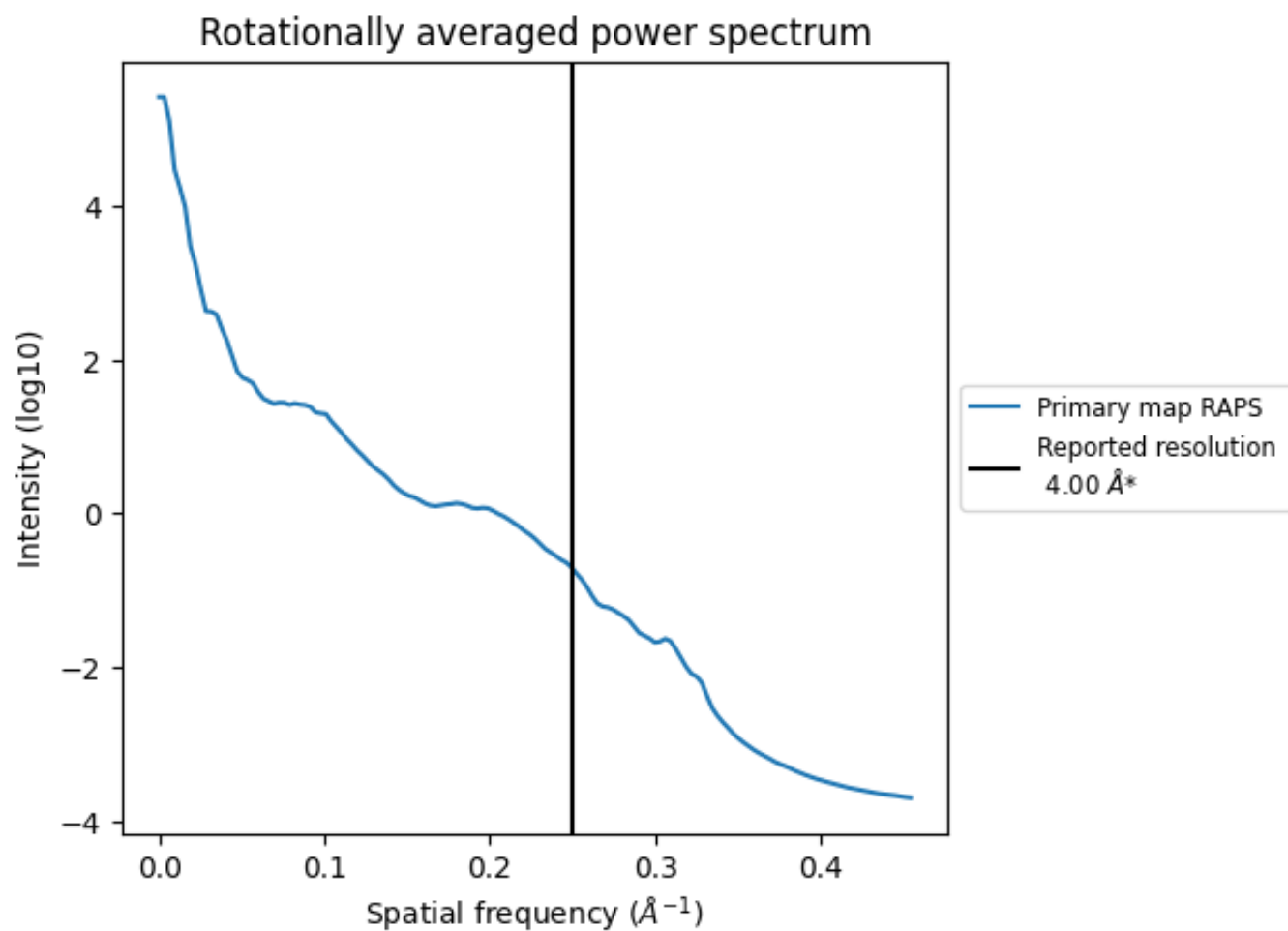
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 306 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation

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

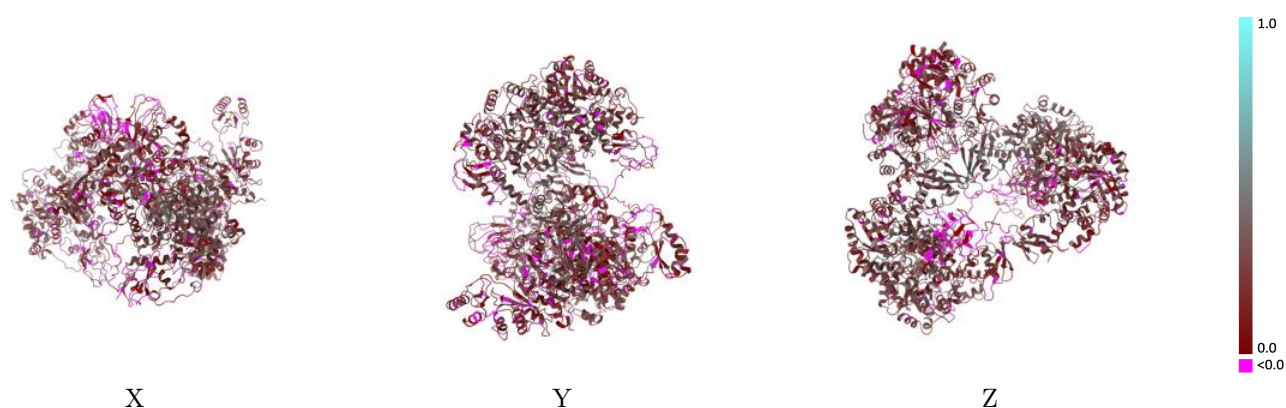
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32778 and PDB model 7WTC. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

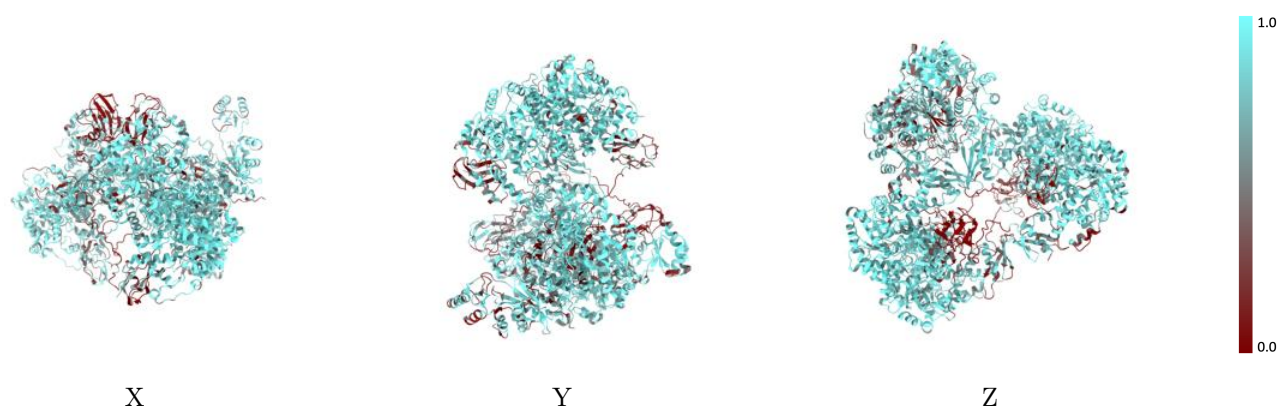
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



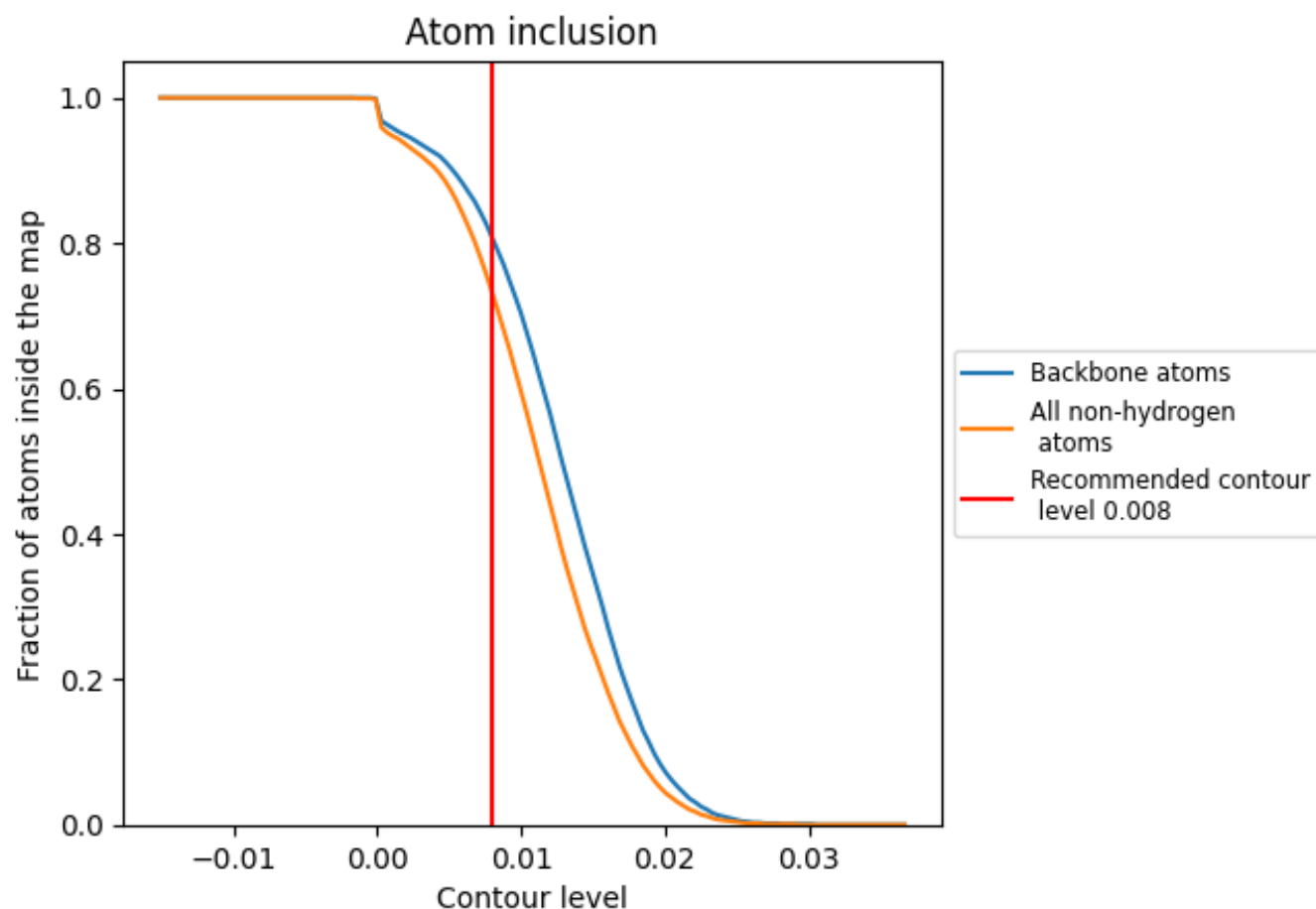
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7320	0.2160
A	0.7570	0.2280
B	0.7290	0.2240
C	0.7310	0.2070
D	0.6970	0.1920

