



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:52 AM UTC

PDB ID : 7CHW / pdb_00007chw
EMDB ID : EMD-30376
Title : Cryo-EM structure of an Escherichia coli RNAP-promoter open complex (RPo)
Authors : Lin, W.; Feng, Y.
Deposited on : 2020-07-06
Resolution : 3.58 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:

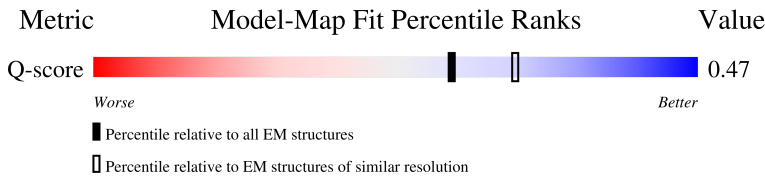
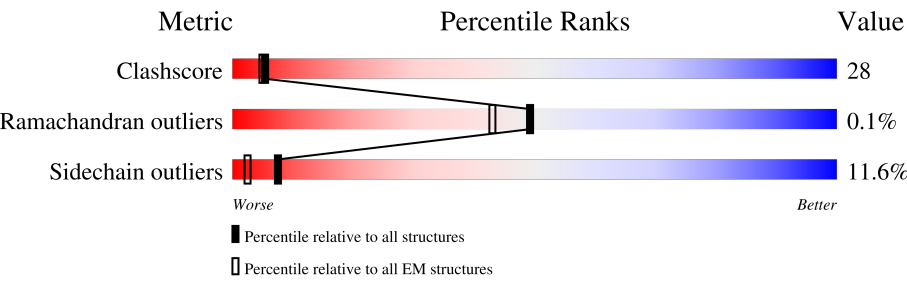
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.58 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	12629 (3.08 - 4.08)

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	H	63	 37% 43% 57%
2	A	329	 36% 31% 30%
2	B	329	 8% 33% 31% 5% 31%
2	K	329	 20% 13% 8% 80%

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Mol	Chain	Length	Quality of chain
3	C	1342	8% 54% 41% 5%
4	D	1407	16% 49% 41% 6% 5%
5	E	91	8% 42% 36% 5% 16%
6	F	613	32% 33% 40% • 23%
7	G	63	30% 17% 60% 22%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 32282 atoms, of which 529 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 DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	63	Total	C	N	O	P	0	0
			1312	623	256	370	63		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	K	67	Total	C	H	N	O	S	0	0
			1046	328	529	88	99	2		
2	A	230	Total	C	N	O	S		0	0
			1787	1112	317	352	6			
2	B	228	Total	C	N	O	S		0	0
			1767	1100	312	349	6			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1339	Total	C	N	O	S	0	0
			10561	6626	1840	2052	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1343	Total	C	N	O	S	0	0
			10363	6509	1846	1958	50		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	76	Total	C	N	O	S	0	0
			606	367	115	123	1		

- Molecule 6 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	472	Total	C	N	O	S	0	0
			3845	2408	685	729	23		

- Molecule 7 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	49	Total	C	N	O	P	0	0
			992	478	164	301	49		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

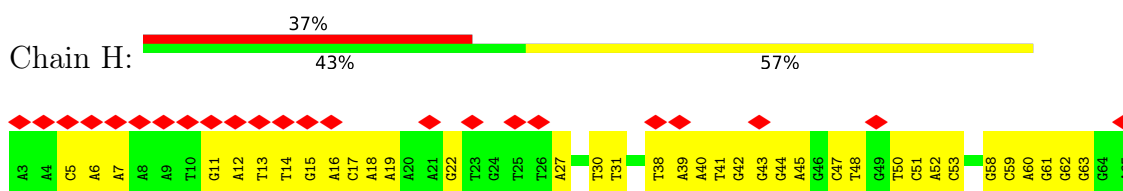
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

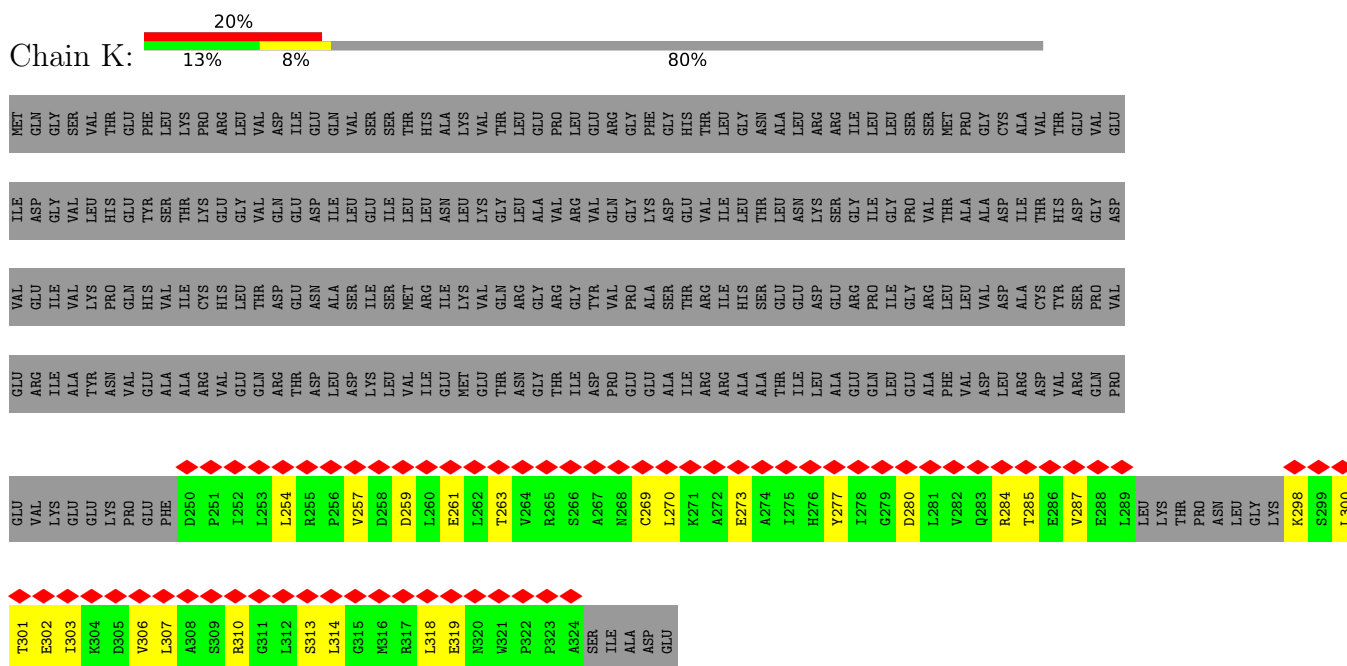
3 Residue-property plots

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.

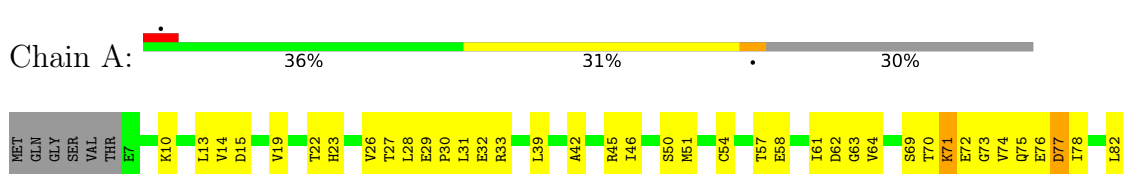
- Molecule 1: DNA (63-MER)

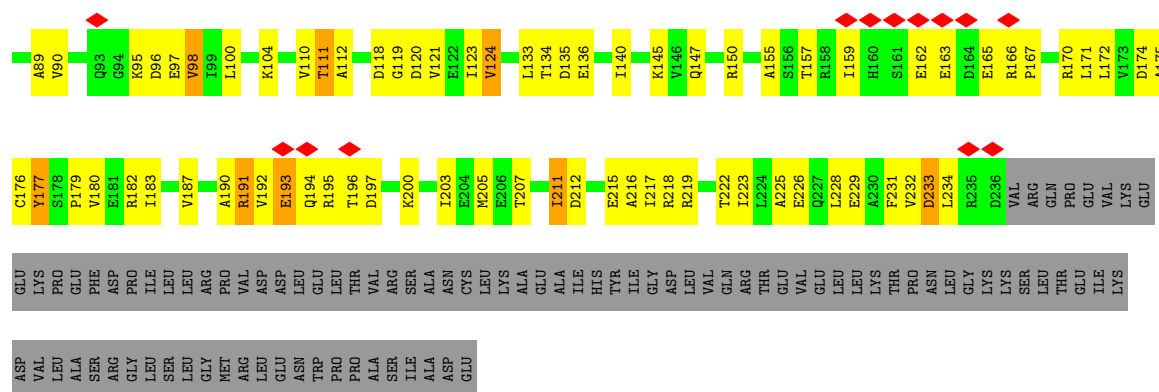


- Molecule 2: DNA-directed RNA polymerase subunit alpha

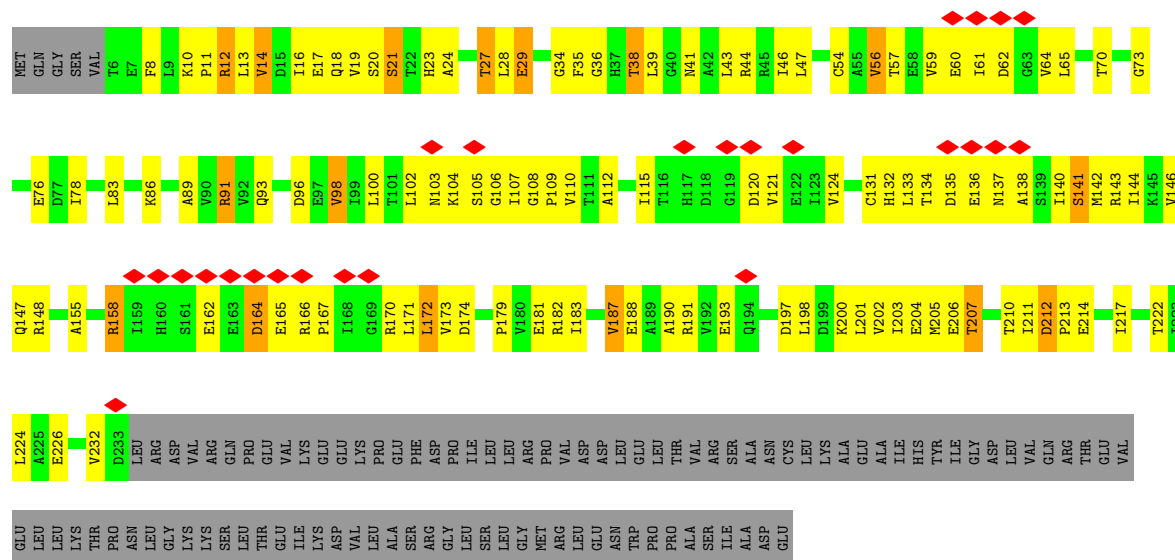


- Molecule 2: DNA-directed RNA polymerase subunit alpha

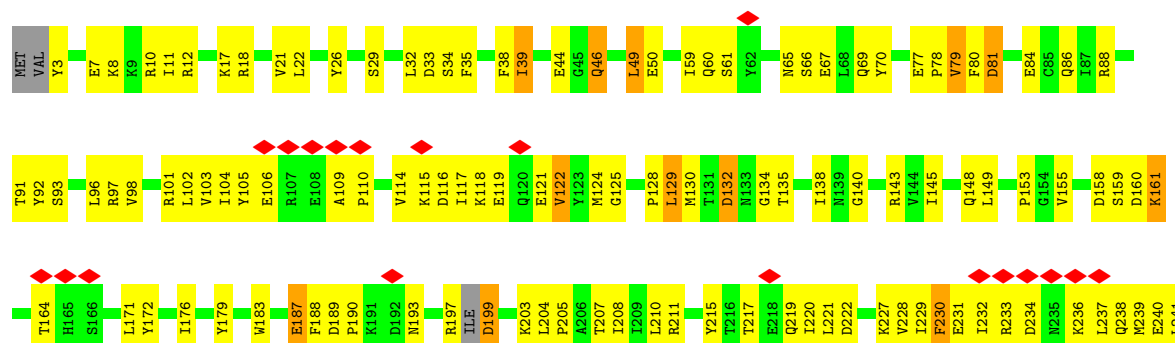


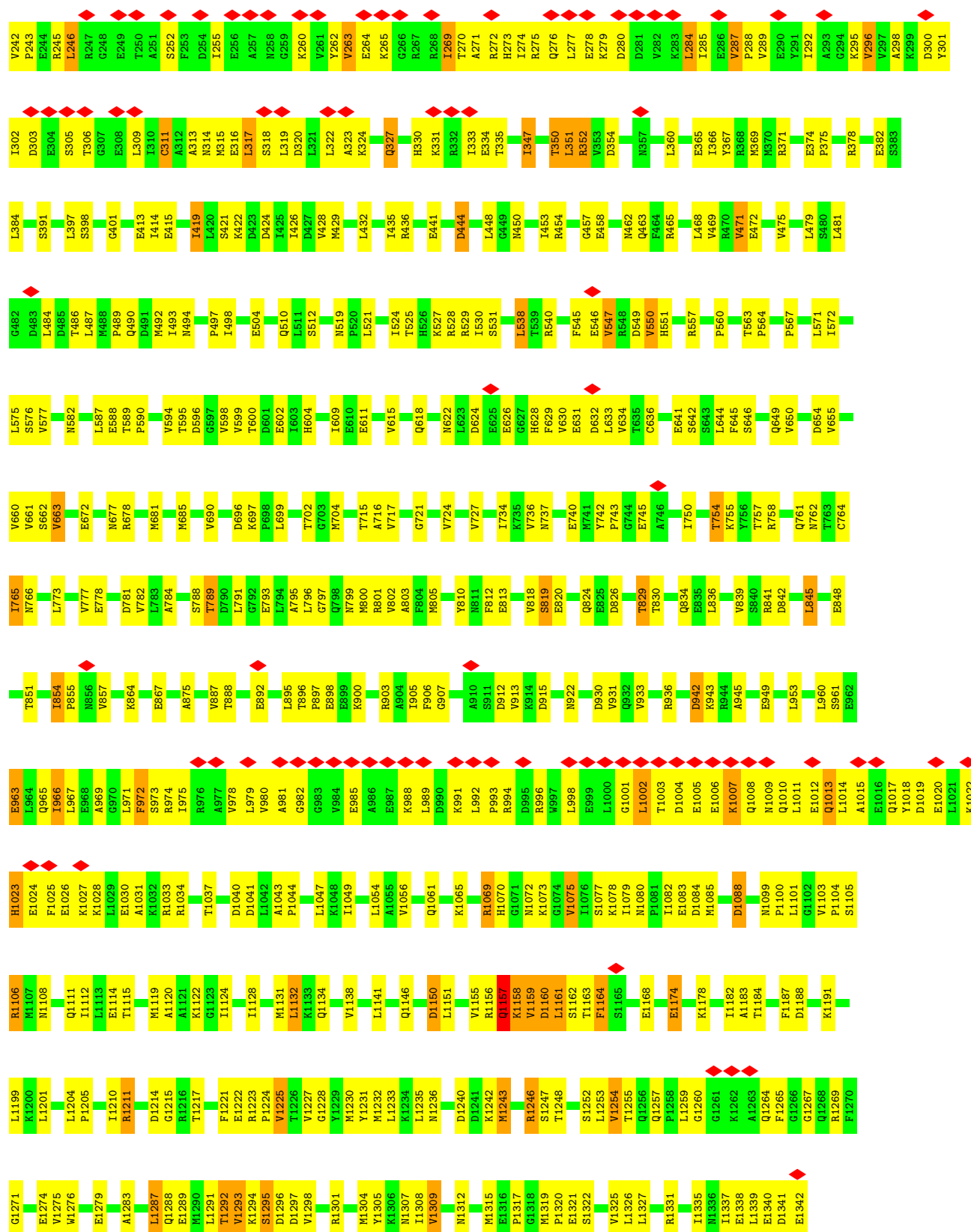


• Molecule 2: DNA-directed RNA polymerase subunit alpha

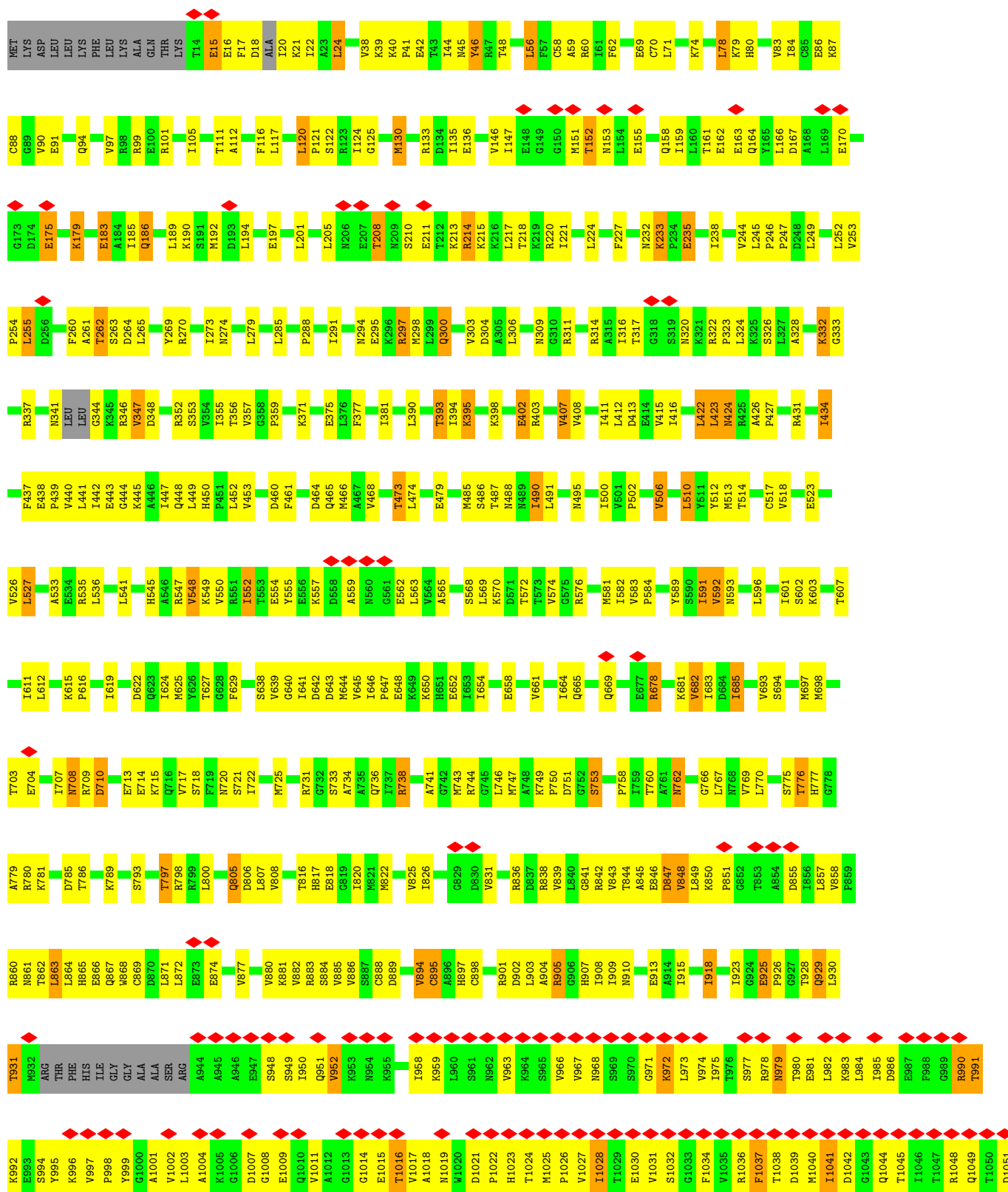


• Molecule 3: DNA-directed RNA polymerase subunit beta

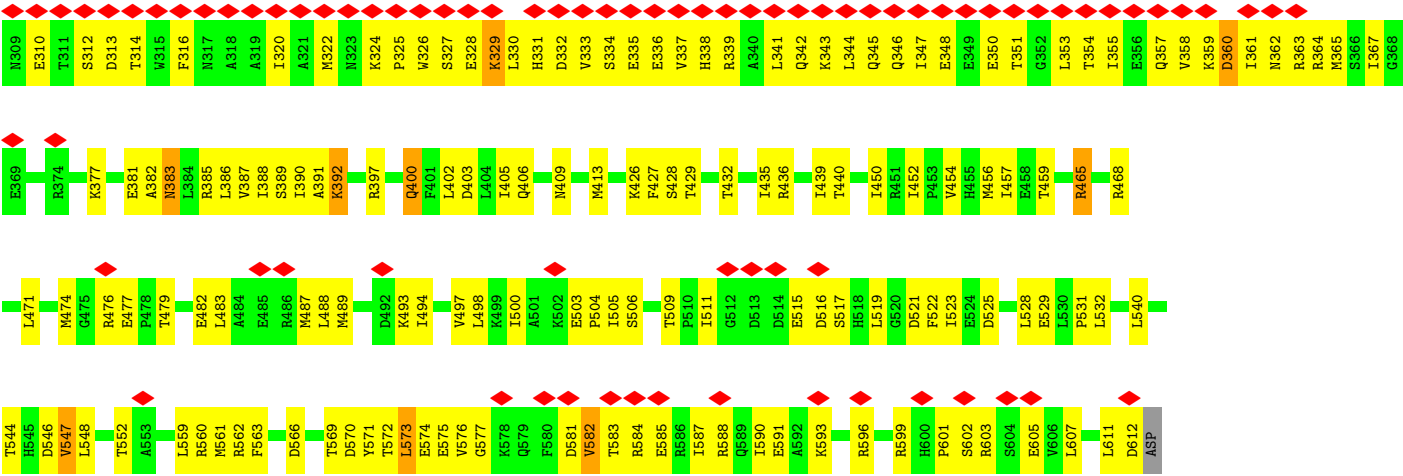




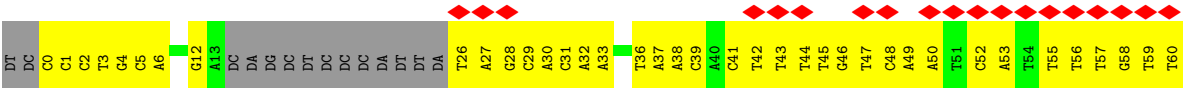
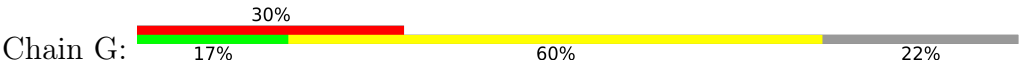
- Molecule 4: DNA-directed RNA polymerase subunit beta'







• Molecule 7: DNA (63-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199208	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 ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.219	Depositor
Minimum map value	-0.168	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0259	Depositor
Map size ($\text{\AA}$)	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3069999, 1.3069999, 1.3069999	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H	0.22	0/1478	0.36	0/2283
2	A	0.33	0/1809	0.52	0/2451
2	B	0.27	0/1789	0.44	0/2425
2	K	0.27	0/523	0.54	0/710
3	C	0.35	0/10729	0.51	2/14474 (0.0%)
4	D	0.33	0/10515	0.51	1/14198 (0.0%)
5	E	0.32	0/604	0.58	0/807
6	F	0.22	0/3896	0.45	0/5236
7	G	0.23	0/1106	0.40	0/1700
All	All	0.32	0/32449	0.49	3/44284 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1160	ASP	N-CA-C	8.04	120.30	110.41
4	D	333	GLY	N-CA-C	5.46	117.75	111.36
3	C	1157	GLN	N-CA-C	5.30	117.13	111.36

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	H	1312	0	709	63	0
2	A	1787	0	1810	91	0
2	B	1767	0	1789	110	0
2	K	517	529	528	9	0
3	C	10561	0	10575	562	0
4	D	10363	0	10510	655	0
5	E	606	0	609	31	0
6	F	3845	0	3913	318	0
7	G	992	0	560	53	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	31753	529	31003	1760	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 28.

All (1760) 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)
4:D:17:PHE:CZ	4:D:1353:VAL:HG11	1.59	1.36
4:D:17:PHE:HZ	4:D:1353:VAL:CG1	1.52	1.23
3:C:1342:GLU:HG3	4:D:18:ASP:OD1	1.45	1.15
3:C:1002:LEU:HD23	3:C:1007:LYS:HB2	1.37	1.06
3:C:1146:GLN:OE1	3:C:1160:ASP:HB3	1.57	1.05
6:F:261:LEU:HD11	6:F:265:GLN:HB3	1.40	1.03
4:D:17:PHE:CZ	4:D:1353:VAL:CG1	2.33	1.03
4:D:930:LEU:HD13	4:D:1244:GLN:HB3	1.40	1.02
3:C:1160:ASP:OD1	3:C:1161:LEU:N	1.91	1.02
4:D:252:LEU:HD12	4:D:262:THR:HB	1.39	1.02
4:D:1109:LEU:HD13	4:D:1115:ILE:HG21	1.44	0.99
4:D:17:PHE:HZ	4:D:1353:VAL:HG11	0.85	0.99
6:F:231:THR:HG21	6:F:252:LEU:HB2	1.40	0.99
3:C:232:ILE:HG12	3:C:237:LEU:HD22	1.45	0.99
3:C:1260:GLY:HA3	3:C:1265:PHE:HA	1.42	0.97
6:F:292:VAL:HG21	6:F:299:LYS:HG3	1.46	0.96
4:D:1280:VAL:HG11	4:D:1304:ARG:HH21	1.27	0.95
4:D:1027:VAL:HG22	4:D:1102:PRO:HD2	1.49	0.95
2:B:86:LYS:HE2	2:B:174:ASP:HB2	1.48	0.95
4:D:982:LEU:HB2	4:D:995:TYR:HB2	1.47	0.95
2:A:104:LYS:HD3	2:A:110:VAL:HG22	1.50	0.94
4:D:1167:LYS:HE3	4:D:1170:LYS:HD3	1.50	0.94
4:D:79:LYS:HB3	6:F:569:THR:HB	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:885:VAL:HG11	4:D:1255:VAL:HG12	1.51	0.92
3:C:119:GLU:HB2	3:C:489:PRO:HD2	1.52	0.90
6:F:364:ARG:HA	6:F:367:ILE:HD12	1.50	0.90
2:B:104:LYS:HG2	2:B:110:VAL:HG22	1.53	0.90
3:C:1158:LYS:HA	3:C:1158:LYS:NZ	1.86	0.90
3:C:398:SER:HB2	3:C:401:GLY:H	1.32	0.90
3:C:982:GLY:HA3	3:C:1002:LEU:HG	1.49	0.90
4:D:845:ALA:HB3	4:D:881:LYS:HG2	1.53	0.90
3:C:164:THR:HG21	3:C:171:LEU:HG	1.54	0.89
2:A:100:LEU:HD21	2:A:121:VAL:HG11	1.55	0.89
3:C:1158:LYS:HA	3:C:1158:LYS:HZ2	1.34	0.89
3:C:1342:GLU:CG	4:D:18:ASP:OD1	2.20	0.89
6:F:288:MET:HG3	6:F:299:LYS:HD2	1.55	0.89
6:F:247:GLU:HA	6:F:250:LEU:HD12	1.55	0.89
3:C:106:GLU:HG2	3:C:109:ALA:HB3	1.54	0.88
2:B:105:SER:HB3	2:B:138:ALA:HB1	1.53	0.88
3:C:982:GLY:HA2	3:C:1003:THR:HG23	1.53	0.88
4:D:1280:VAL:HG21	4:D:1304:ARG:HE	1.36	0.88
4:D:905:ARG:HH21	4:D:907:HIS:HB2	1.39	0.88
6:F:223:GLU:HA	6:F:226:ALA:HB3	1.56	0.87
3:C:975:ILE:HA	3:C:978:VAL:HB	1.57	0.87
6:F:577:GLY:HA3	6:F:583:THR:HG22	1.56	0.86
6:F:331:HIS:HA	6:F:334:SER:HB2	1.56	0.86
6:F:547:VAL:HG11	6:F:607:LEU:HD11	1.57	0.86
5:E:34:GLY:O	5:E:35:LYS:HD3	1.75	0.85
4:D:1024:THR:HG22	4:D:1026:PRO:HD3	1.58	0.85
4:D:1042:ASP:HB3	4:D:1048:ARG:HB2	1.56	0.85
4:D:1341:ARG:HG2	4:D:1341:ARG:HH11	1.38	0.85
4:D:800:LEU:HD22	4:D:1256:ILE:HD13	1.58	0.85
6:F:161:LEU:HG	6:F:162:ILE:HG12	1.58	0.85
4:D:161:THR:HG22	4:D:164:GLN:HG3	1.56	0.85
5:E:4:VAL:HG23	5:E:5:THR:HG23	1.59	0.85
2:A:222:THR:HG22	2:B:232:VAL:HA	1.57	0.85
4:D:322:ARG:HG2	4:D:323:PRO:HD2	1.57	0.85
7:G:47:DT:H1'	7:G:48:DC:H5'	1.57	0.84
4:D:1037:PHE:HB3	4:D:1041:ILE:HD13	1.59	0.83
4:D:929:GLN:HG2	4:D:930:LEU:HG	1.60	0.83
4:D:111:THR:HG23	4:D:300:GLN:HB2	1.58	0.82
3:C:103:VAL:HG12	3:C:116:ASP:HB2	1.60	0.82
4:D:848:VAL:HG22	4:D:858:VAL:HG22	1.61	0.82
3:C:1008:GLN:HA	3:C:1011:LEU:HD12	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:MET:CE	5:E:49:ILE:HG22	2.09	0.82
3:C:453:ILE:HD11	3:C:587:LEU:HD11	1.60	0.81
6:F:144:LEU:HD13	6:F:265:GLN:HG2	1.62	0.81
3:C:1088:ASP:OD1	3:C:1088:ASP:N	2.13	0.81
2:B:166:ARG:HB3	2:B:170:ARG:HB2	1.61	0.81
3:C:1269:ARG:HH21	4:D:344:GLY:HA3	1.44	0.81
4:D:1031:VAL:HG21	4:D:1088:VAL:HG21	1.62	0.81
3:C:642:SER:HB3	4:D:770:LEU:HD21	1.61	0.80
3:C:221:LEU:HD12	3:C:313:ALA:HB1	1.63	0.80
3:C:1065:LYS:HE2	3:C:1235:LEU:HD12	1.64	0.80
6:F:390:ILE:HD11	6:F:432:THR:HG23	1.63	0.80
4:D:559:ALA:HB3	4:D:562:GLU:HG2	1.63	0.80
4:D:218:THR:HA	4:D:221:ILE:HG22	1.64	0.80
4:D:424:ASN:HB2	4:D:434:ILE:HG12	1.64	0.79
3:C:252:SER:HA	3:C:265:LYS:HG3	1.65	0.79
5:E:30:MET:CE	5:E:49:ILE:CG2	2.61	0.79
6:F:573:LEU:HD21	7:G:45:DT:H2'	1.63	0.79
4:D:746:LEU:HD23	4:D:758:PRO:HB3	1.62	0.79
6:F:137:TYR:HB2	6:F:361:ILE:HG21	1.63	0.78
4:D:17:PHE:CE1	4:D:1353:VAL:HG11	2.19	0.78
3:C:979:LEU:HD11	3:C:1011:LEU:HD11	1.65	0.78
4:D:1082:ASP:HB3	4:D:1088:VAL:HB	1.63	0.78
6:F:231:THR:HA	6:F:248:GLU:HB3	1.66	0.78
3:C:678:ARG:HG2	3:C:1108:ASN:HD22	1.49	0.77
4:D:84:ILE:HG22	4:D:91:GLU:HB3	1.64	0.77
4:D:661:VAL:HG23	4:D:682:VAL:HG22	1.67	0.77
6:F:456:MET:HE1	6:F:497:VAL:HG22	1.66	0.77
6:F:229:VAL:HG12	6:F:232:ARG:HH21	1.50	0.77
6:F:134:VAL:HG13	6:F:273:MET:HE1	1.66	0.77
4:D:253:VAL:HG11	6:F:523:ILE:HD12	1.67	0.76
2:B:18:GLN:HE22	2:B:21:SER:HA	1.49	0.76
6:F:561:MET:HE2	6:F:576:VAL:HA	1.66	0.76
3:C:255:ILE:HG22	3:C:262:TYR:HB2	1.68	0.75
3:C:979:LEU:HD11	3:C:1011:LEU:HD21	1.68	0.75
4:D:1341:ARG:HG2	4:D:1341:ARG:NH1	1.98	0.75
6:F:166:VAL:HG22	6:F:258:GLN:HA	1.68	0.75
4:D:839:VAL:HG23	4:D:882:VAL:HG11	1.68	0.75
2:A:64:VAL:HG21	2:A:78:ILE:HG13	1.69	0.75
4:D:1049:GLN:HB2	4:D:1059:LEU:HD11	1.69	0.74
3:C:360:LEU:HD13	3:C:378:ARG:HG3	1.68	0.74
3:C:453:ILE:HD13	3:C:530:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1021:ASP:HB3	4:D:1024:THR:HB	1.68	0.74
2:K:280:ASP:O	2:K:284:ARG:N	2.21	0.74
3:C:594:VAL:HG22	3:C:599:VAL:HG22	1.70	0.74
4:D:857:LEU:HD12	4:D:871:LEU:HD21	1.68	0.74
2:B:61:ILE:HD13	2:B:142:MET:HB3	1.69	0.74
1:H:14:DT:OP2	6:F:584:ARG:NE	2.20	0.73
1:H:22:DG:H22	7:G:41:DC:H1'	1.52	0.73
3:C:3:TYR:N	3:C:7:GLU:OE1	2.22	0.73
3:C:81:ASP:OD1	3:C:81:ASP:N	2.19	0.73
6:F:141:ILE:HG22	6:F:145:LEU:HD23	1.70	0.73
3:C:97:ARG:HG3	3:C:121:GLU:HB3	1.68	0.73
4:D:1162:ILE:HG22	4:D:1178:THR:HB	1.70	0.73
6:F:111:LEU:HD21	6:F:119:ILE:HD12	1.69	0.73
4:D:863:LEU:HD21	4:D:901:ARG:HB2	1.70	0.73
6:F:593:LYS:HG2	6:F:596:ARG:HH12	1.54	0.73
3:C:119:GLU:HG2	3:C:490:GLN:HB2	1.71	0.73
1:H:38:DT:H2''	1:H:39:DA:H5'	1.70	0.72
2:A:192:VAL:HG12	2:A:195:ARG:HB2	1.71	0.72
2:B:73:GLY:O	2:B:134:THR:HG23	1.89	0.72
4:D:112:ALA:HA	4:D:238:ILE:HD13	1.71	0.72
4:D:1045:THR:HG21	4:D:1076:PRO:HB3	1.72	0.72
3:C:230:PHE:HB3	3:C:333:ILE:HB	1.72	0.72
3:C:1159:VAL:HG12	3:C:1160:ASP:N	2.03	0.72
2:A:234:LEU:HD12	2:B:214:GLU:HG2	1.71	0.71
3:C:241:LEU:HD21	3:C:246:LEU:HD11	1.71	0.71
6:F:108:VAL:O	6:F:385:ARG:NH2	2.23	0.71
3:C:960:LEU:HB3	3:C:1025:PHE:HE1	1.53	0.71
3:C:1246:ARG:NH1	4:D:348:ASP:OD1	2.23	0.71
3:C:864:LYS:HD3	3:C:875:ALA:HB1	1.72	0.71
4:D:1060:VAL:HG22	4:D:1106:ILE:HD12	1.72	0.71
6:F:354:THR:HG23	6:F:357:GLN:H	1.55	0.71
3:C:272:ARG:HA	3:C:275:ARG:HB2	1.72	0.71
4:D:262:THR:HG22	6:F:504:PRO:HB2	1.73	0.71
3:C:988:LYS:HA	3:C:991:LYS:HG2	1.71	0.71
4:D:1343:GLU:HB3	4:D:1345:ARG:HG3	1.71	0.71
6:F:574:GLU:OE2	6:F:588:ARG:NH2	2.23	0.71
6:F:336:GLU:HA	6:F:339:ARG:HG2	1.72	0.70
3:C:1131:MET:HE2	3:C:1141:LEU:HD12	1.71	0.70
4:D:816:THR:HG22	4:D:818:GLU:H	1.56	0.70
4:D:836:ARG:NH2	4:D:866:GLU:OE1	2.24	0.70
6:F:102:MET:HA	6:F:105:MET:HE2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:302:GLU:N	7:G:56:DT:OP2	2.23	0.70
2:B:11:PRO:HB2	2:B:28:LEU:HD11	1.73	0.70
6:F:248:GLU:HA	6:F:251:LYS:HE2	1.72	0.70
3:C:199:ASP:OD1	3:C:199:ASP:N	2.23	0.70
3:C:1157:GLN:OE1	3:C:1157:GLN:HA	1.90	0.70
4:D:895:CYS:SG	4:D:898:CYS:N	2.62	0.70
4:D:1057:SER:HB2	4:D:1059:LEU:HD13	1.72	0.70
3:C:796:LEU:N	3:C:1231:TYR:OH	2.25	0.69
3:C:1319:MET:HG3	3:C:1320:PRO:HD2	1.73	0.69
4:D:74:LYS:NZ	4:D:86:GLU:OE2	2.25	0.69
2:A:215:GLU:OE2	2:A:219:ARG:NH2	2.25	0.69
6:F:278:ASP:HA	6:F:281:ARG:HH22	1.57	0.69
7:G:29:DC:H4'	7:G:30:DA:H5'	1.73	0.69
1:H:6:DA:N6	7:G:57:DT:O4	2.26	0.69
3:C:61:SER:OG	3:C:66:SER:N	2.23	0.69
7:G:52:DC:H5'	7:G:52:DC:H6	1.57	0.69
1:H:62:DG:H4'	1:H:63:DG:H5'	1.74	0.69
2:B:181:GLU:HA	4:D:535:ARG:HH12	1.55	0.69
3:C:819:SER:HB2	3:C:1085:MET:HG3	1.75	0.68
4:D:510:LEU:O	4:D:514:THR:HG22	1.93	0.68
6:F:572:THR:O	6:F:576:VAL:N	2.24	0.68
2:A:50:SER:HB3	2:B:8:PHE:HZ	1.57	0.68
4:D:1027:VAL:HB	4:D:1121:LEU:HB2	1.74	0.68
4:D:91:GLU:OE2	4:D:101:ARG:NH2	2.22	0.68
6:F:160:ASP:O	6:F:265:GLN:NE2	2.27	0.68
3:C:323:ALA:O	3:C:327:GLN:NE2	2.27	0.68
4:D:568:SER:OG	4:D:570:LYS:NZ	2.27	0.68
4:D:973:LEU:H	4:D:1003:LEU:HD12	1.59	0.68
6:F:310:GLU:HB3	6:F:344:LEU:HD22	1.75	0.68
2:A:162:GLU:OE1	2:A:165:GLU:N	2.24	0.67
4:D:155:GLU:N	4:D:158:GLN:OE1	2.28	0.67
3:C:933:VAL:HG11	3:C:945:ALA:HB2	1.76	0.67
6:F:348:GLU:HA	6:F:351:THR:HG22	1.77	0.67
4:D:789:LYS:HG3	4:D:931:THR:HG21	1.74	0.67
5:E:34:GLY:C	5:E:35:LYS:HD3	2.20	0.67
4:D:734:ALA:O	4:D:738:ARG:NH1	2.27	0.67
4:D:1089:LEU:HA	4:D:1096:PRO:HA	1.77	0.67
4:D:1215:GLU:OE1	4:D:1215:GLU:N	2.26	0.67
3:C:618:GLN:HE21	4:D:770:LEU:HD22	1.59	0.67
4:D:930:LEU:HD12	4:D:1246:VAL:HG23	1.76	0.67
6:F:222:ALA:O	6:F:226:ALA:N	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:MET:HE1	2:B:217:ILE:HG13	1.77	0.67
3:C:576:SER:OG	3:C:577:VAL:N	2.26	0.66
2:B:100:LEU:HB2	2:B:144:ILE:HG13	1.76	0.66
3:C:230:PHE:O	3:C:333:ILE:N	2.28	0.66
4:D:845:ALA:O	4:D:860:ARG:NH2	2.25	0.66
3:C:529:ARG:HD2	3:C:572:ILE:HG22	1.76	0.66
3:C:300:ASP:OD1	3:C:313:ALA:N	2.27	0.66
4:D:857:LEU:H	4:D:857:LEU:HD23	1.61	0.66
3:C:758:ARG:NH1	3:C:762:ASN:OD1	2.28	0.66
3:C:903:ARG:O	3:C:907:GLY:N	2.27	0.66
4:D:1158:GLU:OE1	4:D:1158:GLU:N	2.28	0.66
3:C:1158:LYS:HA	3:C:1158:LYS:CE	2.25	0.66
4:D:1065:ALA:HB2	4:D:1193:TRP:HB3	1.78	0.66
6:F:248:GLU:HG2	6:F:251:LYS:HE2	1.76	0.66
3:C:67:GLU:HG2	3:C:103:VAL:HG22	1.78	0.66
3:C:189:ASP:HB2	3:C:190:PRO:HD2	1.77	0.66
6:F:143:TYR:O	6:F:150:ARG:NH2	2.28	0.66
4:D:975:ILE:HG22	4:D:1028:ILE:HG21	1.78	0.65
4:D:1115:ILE:HD12	4:D:1119:ASP:HB3	1.78	0.65
3:C:179:TYR:HB2	3:C:398:SER:OG	1.96	0.65
3:C:1339:LEU:HD13	4:D:17:PHE:CD2	2.31	0.65
6:F:261:LEU:HD23	6:F:266:PHE:HD1	1.61	0.65
2:A:190:ALA:HB2	2:A:200:LYS:HB2	1.79	0.65
2:B:182:ARG:NH1	2:B:204:GLU:OE2	2.29	0.65
3:C:690:VAL:HG23	3:C:1236:ASN:HB3	1.78	0.65
3:C:1069:ARG:NH1	3:C:1114:GLU:OE2	2.29	0.65
4:D:479:GLU:HG2	5:E:20:VAL:HG11	1.78	0.65
4:D:986:ASP:OD2	4:D:990:ARG:NH1	2.30	0.65
6:F:474:MET:SD	6:F:476:ARG:NH2	2.70	0.65
4:D:710:ASP:N	4:D:710:ASP:OD1	2.28	0.65
6:F:577:GLY:O	6:F:581:ASP:N	2.28	0.65
7:G:58:DG:H2'	7:G:59:DT:H72	1.79	0.65
3:C:101:ARG:HG2	3:C:118:LYS:HB2	1.78	0.65
6:F:601:PRO:O	6:F:603:ARG:NH2	2.29	0.65
4:D:161:THR:HG23	4:D:163:GLU:H	1.60	0.65
6:F:338:HIS:HA	6:F:341:LEU:HG	1.77	0.65
4:D:398:LYS:HD3	6:F:532:LEU:CD2	2.27	0.65
3:C:975:ILE:O	3:C:979:LEU:N	2.30	0.64
2:A:61:ILE:HB	2:A:64:VAL:HG12	1.78	0.64
6:F:225:ARG:HA	6:F:228:TYR:HB3	1.79	0.64
3:C:564:PRO:HD3	3:C:572:ILE:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:MET:HB2	5:E:46:THR:HG22	1.79	0.64
4:D:1136:GLY:HA2	4:D:1140:ARG:HB2	1.79	0.64
3:C:1271:GLY:N	3:C:1274:GLU:OE1	2.30	0.64
6:F:150:ARG:CB	6:F:155:GLU:HB3	2.28	0.64
6:F:299:LYS:HG2	6:F:302:PHE:HE2	1.63	0.64
3:C:715:THR:HG21	3:C:782:VAL:HG22	1.79	0.64
4:D:1059:LEU:HB3	4:D:1107:VAL:HG23	1.80	0.64
3:C:276:GLN:HA	3:C:279:LYS:HZ2	1.61	0.64
6:F:294:GLN:HE22	6:F:333:VAL:HG11	1.63	0.64
6:F:358:VAL:O	6:F:362:ASN:ND2	2.30	0.64
6:F:391:ALA:HB2	6:F:439:ILE:HD13	1.80	0.64
2:A:191:ARG:NH1	2:A:195:ARG:O	2.30	0.64
4:D:1062:LEU:HD22	4:D:1066:GLU:HB3	1.81	0.63
4:D:1108:GLN:NE2	4:D:1120:THR:OG1	2.32	0.63
6:F:157:ARG:HD2	6:F:160:ASP:HB2	1.79	0.63
6:F:351:THR:HG23	6:F:353:LEU:H	1.63	0.63
3:C:1014:LEU:O	3:C:1018:TYR:N	2.31	0.63
3:C:1164:PHE:HB2	3:C:1168:GLU:HB3	1.79	0.63
4:D:709:ARG:HD2	4:D:714:GLU:HB2	1.80	0.63
4:D:750:PRO:HA	4:D:777:HIS:NE2	2.13	0.63
4:D:1025:MET:N	4:D:1124:ILE:O	2.28	0.63
6:F:150:ARG:HB3	6:F:155:GLU:HB3	1.81	0.63
2:A:195:ARG:NH2	2:A:197:ASP:OD1	2.31	0.63
6:F:360:ASP:HA	6:F:363:ARG:HB3	1.79	0.63
4:D:298:MET:HE1	6:F:406:GLN:HG3	1.80	0.63
1:H:13:DT:H2''	1:H:14:DT:H71	1.79	0.63
3:C:896:THR:HB	3:C:897:PRO:HD2	1.80	0.63
3:C:1264:GLN:NE2	4:D:375:GLU:OE2	2.31	0.63
4:D:968:ASN:HD22	4:D:1117:SER:HB3	1.64	0.63
4:D:972:LYS:NZ	4:D:973:LEU:O	2.31	0.63
4:D:80:HIS:HB3	4:D:83:VAL:CG1	2.29	0.63
4:D:443:GLU:OE2	4:D:444:GLY:N	2.31	0.63
6:F:390:ILE:CD1	6:F:432:THR:HG23	2.29	0.63
3:C:12:ARG:HD3	3:C:1183:ALA:HB2	1.81	0.63
6:F:145:LEU:O	6:F:225:ARG:NH2	2.32	0.63
2:A:61:ILE:HB	2:A:64:VAL:CG1	2.29	0.62
1:H:30:DT:H73	1:H:31:DT:H72	1.81	0.62
1:H:42:DG:H22	3:C:375:PRO:HD2	1.64	0.62
3:C:119:GLU:HB2	3:C:489:PRO:CD	2.27	0.62
7:G:49:DA:H2''	7:G:50:DA:C5	2.34	0.62
2:A:22:THR:HB	2:A:207:THR:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:ARG:NH2	3:C:793:GLU:OE1	2.32	0.62
4:D:847:ASP:OD1	4:D:847:ASP:N	2.25	0.62
5:E:30:MET:HE1	5:E:49:ILE:HG22	1.80	0.62
6:F:322:MET:HG3	6:F:324:LYS:HD3	1.81	0.62
4:D:1068:THR:HG22	4:D:1069:ALA:H	1.65	0.62
2:A:58:GLU:OE1	2:A:170:ARG:HD2	1.99	0.62
3:C:754:THR:O	3:C:754:THR:OG1	2.16	0.62
6:F:227:GLN:HE21	6:F:231:THR:HG22	1.64	0.62
2:B:104:LYS:NZ	2:B:105:SER:O	2.21	0.62
3:C:44:GLU:HG3	3:C:46:GLN:H	1.64	0.62
4:D:300:GLN:NE2	4:D:304:ASP:OD2	2.33	0.62
3:C:275:ARG:O	3:C:279:LYS:HG2	2.00	0.62
5:E:72:GLN:O	5:E:76:GLU:N	2.31	0.62
4:D:442:ILE:HD13	4:D:448:GLN:HG3	1.82	0.62
5:E:38:LEU:HD12	5:E:38:LEU:N	2.15	0.62
6:F:282:THR:O	6:F:286:LEU:N	2.31	0.62
2:B:60:GLU:HB3	2:B:143:ARG:HB2	1.82	0.62
3:C:302:ILE:HA	3:C:309:LEU:HA	1.82	0.62
4:D:1037:PHE:HB3	4:D:1041:ILE:CD1	2.30	0.62
4:D:1057:SER:OG	4:D:1108:GLN:HA	1.99	0.62
4:D:1346:GLY:O	4:D:1350:ASN:HB2	2.00	0.61
1:H:40:DA:H5'	1:H:41:DT:H72	1.83	0.61
3:C:1023:HIS:O	3:C:1027:LYS:N	2.21	0.61
4:D:255:LEU:HD23	4:D:261:ALA:HB2	1.82	0.61
3:C:960:LEU:HB3	3:C:1025:PHE:CE1	2.36	0.61
2:A:29:GLU:HB3	2:A:30:PRO:HD3	1.83	0.61
6:F:345:GLN:HA	6:F:348:GLU:HG3	1.81	0.61
2:A:97:GLU:OE2	2:A:145:LYS:HD2	2.01	0.61
4:D:120:LEU:HB3	4:D:121:PRO:HD3	1.82	0.61
3:C:106:GLU:HB2	3:C:114:VAL:HG21	1.82	0.61
3:C:813:GLU:HB2	4:D:461:PHE:HD2	1.64	0.61
4:D:426:ALA:HB3	4:D:427:PRO:HD3	1.83	0.61
4:D:826:ILE:HG12	4:D:831:VAL:HG12	1.83	0.61
4:D:1314:LEU:HD21	4:D:1331:VAL:HG21	1.83	0.61
3:C:988:LYS:HA	3:C:991:LYS:HE3	1.81	0.61
3:C:1338:GLU:O	4:D:20:ILE:HG23	2.01	0.61
4:D:70:CYS:SG	4:D:71:LEU:N	2.73	0.61
4:D:1215:GLU:HG3	4:D:1220:ILE:HD11	1.82	0.61
6:F:585:GLU:HA	6:F:588:ARG:CG	2.31	0.61
2:A:31:LEU:HD21	2:A:39:LEU:HD12	1.82	0.61
2:B:108:GLY:O	2:B:133:LEU:N	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:819:SER:OG	3:C:820:GLU:N	2.33	0.61
3:C:1002:LEU:HB2	3:C:1011:LEU:CD1	2.31	0.61
4:D:999:TYR:CD2	4:D:1102:PRO:HG3	2.36	0.61
3:C:378:ARG:NH1	3:C:382:GLU:OE2	2.34	0.60
4:D:263:SER:OG	4:D:264:ASP:N	2.33	0.60
4:D:1175:LEU:HD22	4:D:1190:ILE:HD11	1.83	0.60
6:F:313:ASP:HB3	6:F:316:PHE:HB2	1.82	0.60
3:C:172:TYR:O	3:C:432:LEU:HD11	2.01	0.60
4:D:17:PHE:CZ	4:D:1353:VAL:HG13	2.33	0.60
4:D:45:ASN:HB3	4:D:48:THR:O	2.01	0.60
4:D:1060:VAL:HG22	4:D:1106:ILE:CD1	2.32	0.60
2:A:74:VAL:HG12	2:A:133:LEU:HD13	1.83	0.60
3:C:84:GLU:N	3:C:84:GLU:OE1	2.35	0.60
3:C:662:SER:OG	3:C:663:VAL:N	2.33	0.60
3:C:69:GLN:HG2	3:C:101:ARG:O	2.01	0.60
3:C:272:ARG:O	3:C:276:GLN:N	2.34	0.60
3:C:971:LEU:HD21	3:C:1014:LEU:HD13	1.81	0.60
4:D:1163:VAL:HG21	4:D:1202:GLU:HB3	1.84	0.60
2:B:12:ARG:HD3	2:B:13:LEU:H	1.67	0.60
3:C:444:ASP:O	3:C:450:ASN:ND2	2.34	0.60
3:C:529:ARG:HD2	3:C:572:ILE:CG2	2.30	0.60
4:D:518:VAL:HG23	4:D:547:ARG:HH22	1.67	0.60
2:A:191:ARG:NH2	2:A:196:THR:O	2.25	0.60
3:C:65:ASN:O	3:C:105:TYR:HB2	2.00	0.60
3:C:415:GLU:OE1	3:C:415:GLU:N	2.33	0.60
3:C:1103:VAL:HG11	3:C:1112:ILE:CD1	2.32	0.60
4:D:1044:GLN:HB3	4:D:1074:LEU:CD1	2.31	0.60
6:F:494:ILE:O	6:F:498:LEU:HG	2.02	0.60
2:B:41:ASN:OD1	2:B:44:ARG:NH2	2.34	0.60
3:C:421:SER:OG	3:C:422:LYS:N	2.35	0.60
3:C:1072:ASN:ND2	3:C:1111:GLN:OE1	2.34	0.60
4:D:972:LYS:HD3	4:D:1003:LEU:HG	1.83	0.60
2:B:60:GLU:OE1	2:B:143:ARG:NH1	2.33	0.59
3:C:484:LEU:HA	3:C:487:LEU:HD22	1.84	0.59
3:C:1304:MET:O	3:C:1308:ILE:HG12	2.02	0.59
5:E:30:MET:HE3	5:E:49:ILE:HG21	1.83	0.59
6:F:295:CYS:O	6:F:296:LYS:HG2	2.02	0.59
4:D:905:ARG:NH1	4:D:910:ASN:OD1	2.34	0.59
4:D:949:SER:HB3	4:D:1016:THR:HB	1.84	0.59
4:D:1032:SER:OG	4:D:1115:ILE:O	2.20	0.59
4:D:1078:LEU:O	4:D:1098:GLN:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:14:VAL:HG22	2:A:15:ASP:H	1.66	0.59
4:D:860:ARG:O	4:D:862:THR:HG23	2.01	0.59
6:F:138:PRO:HD3	6:F:353:LEU:HD11	1.84	0.59
6:F:250:LEU:HA	6:F:253:SER:OG	2.01	0.59
6:F:585:GLU:HA	6:F:588:ARG:HG2	1.83	0.59
3:C:271:ALA:O	3:C:275:ARG:HG3	2.02	0.59
3:C:324:LYS:HA	3:C:327:GLN:HE22	1.68	0.59
4:D:929:GLN:O	4:D:930:LEU:HD23	2.02	0.59
4:D:1062:LEU:O	4:D:1067:ARG:NH2	2.27	0.59
6:F:359:LYS:O	6:F:363:ARG:N	2.35	0.59
3:C:269:ILE:HG13	3:C:269:ILE:O	2.03	0.59
6:F:146:GLU:OE1	6:F:150:ARG:HG3	2.03	0.59
3:C:272:ARG:O	3:C:276:GLN:HG3	2.01	0.59
6:F:571:TYR:HB3	6:F:575:GLU:HG3	1.83	0.59
6:F:227:GLN:O	6:F:231:THR:HG23	2.03	0.59
3:C:102:LEU:HB3	3:C:489:PRO:HG3	1.84	0.59
3:C:757:THR:HG22	3:C:765:ILE:O	2.03	0.59
4:D:1036:ARG:NH2	4:D:1085:GLY:O	2.36	0.59
4:D:843:VAL:CG2	4:D:883:ARG:HD3	2.33	0.59
1:H:63:DG:H5''	4:D:1170:LYS:CG	2.32	0.58
2:K:298:LYS:HB3	7:G:55:DT:H2'	1.85	0.58
3:C:114:VAL:HG12	3:C:115:LYS:HD2	1.85	0.58
3:C:215:TYR:HB3	3:C:220:ILE:HD11	1.83	0.58
3:C:360:LEU:CD1	3:C:378:ARG:HG3	2.33	0.58
3:C:854:ILE:HG22	3:C:855:PRO:HD2	1.84	0.58
3:C:982:GLY:CA	3:C:1002:LEU:HG	2.28	0.58
3:C:1225:VAL:HG13	4:D:638:SER:HB2	1.83	0.58
4:D:201:LEU:HB2	4:D:221:ILE:HD13	1.85	0.58
3:C:594:VAL:CG2	3:C:599:VAL:HG22	2.33	0.58
3:C:757:THR:CG2	3:C:765:ILE:HG23	2.34	0.58
4:D:793:SER:O	4:D:797:THR:HG22	2.03	0.58
6:F:515:GLU:HG2	6:F:516:ASP:H	1.68	0.58
2:B:91:ARG:HD3	2:B:124:VAL:CG1	2.33	0.58
3:C:545:PHE:CE2	4:D:781:LYS:HD3	2.38	0.58
4:D:44:ILE:HD11	6:F:450:ILE:CD1	2.32	0.58
4:D:317:THR:HG21	4:D:320:ASN:HB3	1.86	0.58
4:D:1226:VAL:O	4:D:1229:VAL:HG12	2.03	0.58
5:E:70:GLN:O	5:E:74:GLU:HG2	2.03	0.58
6:F:572:THR:HB	6:F:575:GLU:HB3	1.84	0.58
6:F:612:ASP:OD1	6:F:612:ASP:N	2.36	0.58
2:K:301:THR:H	7:G:56:DT:H5'	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1172:LYS:HE2	4:D:1189:MET:CE	2.33	0.58
1:H:16:DA:H1'	1:H:17:DC:H5'	1.85	0.58
4:D:1106:ILE:O	4:D:1122:ALA:HA	2.03	0.58
4:D:1281:GLU:OE1	4:D:1281:GLU:N	2.36	0.58
6:F:353:LEU:HD22	6:F:357:GLN:NE2	2.19	0.58
1:H:63:DG:H5''	4:D:1170:LYS:HG2	1.84	0.58
3:C:867:GLU:OE1	3:C:867:GLU:N	2.35	0.58
3:C:1103:VAL:HG11	3:C:1112:ILE:HD12	1.84	0.58
4:D:818:GLU:N	4:D:818:GLU:OE2	2.37	0.58
4:D:1051:ASP:OD1	4:D:1052:GLU:N	2.35	0.58
4:D:1176:VAL:HG13	4:D:1186:TYR:O	2.04	0.58
7:G:0:DC:H2''	7:G:1:DC:C5	2.38	0.58
1:H:62:DG:C4'	1:H:63:DG:H5'	2.33	0.58
4:D:979:ASN:OD1	4:D:979:ASN:N	2.37	0.58
5:E:30:MET:CE	5:E:49:ILE:HG21	2.33	0.58
3:C:210:LEU:HD21	3:C:429:MET:HE1	1.84	0.58
4:D:1163:VAL:HG23	4:D:1202:GLU:O	2.03	0.58
7:G:43:DT:H2''	7:G:44:DT:H5'	1.86	0.58
4:D:317:THR:CG2	4:D:320:ASN:HB3	2.33	0.58
4:D:822:MET:HE3	4:D:838:ARG:HB3	1.86	0.58
4:D:980:THR:HB	4:D:997:VAL:HB	1.85	0.58
2:B:167:PRO:HD2	2:B:170:ARG:HG3	1.84	0.58
4:D:552:ILE:HD12	4:D:589:TYR:CE1	2.39	0.58
4:D:973:LEU:HB2	4:D:1003:LEU:CD1	2.34	0.58
4:D:1002:VAL:O	4:D:1003:LEU:HD23	2.04	0.58
4:D:1025:MET:HB3	4:D:1124:ILE:CG2	2.34	0.58
4:D:1106:ILE:HG12	4:D:1123:ARG:O	2.04	0.58
2:A:58:GLU:HG2	2:A:145:LYS:HE2	1.86	0.57
2:B:56:VAL:HG23	2:B:173:VAL:HG11	1.85	0.57
2:B:61:ILE:HG22	2:B:64:VAL:H	1.69	0.57
3:C:560:PRO:HB2	4:D:776:THR:HG21	1.85	0.57
4:D:846:GLU:HA	4:D:860:ARG:CZ	2.34	0.57
4:D:966:VAL:O	4:D:973:LEU:HA	2.03	0.57
4:D:1025:MET:O	4:D:1124:ILE:HB	2.03	0.57
3:C:161:LYS:HD3	3:C:161:LYS:H	1.68	0.57
3:C:1010:GLN:HA	3:C:1013:GLN:CB	2.34	0.57
3:C:1101:LEU:O	4:D:731:ARG:HG2	2.04	0.57
3:C:1304:MET:HE3	3:C:1308:ILE:HD11	1.87	0.57
3:C:1338:GLU:O	3:C:1339:LEU:HD23	2.04	0.57
4:D:562:GLU:O	4:D:563:LEU:HD13	2.04	0.57
4:D:986:ASP:OD1	4:D:990:ARG:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:525:ASP:OD1	6:F:528:LEU:HD13	2.04	0.57
4:D:208:THR:HG21	4:D:213:LYS:HE3	1.86	0.57
6:F:130:VAL:O	6:F:134:VAL:HG23	2.04	0.57
6:F:355:ILE:HG22	6:F:359:LYS:HG3	1.86	0.57
4:D:390:LEU:CD2	4:D:407:VAL:HG11	2.34	0.57
4:D:805:GLN:HA	4:D:805:GLN:HE21	1.68	0.57
4:D:839:VAL:HG22	4:D:864:LEU:HD12	1.85	0.57
4:D:868:TRP:O	4:D:872:LEU:HG	2.03	0.57
4:D:974:VAL:HG21	4:D:1030:GLU:CG	2.34	0.57
4:D:1036:ARG:NH2	4:D:1081:VAL:HG11	2.20	0.57
3:C:272:ARG:HA	3:C:275:ARG:HD2	1.86	0.57
3:C:557:ARG:NH2	3:C:611:GLU:OE1	2.25	0.57
3:C:1010:GLN:CD	3:C:1013:GLN:HB3	2.29	0.57
3:C:1326:LEU:HD21	4:D:337:ARG:NH2	2.19	0.57
4:D:84:ILE:HG22	4:D:91:GLU:CB	2.34	0.57
4:D:744:ARG:HH12	4:D:747:MET:HE2	1.70	0.57
3:C:602:GLU:OE2	3:C:604:HIS:NE2	2.36	0.57
4:D:885:VAL:HG22	4:D:1258:ARG:HD2	1.86	0.57
3:C:103:VAL:HA	3:C:116:ASP:HA	1.86	0.57
3:C:716:ALA:HB3	3:C:784:ALA:HB3	1.85	0.57
4:D:930:LEU:HD12	4:D:1246:VAL:CG2	2.34	0.57
4:D:930:LEU:CD1	4:D:1244:GLN:HB3	2.25	0.57
2:B:179:PRO:O	2:B:207:THR:HG22	2.03	0.57
3:C:309:LEU:HD23	3:C:309:LEU:H	1.70	0.57
3:C:314:ASN:OD1	3:C:352:ARG:NH2	2.36	0.57
4:D:473:THR:OG1	4:D:474:LEU:N	2.37	0.57
4:D:533:ALA:HB1	4:D:574:VAL:HG13	1.87	0.57
4:D:1172:LYS:HE2	4:D:1189:MET:HE2	1.87	0.57
6:F:129:GLN:O	6:F:133:SER:OG	2.20	0.57
6:F:290:LEU:HD12	6:F:294:GLN:OE1	2.05	0.57
3:C:164:THR:CG2	3:C:171:LEU:HG	2.32	0.57
4:D:513:MET:HE1	4:D:627:THR:HG22	1.87	0.57
7:G:49:DA:H2"	7:G:50:DA:N7	2.20	0.57
2:K:259:ASP:O	2:K:310:ARG:NH1	2.38	0.56
2:A:118:ASP:OD1	2:A:119:GLY:N	2.36	0.56
2:B:46:ILE:CD1	2:B:224:LEU:HB2	2.35	0.56
2:B:104:LYS:HB3	2:B:140:ILE:CG2	2.35	0.56
3:C:298:ALA:HB3	3:C:334:GLU:HB3	1.86	0.56
2:B:155:ALA:HA	2:B:158:ARG:HE	1.70	0.56
4:D:1343:GLU:C	4:D:1344:LEU:HG	2.28	0.56
6:F:246:GLN:O	6:F:250:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:397:ARG:NH1	7:G:26:DT:O4	2.26	0.56
6:F:400:GLN:HB2	6:F:403:ASP:OD1	2.05	0.56
7:G:52:DC:H5'	7:G:52:DC:C6	2.39	0.56
1:H:5:DC:H1'	1:H:6:DA:C8	2.40	0.56
2:A:180:VAL:HG12	2:A:207:THR:HG22	1.86	0.56
2:B:19:VAL:O	2:B:23:HIS:HB3	2.04	0.56
3:C:255:ILE:CG2	3:C:262:TYR:HB2	2.35	0.56
3:C:397:LEU:O	3:C:398:SER:OG	2.22	0.56
4:D:21:LYS:CG	4:D:22:ILE:N	2.68	0.56
4:D:146:VAL:O	4:D:147:ILE:HD13	2.05	0.56
4:D:355:ILE:HG12	4:D:464:ASP:O	2.05	0.56
4:D:393:THR:OG1	4:D:394:ILE:N	2.36	0.56
4:D:664:ILE:HD13	4:D:681:LYS:HG2	1.87	0.56
6:F:310:GLU:HB3	6:F:344:LEU:CD2	2.34	0.56
3:C:1267:GLY:HA3	4:D:347:VAL:O	2.06	0.56
4:D:1034:PHE:HB2	4:D:1081:VAL:HG23	1.88	0.56
5:E:3:ARG:HH21	5:E:52:ARG:HD3	1.69	0.56
6:F:221:PHE:O	6:F:224:LEU:HB3	2.06	0.56
7:G:4:DG:H2''	7:G:5:DC:C5	2.41	0.56
3:C:642:SER:CB	4:D:770:LEU:HD21	2.33	0.56
3:C:993:PRO:HG2	3:C:996:ARG:CB	2.36	0.56
4:D:423:LEU:HG	4:D:466:MET:HE3	1.87	0.56
4:D:643:ASP:O	4:D:645:VAL:HG23	2.05	0.56
3:C:813:GLU:HB2	4:D:461:PHE:CD2	2.41	0.56
2:B:59:VAL:HA	2:B:143:ARG:O	2.06	0.56
3:C:276:GLN:O	3:C:280:ASP:HB2	2.05	0.56
3:C:301:TYR:HB2	3:C:311:CYS:SG	2.46	0.56
3:C:453:ILE:HD11	3:C:587:LEU:CD1	2.34	0.56
4:D:1163:VAL:HG21	4:D:1198:VAL:HG21	1.87	0.56
6:F:529:GLU:OE1	6:F:529:GLU:N	2.38	0.56
7:G:59:DT:H2'	7:G:60:DT:H71	1.88	0.56
3:C:582:ASN:HA	3:C:588:GLU:OE2	2.06	0.56
3:C:672:GLU:HB3	3:C:1187:PHE:CD1	2.41	0.56
3:C:1252:SER:HB3	3:C:1255:THR:O	2.06	0.56
4:D:850:LYS:NZ	4:D:855:ASP:HB3	2.21	0.56
6:F:233:ASP:O	6:F:236:LYS:NZ	2.25	0.56
6:F:303:ILE:O	6:F:307:THR:N	2.39	0.56
7:G:47:DT:H1'	7:G:48:DC:C5'	2.33	0.56
2:B:64:VAL:O	2:B:65:LEU:HD23	2.05	0.56
2:B:197:ASP:O	2:B:198:LEU:HD22	2.06	0.56
3:C:745:GLU:HG2	3:C:1017:GLN:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:210:SER:HB3	4:D:213:LYS:HB2	1.88	0.56
4:D:1152:GLU:O	4:D:1214:PRO:HD2	2.06	0.56
3:C:519:ASN:HB3	3:C:521:LEU:H	1.71	0.56
3:C:1072:ASN:HD21	3:C:1230:MET:HE1	1.70	0.56
4:D:255:LEU:HD23	4:D:261:ALA:CB	2.35	0.56
4:D:1080:ILE:N	4:D:1097:ALA:O	2.38	0.56
6:F:144:LEU:HD12	6:F:147:GLN:HG3	1.87	0.56
6:F:234:THR:CG2	6:F:248:GLU:HB2	2.36	0.56
2:B:83:LEU:HD21	4:D:526:VAL:CG2	2.36	0.55
3:C:217:THR:HG23	3:C:351:LEU:HD22	1.87	0.55
3:C:398:SER:HB2	3:C:401:GLY:N	2.14	0.55
3:C:721:GLY:N	3:C:740:GLU:OE1	2.37	0.55
3:C:801:ARG:HH21	3:C:1119:MET:HE1	1.71	0.55
3:C:1298:VAL:HG23	3:C:1321:GLU:HG3	1.89	0.55
4:D:981:GLU:OE1	4:D:981:GLU:N	2.38	0.55
4:D:1162:ILE:HD12	4:D:1202:GLU:O	2.06	0.55
6:F:223:GLU:HA	6:F:226:ALA:CB	2.34	0.55
4:D:1162:ILE:CG2	4:D:1178:THR:HB	2.35	0.55
6:F:585:GLU:HG2	6:F:588:ARG:HH11	1.71	0.55
1:H:17:DC:H1'	1:H:18:DA:O4'	2.06	0.55
2:A:218:ARG:O	2:A:222:THR:HG23	2.05	0.55
3:C:102:LEU:CB	3:C:489:PRO:HG3	2.36	0.55
3:C:1164:PHE:HB2	3:C:1168:GLU:CB	2.36	0.55
4:D:297:ARG:NH2	6:F:104:GLU:OE1	2.38	0.55
4:D:390:LEU:HD21	4:D:407:VAL:HG11	1.88	0.55
4:D:1101:LEU:HD13	4:D:1107:VAL:HG11	1.88	0.55
4:D:1105:ALA:HB1	4:D:1122:ALA:CB	2.36	0.55
2:A:14:VAL:CG1	2:A:27:THR:HB	2.37	0.55
3:C:231:GLU:HA	3:C:331:LYS:O	2.05	0.55
3:C:699:LEU:HG	3:C:799:ASN:ND2	2.22	0.55
3:C:942:ASP:OD1	3:C:942:ASP:N	2.29	0.55
4:D:402:GLU:OE1	4:D:403:ARG:HG3	2.06	0.55
5:E:29:GLN:O	5:E:32:VAL:O	2.25	0.55
6:F:247:GLU:O	6:F:251:LYS:HG3	2.06	0.55
6:F:306:PHE:CE2	6:F:310:GLU:HA	2.42	0.55
3:C:1115:THR:CG2	3:C:1228:GLY:HA3	2.37	0.55
3:C:1315:MET:HE2	3:C:1317:PRO:HB3	1.89	0.55
4:D:1105:ALA:HB1	4:D:1122:ALA:HB1	1.88	0.55
6:F:234:THR:HG21	6:F:248:GLU:HB2	1.87	0.55
6:F:506:SER:O	6:F:509:THR:HG22	2.07	0.55
2:B:93:GLN:HG2	2:B:120:ASP:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1009:ASN:O	3:C:1013:GLN:HB2	2.07	0.55
4:D:807:LEU:HD21	4:D:894:VAL:CG1	2.37	0.55
4:D:807:LEU:HD21	4:D:894:VAL:HG13	1.89	0.55
4:D:999:TYR:CE2	4:D:1027:VAL:HA	2.42	0.55
3:C:596:ASP:N	3:C:596:ASP:OD1	2.40	0.55
4:D:929:GLN:CG	4:D:930:LEU:HG	2.35	0.55
4:D:1191:PRO:HB3	4:D:1193:TRP:CZ3	2.42	0.55
6:F:256:PHE:HA	6:F:259:PHE:CE2	2.42	0.55
6:F:324:LYS:HB3	6:F:325:PRO:HD2	1.89	0.55
2:B:35:PHE:HA	2:B:38:THR:CG2	2.36	0.55
3:C:1010:GLN:O	3:C:1014:LEU:N	2.23	0.55
3:C:1259:LEU:HD22	6:F:521:ASP:O	2.07	0.55
4:D:44:ILE:HD11	6:F:450:ILE:HD13	1.89	0.55
4:D:591:ILE:HG22	4:D:592:VAL:HG13	1.88	0.55
6:F:108:VAL:HG21	6:F:381:GLU:O	2.06	0.55
6:F:261:LEU:HD23	6:F:266:PHE:CD1	2.41	0.55
3:C:820:GLU:HB2	3:C:1080:ASN:O	2.06	0.55
4:D:518:VAL:HG23	4:D:547:ARG:NH2	2.22	0.55
4:D:1031:VAL:HG21	4:D:1088:VAL:CG2	2.36	0.55
4:D:1039:ASP:OD1	4:D:1074:LEU:HD22	2.07	0.55
4:D:1089:LEU:HD12	4:D:1096:PRO:HA	1.88	0.55
6:F:322:MET:CG	6:F:324:LYS:HD3	2.36	0.55
2:B:36:GLY:HA3	2:B:187:VAL:HG21	1.87	0.54
2:B:109:PRO:HA	2:B:132:HIS:HA	1.90	0.54
4:D:697:MET:HE3	4:D:698:MET:SD	2.47	0.54
4:D:1048:ARG:HA	4:D:1048:ARG:HE	1.71	0.54
6:F:150:ARG:O	6:F:155:GLU:N	2.26	0.54
6:F:435:ILE:O	6:F:439:ILE:HG13	2.07	0.54
3:C:761:GLN:N	3:C:761:GLN:OE1	2.41	0.54
4:D:79:LYS:CB	6:F:569:THR:HB	2.31	0.54
4:D:328:ALA:O	4:D:332:LYS:HB2	2.07	0.54
4:D:713:GLU:HG2	4:D:714:GLU:H	1.73	0.54
4:D:746:LEU:CD2	4:D:758:PRO:HB3	2.35	0.54
4:D:857:LEU:HD12	4:D:871:LEU:CD2	2.36	0.54
4:D:1268:ASN:HA	4:D:1274:PHE:CE1	2.42	0.54
2:B:191:ARG:NH1	2:B:193:GLU:HA	2.21	0.54
6:F:144:LEU:O	6:F:147:GLN:HB2	2.06	0.54
7:G:29:DC:H2''	7:G:30:DA:C8	2.43	0.54
1:H:48:DT:O2	3:C:199:ASP:HB3	2.07	0.54
3:C:979:LEU:HA	3:C:1002:LEU:CD2	2.36	0.54
3:C:1070:HIS:NE2	3:C:1114:GLU:OE1	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:MET:HB3	4:D:175:GLU:OE2	2.07	0.54
4:D:161:THR:HG22	4:D:164:GLN:CG	2.32	0.54
4:D:1087:ASP:HB2	4:D:1096:PRO:HG3	1.89	0.54
6:F:163:THR:OG1	6:F:260:ARG:HD2	2.07	0.54
2:B:100:LEU:HB2	2:B:144:ILE:CG1	2.37	0.54
3:C:171:LEU:HD13	3:C:189:ASP:HA	1.90	0.54
3:C:985:GLU:HA	3:C:988:LYS:HG2	1.89	0.54
3:C:1010:GLN:OE1	3:C:1014:LEU:N	2.40	0.54
4:D:152:THR:HG22	4:D:153:ASN:H	1.73	0.54
4:D:1155:ILE:H	4:D:1155:ILE:HD13	1.73	0.54
6:F:133:SER:O	6:F:361:ILE:HG23	2.07	0.54
3:C:103:VAL:HG12	3:C:116:ASP:CB	2.36	0.54
3:C:575:LEU:HD12	3:C:576:SER:H	1.71	0.54
3:C:1075:VAL:CG1	4:D:356:THR:HG22	2.37	0.54
3:C:1161:LEU:HD12	3:C:1161:LEU:O	2.06	0.54
4:D:901:ARG:O	4:D:903:LEU:HG	2.07	0.54
2:A:45:ARG:NH2	3:C:1084:ASP:OD1	2.41	0.54
3:C:1002:LEU:HD23	3:C:1007:LYS:CB	2.26	0.54
3:C:1296:ASP:OD1	3:C:1321:GLU:N	2.41	0.54
6:F:572:THR:O	6:F:576:VAL:HG23	2.08	0.54
2:B:54:CYS:SG	2:B:148:ARG:HG2	2.47	0.54
2:B:91:ARG:HH11	2:B:124:VAL:HG11	1.73	0.54
3:C:1163:THR:O	3:C:1164:PHE:O	2.26	0.54
4:D:69:GLU:HG3	4:D:70:CYS:O	2.08	0.54
4:D:1102:PRO:HG2	4:D:1124:ILE:CD1	2.38	0.54
4:D:1106:ILE:N	4:D:1122:ALA:HB1	2.23	0.54
6:F:298:PRO:HB2	6:F:301:ASN:ND2	2.23	0.54
3:C:276:GLN:HA	3:C:279:LYS:NZ	2.23	0.54
3:C:540:ARG:NH2	3:C:567:PRO:HG2	2.23	0.54
3:C:1106:ARG:H	3:C:1106:ARG:HD2	1.72	0.54
4:D:291:ILE:HD13	6:F:409:ASN:HB3	1.90	0.54
4:D:1078:LEU:O	4:D:1080:ILE:HG13	2.08	0.54
4:D:1314:LEU:HD11	4:D:1331:VAL:HG22	1.90	0.54
4:D:1317:GLU:OE2	4:D:1345:ARG:NH2	2.41	0.54
7:G:56:DT:H2"	7:G:57:DT:H72	1.90	0.54
1:H:42:DG:O6	6:F:106:GLY:HA3	2.08	0.54
3:C:1158:LYS:CE	3:C:1158:LYS:CA	2.86	0.54
3:C:1260:GLY:HA3	3:C:1265:PHE:CA	2.28	0.54
4:D:697:MET:SD	4:D:741:ALA:HB3	2.48	0.54
4:D:968:ASN:OD1	4:D:972:LYS:N	2.41	0.54
6:F:561:MET:SD	6:F:576:VAL:HG13	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:231:GLU:OE2	3:C:284:LEU:HD11	2.08	0.53
3:C:1325:VAL:HG13	4:D:249:LEU:HD13	1.90	0.53
4:D:245:LEU:HG	4:D:246:PRO:HD2	1.91	0.53
4:D:603:LYS:O	4:D:607:THR:HG23	2.08	0.53
3:C:453:ILE:HD13	3:C:530:ILE:CD1	2.36	0.53
4:D:1105:ALA:O	4:D:1106:ILE:HD13	2.08	0.53
6:F:602:SER:HA	6:F:605:GLU:HB2	1.90	0.53
2:B:158:ARG:HD2	2:B:172:LEU:CD2	2.38	0.53
3:C:239:MET:HG2	3:C:240:GLU:O	2.08	0.53
3:C:1204:LEU:HB3	3:C:1205:PRO:HD2	1.90	0.53
4:D:518:VAL:CG1	4:D:707:ILE:HB	2.38	0.53
4:D:703:THR:HG21	4:D:715:LYS:HD3	1.90	0.53
4:D:1002:VAL:O	4:D:1018:ALA:HA	2.09	0.53
6:F:252:LEU:HA	6:F:255:VAL:HG22	1.91	0.53
2:A:58:GLU:OE2	2:A:145:LYS:NZ	2.24	0.53
2:B:107:ILE:HG12	2:B:135:ASP:CG	2.33	0.53
4:D:438:GLU:HG3	4:D:485:MET:HE1	1.89	0.53
4:D:952:VAL:O	4:D:1014:GLY:N	2.41	0.53
4:D:1144:LEU:HD21	4:D:1236:GLU:HB2	1.90	0.53
6:F:165:PHE:CZ	6:F:220:LYS:HB2	2.42	0.53
1:H:27:DA:H5'	1:H:27:DA:C8	2.43	0.53
2:A:212:ASP:HB3	2:A:215:GLU:HB3	1.89	0.53
3:C:211:ARG:NE	3:C:354:ASP:OD2	2.37	0.53
3:C:1040:ASP:OD1	3:C:1041:ASP:N	2.41	0.53
3:C:1321:GLU:O	3:C:1325:VAL:HG23	2.09	0.53
4:D:314:ARG:HH12	4:D:323:PRO:HG3	1.74	0.53
4:D:416:ILE:CG2	4:D:439:PRO:HG2	2.37	0.53
4:D:894:VAL:HG23	4:D:895:CYS:O	2.09	0.53
6:F:161:LEU:O	6:F:261:LEU:HD12	2.08	0.53
6:F:363:ARG:O	6:F:367:ILE:HG13	2.08	0.53
7:G:3:DT:C2	7:G:4:DG:N7	2.76	0.53
1:H:58:DG:H4'	1:H:59:DC:OP2	2.08	0.53
2:A:233:ASP:N	2:A:233:ASP:OD1	2.41	0.53
4:D:201:LEU:HD11	4:D:220:ARG:NH1	2.24	0.53
4:D:1021:ASP:CB	4:D:1024:THR:HB	2.35	0.53
6:F:96:ASP:OD1	6:F:96:ASP:N	2.41	0.53
6:F:456:MET:CE	6:F:497:VAL:HG22	2.36	0.53
3:C:724:VAL:HG11	3:C:727:VAL:HG23	1.91	0.53
3:C:985:GLU:O	3:C:989:LEU:HB2	2.08	0.53
4:D:682:VAL:O	4:D:685:ILE:HG23	2.09	0.53
5:E:7:GLN:O	5:E:11:GLU:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:141:ILE:HG22	6:F:145:LEU:CD2	2.39	0.53
6:F:355:ILE:HA	6:F:358:VAL:HB	1.91	0.53
6:F:547:VAL:HG11	6:F:607:LEU:CD1	2.34	0.53
1:H:39:DA:H3'	6:F:429:THR:CG2	2.39	0.53
2:A:110:VAL:HG23	2:A:133:LEU:HD23	1.91	0.53
3:C:29:SER:O	3:C:33:ASP:HB2	2.09	0.53
3:C:130:MET:SD	3:C:134:GLY:HA2	2.49	0.53
3:C:233:ARG:HD3	3:C:238:GLN:OE1	2.09	0.53
3:C:757:THR:HG23	3:C:765:ILE:HG23	1.89	0.53
3:C:979:LEU:HA	3:C:1002:LEU:HD21	1.91	0.53
3:C:988:LYS:CA	3:C:991:LYS:HE3	2.38	0.53
4:D:1051:ASP:OD2	4:D:1056:LEU:HB2	2.08	0.53
2:B:83:LEU:HD21	4:D:526:VAL:HG22	1.91	0.53
3:C:1010:GLN:HA	3:C:1013:GLN:HB3	1.90	0.53
3:C:1164:PHE:HD1	3:C:1168:GLU:HB2	1.72	0.53
3:C:1243:MET:HE3	4:D:445:LYS:HE2	1.89	0.53
4:D:1215:GLU:CG	4:D:1220:ILE:HD11	2.38	0.53
2:B:60:GLU:HB2	2:B:170:ARG:NH1	2.23	0.53
3:C:805:MET:HE1	3:C:1221:PHE:CE2	2.44	0.53
4:D:789:LYS:HG3	4:D:931:THR:CG2	2.39	0.53
4:D:1057:SER:CB	4:D:1059:LEU:HD13	2.39	0.53
4:D:1110:GLU:O	4:D:1113:VAL:HG22	2.09	0.53
1:H:44:DG:O5'	6:F:392:LYS:HD3	2.10	0.52
2:B:135:ASP:OD1	2:B:136:GLU:N	2.40	0.52
3:C:887:VAL:HB	3:C:913:VAL:CG2	2.40	0.52
4:D:40:LYS:HD3	4:D:42:GLU:OE1	2.08	0.52
4:D:337:ARG:N	4:D:341:ASN:O	2.42	0.52
6:F:341:LEU:O	6:F:344:LEU:HG	2.09	0.52
2:B:83:LEU:HD11	4:D:527:LEU:O	2.09	0.52
3:C:149:LEU:HD12	3:C:453:ILE:HG12	1.90	0.52
6:F:402:LEU:HD12	6:F:405:ILE:HD11	1.91	0.52
6:F:479:THR:HG22	6:F:482:GLU:OE1	2.09	0.52
2:B:112:ALA:O	2:B:115:ILE:HG13	2.08	0.52
3:C:172:TYR:CD2	3:C:435:ILE:HG22	2.44	0.52
3:C:1288:GLN:O	3:C:1292:THR:HB	2.09	0.52
6:F:166:VAL:CG2	6:F:258:GLN:HA	2.38	0.52
2:A:98:VAL:HG11	2:A:121:VAL:HG21	1.90	0.52
2:A:192:VAL:CG1	2:A:195:ARG:HB2	2.39	0.52
3:C:1254:VAL:O	4:D:99:ARG:NH2	2.32	0.52
4:D:46:TYR:CD2	6:F:452:ILE:HG22	2.43	0.52
4:D:1251:LYS:O	4:D:1255:VAL:HG13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:685:MET:SD	3:C:1073:LYS:HG3	2.49	0.52
3:C:1275:VAL:O	3:C:1279:GLU:HG3	2.10	0.52
6:F:292:VAL:HG22	6:F:297:MET:O	2.09	0.52
6:F:511:ILE:HD11	6:F:517:SER:OG	2.09	0.52
3:C:67:GLU:HG2	3:C:103:VAL:CG2	2.38	0.52
3:C:155:VAL:HG12	3:C:176:ILE:HG12	1.91	0.52
3:C:302:ILE:O	3:C:330:HIS:NE2	2.40	0.52
4:D:808:VAL:HG21	4:D:1359:ALA:HB2	1.92	0.52
4:D:1025:MET:HB3	4:D:1124:ILE:HB	1.92	0.52
6:F:111:LEU:CD2	6:F:119:ILE:HD12	2.39	0.52
2:A:77:ASP:OD1	2:A:77:ASP:N	2.43	0.52
3:C:311:CYS:HA	3:C:315:MET:SD	2.50	0.52
4:D:972:LYS:HZ1	4:D:1028:ILE:HD12	1.75	0.52
3:C:528:ARG:HD3	3:C:663:VAL:HG11	1.92	0.52
3:C:979:LEU:HD11	3:C:1011:LEU:CD1	2.39	0.52
3:C:1252:SER:HB2	3:C:1259:LEU:HD23	1.90	0.52
4:D:985:ILE:HA	4:D:990:ARG:O	2.10	0.52
6:F:148:TYR:HA	6:F:151:VAL:HB	1.91	0.52
1:H:42:DG:H4'	1:H:43:DG:O4'	2.09	0.52
3:C:696:ASP:OD2	3:C:696:ASP:N	2.39	0.52
3:C:993:PRO:HG2	3:C:996:ARG:HB2	1.92	0.52
4:D:502:PRO:HB2	4:D:506:VAL:HG22	1.92	0.52
4:D:704:GLU:HB2	4:D:718:SER:HB3	1.91	0.52
4:D:1038:THR:CG2	4:D:1079:LYS:H	2.23	0.52
4:D:1266:ILE:HG13	4:D:1276:GLU:O	2.10	0.52
6:F:136:GLU:HG3	6:F:361:ILE:CD1	2.39	0.52
6:F:353:LEU:HB3	6:F:357:GLN:CB	2.40	0.52
1:H:11:DG:N2	7:G:53:DA:N3	2.48	0.52
1:H:12:DA:OP2	6:F:593:LYS:HE2	2.10	0.52
3:C:188:PHE:HE2	3:C:436:ARG:HB2	1.73	0.52
3:C:1243:MET:HE2	4:D:445:LYS:HG2	1.90	0.52
4:D:798:ARG:HD2	4:D:798:ARG:O	2.10	0.52
4:D:1030:GLU:OE2	4:D:1090:ILE:HG23	2.10	0.52
4:D:1160:SER:OG	4:D:1206:ARG:N	2.43	0.52
2:B:24:ALA:HB3	2:B:213:PRO:HB2	1.92	0.51
3:C:672:GLU:OE1	3:C:672:GLU:N	2.34	0.51
3:C:1006:GLU:HA	3:C:1009:ASN:HB2	1.91	0.51
3:C:1257:GLN:NE2	3:C:1322:SER:OG	2.42	0.51
4:D:518:VAL:HG11	4:D:707:ILE:HB	1.90	0.51
5:E:68:GLU:O	5:E:71:GLU:HB2	2.10	0.51
6:F:281:ARG:HB3	6:F:281:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:228:LEU:O	2:A:232:VAL:HG23	2.11	0.51
3:C:104:ILE:HB	3:C:115:LYS:HB2	1.91	0.51
3:C:898:GLU:OE1	3:C:898:GLU:N	2.43	0.51
3:C:1031:ALA:HA	3:C:1034:ARG:HH12	1.74	0.51
3:C:1157:GLN:NE2	3:C:1159:VAL:CG2	2.73	0.51
3:C:1339:LEU:HD22	4:D:20:ILE:HG12	1.92	0.51
4:D:708:ASN:OD1	4:D:708:ASN:N	2.41	0.51
4:D:872:LEU:HB3	4:D:877:VAL:HG11	1.91	0.51
6:F:125:ASP:HA	6:F:128:ASN:HB2	1.93	0.51
6:F:213:ASP:HB3	6:F:215:GLU:OE1	2.09	0.51
1:H:16:DA:H1'	1:H:17:DC:C5'	2.40	0.51
3:C:128:PRO:C	3:C:129:LEU:HD23	2.35	0.51
3:C:1248:THR:HG21	6:F:531:PRO:HG3	1.92	0.51
4:D:485:MET:HB3	4:D:488:ASN:HD22	1.75	0.51
4:D:807:LEU:HD22	4:D:915:ILE:HG13	1.91	0.51
6:F:489:MET:HE2	6:F:493:LYS:HB2	1.93	0.51
2:A:10:LYS:HZ3	2:B:226:GLU:HB3	1.75	0.51
2:A:110:VAL:HG21	2:A:140:ILE:HD11	1.92	0.51
2:A:134:THR:OG1	3:C:773:LEU:HD11	2.10	0.51
2:B:91:ARG:HD3	2:B:124:VAL:HG11	1.92	0.51
3:C:564:PRO:HG3	3:C:572:ILE:HG13	1.91	0.51
3:C:618:GLN:NE2	4:D:770:LEU:HD22	2.25	0.51
3:C:690:VAL:CG2	3:C:1236:ASN:HB3	2.39	0.51
4:D:991:THR:O	4:D:992:LYS:HD2	2.11	0.51
4:D:1023:HIS:C	4:D:1125:PRO:HA	2.35	0.51
4:D:1175:LEU:CD2	4:D:1190:ILE:HD11	2.39	0.51
6:F:247:GLU:O	6:F:250:LEU:HB2	2.11	0.51
6:F:329:LYS:NZ	6:F:333:VAL:HG23	2.26	0.51
6:F:577:GLY:CA	6:F:583:THR:HG22	2.34	0.51
4:D:506:VAL:HG12	4:D:629:PHE:CE1	2.45	0.51
4:D:1027:VAL:CG1	4:D:1121:LEU:HB2	2.41	0.51
6:F:141:ILE:HG12	6:F:256:PHE:CE1	2.45	0.51
3:C:961:SER:O	3:C:965:GLN:HG3	2.11	0.51
4:D:262:THR:OG1	4:D:263:SER:N	2.43	0.51
4:D:416:ILE:HG22	4:D:439:PRO:HG2	1.93	0.51
4:D:554:GLU:OE1	4:D:589:TYR:N	2.44	0.51
4:D:1138:LEU:HB3	4:D:1139:PRO:HD3	1.91	0.51
4:D:1175:LEU:HD12	4:D:1176:VAL:H	1.74	0.51
6:F:278:ASP:HA	6:F:281:ARG:NH2	2.26	0.51
6:F:345:GLN:HA	6:F:348:GLU:CG	2.40	0.51
1:H:6:DA:H2''	1:H:7:DA:H5'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:DA:H2"	1:H:61:DG:C8	2.45	0.51
3:C:236:LYS:HE2	3:C:236:LYS:HA	1.92	0.51
3:C:577:VAL:HG23	3:C:661:VAL:O	2.11	0.51
4:D:611:ILE:C	4:D:612:LEU:HD12	2.35	0.51
4:D:749:LYS:HE3	4:D:753:SER:OG	2.10	0.51
4:D:952:VAL:CG1	4:D:984:LEU:HD22	2.40	0.51
4:D:1011:VAL:CG1	4:D:1015:GLU:HB3	2.41	0.51
4:D:1109:LEU:CD1	4:D:1115:ILE:HD13	2.41	0.51
6:F:157:ARG:HD2	6:F:160:ASP:OD2	2.11	0.51
6:F:348:GLU:HB2	6:F:353:LEU:O	2.11	0.51
7:G:3:DT:O2	7:G:4:DG:N7	2.44	0.51
2:A:155:ALA:O	2:A:159:ILE:HG12	2.11	0.51
2:A:219:ARG:HG3	2:A:219:ARG:O	2.09	0.51
3:C:135:THR:HG22	3:C:527:LYS:HE2	1.93	0.51
3:C:215:TYR:HE2	3:C:426:ILE:HD11	1.76	0.51
3:C:594:VAL:HG11	3:C:650:VAL:HG23	1.93	0.51
4:D:311:ARG:NH2	4:D:1329:THR:HG21	2.26	0.51
4:D:797:THR:O	4:D:797:THR:OG1	2.25	0.51
6:F:362:ASN:HA	6:F:365:MET:HE3	1.92	0.51
7:G:48:DC:H2"	7:G:49:DA:C8	2.46	0.51
2:A:26:VAL:HG11	2:A:217:ILE:HD12	1.93	0.51
3:C:319:LEU:HA	3:C:322:LEU:HB2	1.92	0.51
3:C:563:THR:HB	3:C:564:PRO:HD2	1.93	0.51
3:C:1305:TYR:O	3:C:1309:VAL:HG13	2.11	0.51
4:D:437:PHE:HZ	4:D:453:VAL:HG11	1.75	0.51
4:D:704:GLU:HB2	4:D:718:SER:CB	2.40	0.51
4:D:966:VAL:HA	4:D:973:LEU:HD23	1.93	0.51
4:D:998:PRO:O	4:D:1001:ALA:HB2	2.11	0.51
4:D:1272:SER:HB2	4:D:1286:LYS:NZ	2.26	0.51
2:A:134:THR:HG21	3:C:727:VAL:O	2.11	0.51
3:C:18:ARG:HD3	3:C:1188:ASP:OD1	2.11	0.51
3:C:153:PRO:O	3:C:401:GLY:HA2	2.11	0.51
3:C:1017:GLN:HA	3:C:1017:GLN:HE21	1.75	0.51
4:D:514:THR:HG21	4:D:596:LEU:CB	2.41	0.51
4:D:1027:VAL:CB	4:D:1121:LEU:HB2	2.39	0.51
4:D:1102:PRO:O	4:D:1105:ALA:HB2	2.11	0.51
6:F:320:ILE:HA	6:F:327:SER:HB2	1.92	0.51
6:F:571:TYR:HB3	6:F:575:GLU:CG	2.40	0.51
2:B:23:HIS:ND1	2:B:206:GLU:HG2	2.25	0.50
2:B:57:THR:O	2:B:173:VAL:HG12	2.12	0.50
3:C:979:LEU:HG	3:C:1002:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1163:THR:HG22	3:C:1168:GLU:OE2	2.10	0.50
3:C:1243:MET:CE	4:D:445:LYS:HE2	2.41	0.50
4:D:495:ASN:N	4:D:495:ASN:OD1	2.45	0.50
4:D:513:MET:HE1	4:D:627:THR:CG2	2.41	0.50
3:C:98:VAL:O	3:C:121:GLU:HA	2.11	0.50
3:C:208:ILE:HD11	3:C:365:GLU:HB3	1.93	0.50
4:D:16:GLU:OE1	4:D:1369:ARG:NH2	2.44	0.50
4:D:557:LYS:HA	4:D:562:GLU:O	2.11	0.50
4:D:843:VAL:HG21	4:D:883:ARG:HD3	1.94	0.50
5:E:30:MET:HE1	5:E:49:ILE:CG2	2.36	0.50
7:G:38:DA:H2''	7:G:39:DC:C6	2.47	0.50
2:A:71:LYS:NZ	2:A:140:ILE:HG22	2.26	0.50
4:D:298:MET:CE	6:F:406:GLN:HG3	2.41	0.50
4:D:929:GLN:HG2	4:D:930:LEU:CG	2.36	0.50
4:D:1104:LYS:O	4:D:1124:ILE:HA	2.11	0.50
3:C:494:ASN:HB3	3:C:497:PRO:HD2	1.93	0.50
3:C:982:GLY:CA	3:C:1003:THR:HG23	2.36	0.50
4:D:210:SER:O	4:D:214:ARG:NE	2.44	0.50
5:E:78:ALA:O	5:E:80:LEU:HG	2.12	0.50
3:C:274:ILE:O	3:C:278:GLU:HG3	2.11	0.50
4:D:285:LEU:HG	6:F:413:MET:HE1	1.93	0.50
4:D:975:ILE:CG2	4:D:1028:ILE:HG21	2.41	0.50
6:F:143:TYR:O	6:F:147:GLN:HG2	2.12	0.50
6:F:331:HIS:HA	6:F:334:SER:CB	2.37	0.50
1:H:43:DG:N3	6:F:102:MET:HE3	2.26	0.50
3:C:979:LEU:CD1	3:C:1011:LEU:HD11	2.40	0.50
3:C:1099:ASN:OD1	3:C:1100:PRO:HD2	2.11	0.50
3:C:1157:GLN:HB3	3:C:1159:VAL:HG23	1.94	0.50
4:D:583:VAL:HG13	4:D:584:PRO:HD2	1.94	0.50
4:D:884:SER:OG	4:D:886:VAL:HG12	2.11	0.50
4:D:1163:VAL:CG2	4:D:1202:GLU:HB3	2.41	0.50
6:F:290:LEU:HB2	6:F:337:VAL:HG12	1.93	0.50
6:F:582:VAL:HG23	6:F:584:ARG:NH1	2.25	0.50
3:C:272:ARG:O	3:C:272:ARG:HG2	2.11	0.50
3:C:571:LEU:O	3:C:572:ILE:HD13	2.12	0.50
3:C:589:THR:HG22	3:C:590:PRO:HD2	1.94	0.50
3:C:1061:GLN:NE2	3:C:1240:ASP:OD1	2.45	0.50
4:D:766:GLY:C	4:D:767:LEU:HD12	2.36	0.50
4:D:959:LYS:HA	4:D:1007:ASP:OD2	2.12	0.50
4:D:1032:SER:OG	4:D:1116:SER:HA	2.12	0.50
4:D:1272:SER:HB2	4:D:1286:LYS:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:561:MET:CE	6:F:576:VAL:HA	2.38	0.50
3:C:228:VAL:HB	3:C:335:THR:HG23	1.94	0.50
3:C:1023:HIS:HA	3:C:1026:GLU:HB3	1.92	0.50
4:D:279:LEU:HD13	4:D:295:GLU:CG	2.42	0.50
4:D:959:LYS:HD2	4:D:985:ILE:HG13	1.94	0.50
5:E:49:ILE:O	5:E:53:GLU:HG3	2.12	0.50
6:F:476:ARG:HB3	6:F:476:ARG:CZ	2.42	0.50
6:F:476:ARG:HB3	6:F:476:ARG:NH1	2.27	0.50
6:F:487:MET:O	6:F:488:LEU:HD13	2.12	0.50
3:C:263:VAL:HG12	3:C:264:GLU:H	1.77	0.50
3:C:272:ARG:HA	3:C:275:ARG:CB	2.42	0.50
3:C:632:ASP:OD1	3:C:632:ASP:N	2.45	0.50
3:C:979:LEU:CD1	3:C:1011:LEU:HD21	2.41	0.50
4:D:1037:PHE:CZ	4:D:1111:ASP:HB2	2.47	0.50
6:F:354:THR:O	6:F:358:VAL:N	2.35	0.50
2:B:57:THR:C	2:B:173:VAL:HG12	2.36	0.49
3:C:631:GLU:OE1	3:C:631:GLU:N	2.45	0.49
3:C:897:PRO:HG2	3:C:898:GLU:OE1	2.12	0.49
3:C:974:ARG:O	3:C:978:VAL:N	2.45	0.49
4:D:412:LEU:O	4:D:416:ILE:HG12	2.12	0.49
1:H:50:DT:C2'	1:H:51:DC:H5'	2.43	0.49
3:C:702:THR:HG22	3:C:1184:THR:O	2.12	0.49
3:C:1150:ASP:N	3:C:1150:ASP:OD1	2.44	0.49
4:D:1059:LEU:HB2	4:D:1107:VAL:O	2.11	0.49
6:F:286:LEU:HG	6:F:290:LEU:CD2	2.42	0.49
7:G:6:DA:C8	7:G:6:DA:H5'	2.47	0.49
2:A:57:THR:HG21	2:A:147:GLN:NE2	2.28	0.49
3:C:84:GLU:O	3:C:88:ARG:HG3	2.12	0.49
3:C:778:GLU:O	3:C:781:ASP:HB2	2.13	0.49
3:C:826:ASP:OD1	3:C:829:THR:HB	2.12	0.49
3:C:1157:GLN:NE2	3:C:1159:VAL:HG21	2.28	0.49
4:D:218:THR:HA	4:D:221:ILE:CG2	2.39	0.49
4:D:844:THR:OG1	4:D:861:ASN:HA	2.12	0.49
4:D:1087:ASP:HB2	4:D:1096:PRO:CG	2.41	0.49
2:A:183:ILE:HD12	2:A:205:MET:HB2	1.94	0.49
2:B:28:LEU:HD12	2:B:29:GLU:H	1.78	0.49
3:C:104:ILE:N	3:C:115:LYS:O	2.31	0.49
3:C:484:LEU:HA	3:C:487:LEU:CD2	2.41	0.49
3:C:1339:LEU:HD22	4:D:17:PHE:HD2	1.77	0.49
4:D:205:LEU:HD12	4:D:214:ARG:HB2	1.95	0.49
4:D:1196:LEU:HD11	4:D:1210:ILE:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:SER:CB	2:B:138:ALA:HB1	2.35	0.49
3:C:204:LEU:HD11	3:C:369:MET:HE3	1.94	0.49
3:C:972:PHE:CD2	3:C:975:ILE:HD11	2.47	0.49
4:D:1027:VAL:HG22	4:D:1102:PRO:CD	2.33	0.49
6:F:283:GLN:HE22	6:F:286:LEU:HD22	1.78	0.49
6:F:341:LEU:HB2	6:F:344:LEU:CD2	2.42	0.49
1:H:43:DG:H2'	1:H:44:DG:C8	2.48	0.49
1:H:63:DG:OP1	4:D:1170:LYS:HA	2.12	0.49
3:C:971:LEU:HD21	3:C:1014:LEU:CD1	2.42	0.49
3:C:1157:GLN:HE21	3:C:1159:VAL:HG21	1.77	0.49
4:D:709:ARG:NH1	4:D:714:GLU:OE1	2.33	0.49
4:D:975:ILE:HD11	4:D:977:SER:O	2.12	0.49
4:D:1069:ALA:O	4:D:1072:LYS:HE2	2.12	0.49
3:C:230:PHE:CB	3:C:333:ILE:HB	2.41	0.49
3:C:319:LEU:O	3:C:323:ALA:N	2.46	0.49
3:C:1103:VAL:HG21	3:C:1112:ILE:HD11	1.95	0.49
6:F:148:TYR:HB2	6:F:221:PHE:CE1	2.48	0.49
6:F:360:ASP:N	6:F:360:ASP:OD1	2.46	0.49
1:H:62:DG:H1'	1:H:63:DG:O4'	2.12	0.49
2:A:183:ILE:CD1	2:A:205:MET:HB2	2.42	0.49
3:C:800:MET:HE2	3:C:800:MET:HB3	1.63	0.49
4:D:84:ILE:HA	4:D:91:GLU:HA	1.94	0.49
5:E:10:VAL:O	5:E:14:GLY:HA2	2.12	0.49
6:F:479:THR:HG23	6:F:482:GLU:H	1.78	0.49
2:K:298:LYS:O	7:G:55:DT:H2'	2.13	0.49
3:C:444:ASP:OD1	3:C:444:ASP:N	2.35	0.49
3:C:949:GLU:OE2	3:C:1037:THR:HG22	2.13	0.49
3:C:985:GLU:HG2	3:C:988:LYS:HD3	1.93	0.49
3:C:1078:LYS:NZ	3:C:1080:ASN:OD1	2.44	0.49
4:D:179:LYS:NZ	4:D:183:GLU:HG3	2.28	0.49
6:F:283:GLN:NE2	6:F:286:LEU:HD22	2.28	0.49
1:H:62:DG:H2''	1:H:63:DG:O5'	2.13	0.49
3:C:595:THR:HG23	3:C:600:THR:CG2	2.42	0.49
4:D:208:THR:HG21	4:D:213:LYS:HB3	1.94	0.49
4:D:371:LYS:NZ	4:D:443:GLU:OE2	2.46	0.49
4:D:622:ASP:O	4:D:625:MET:N	2.43	0.49
4:D:640:GLY:N	4:D:643:ASP:OD2	2.45	0.49
6:F:144:LEU:HD12	6:F:147:GLN:HB2	1.95	0.49
1:H:42:DG:H2''	1:H:43:DG:OP2	2.13	0.48
1:H:43:DG:O6	3:C:371:ARG:NH1	2.46	0.48
2:A:58:GLU:HB3	2:A:172:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:GLU:O	2:B:142:MET:HA	2.13	0.48
3:C:193:ASN:OD1	3:C:350:THR:HG23	2.13	0.48
3:C:812:PHE:CD2	3:C:813:GLU:HG2	2.49	0.48
4:D:398:LYS:HD3	6:F:532:LEU:HD23	1.95	0.48
4:D:591:ILE:HG22	4:D:592:VAL:CG1	2.42	0.48
4:D:709:ARG:HD2	4:D:714:GLU:CB	2.43	0.48
6:F:275:VAL:HA	6:F:278:ASP:OD2	2.13	0.48
6:F:354:THR:N	6:F:357:GLN:OE1	2.45	0.48
2:B:164:ASP:OD1	2:B:164:ASP:N	2.45	0.48
3:C:303:ASP:HB3	3:C:306:THR:OG1	2.12	0.48
4:D:1089:LEU:HD12	4:D:1096:PRO:CA	2.42	0.48
4:D:1162:ILE:O	4:D:1177:ILE:HA	2.13	0.48
6:F:140:ALA:HB1	6:F:269:LEU:HD22	1.95	0.48
6:F:277:MET:HE1	6:F:359:LYS:NZ	2.29	0.48
6:F:573:LEU:HG	7:G:45:DT:OP2	2.14	0.48
7:G:29:DC:C4'	7:G:30:DA:H5'	2.39	0.48
2:K:285:THR:HG22	2:K:287:VAL:H	1.78	0.48
2:B:60:GLU:HB2	2:B:170:ARG:HH11	1.79	0.48
3:C:44:GLU:OE2	3:C:46:GLN:HB2	2.14	0.48
3:C:270:THR:O	3:C:273:HIS:HB2	2.12	0.48
4:D:733:SER:OG	4:D:734:ALA:N	2.46	0.48
4:D:972:LYS:CD	4:D:1003:LEU:HG	2.42	0.48
4:D:1060:VAL:HA	4:D:1105:ALA:O	2.14	0.48
6:F:133:SER:OG	6:F:364:ARG:HG2	2.13	0.48
7:G:29:DC:H1'	7:G:30:DA:O4'	2.13	0.48
2:K:300:LEU:HB3	7:G:56:DT:H3'	1.94	0.48
2:A:82:LEU:HD11	2:A:171:LEU:HD23	1.95	0.48
3:C:273:HIS:O	3:C:277:LEU:HG	2.13	0.48
3:C:799:ASN:OD1	3:C:799:ASN:N	2.47	0.48
3:C:1115:THR:HG22	3:C:1228:GLY:HA3	1.96	0.48
4:D:158:GLN:C	4:D:159:ILE:HD12	2.39	0.48
4:D:449:LEU:CD1	4:D:466:MET:HE1	2.44	0.48
4:D:514:THR:HG21	4:D:596:LEU:HB3	1.94	0.48
4:D:826:ILE:CG1	4:D:831:VAL:HG12	2.43	0.48
6:F:286:LEU:HA	6:F:289:LYS:HB2	1.95	0.48
6:F:336:GLU:HG3	6:F:339:ARG:HH11	1.78	0.48
2:B:162:GLU:HG3	2:B:166:ARG:CZ	2.44	0.48
2:B:166:ARG:HB3	2:B:170:ARG:CB	2.40	0.48
3:C:119:GLU:CG	3:C:490:GLN:HB2	2.42	0.48
4:D:353:SER:OG	4:D:447:ILE:HG13	2.13	0.48
6:F:523:ILE:HG13	6:F:523:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:DT:H72	6:F:428:SER:OG	2.13	0.48
3:C:122:VAL:HG21	3:C:493:ILE:HB	1.96	0.48
3:C:848:GLU:CD	3:C:888:THR:HG22	2.38	0.48
3:C:1004:ASP:O	3:C:1005:GLU:HG3	2.14	0.48
4:D:950:ILE:HD13	4:D:982:LEU:HD12	1.94	0.48
6:F:144:LEU:HD12	6:F:147:GLN:CB	2.43	0.48
6:F:326:TRP:O	6:F:330:LEU:HG	2.14	0.48
6:F:341:LEU:HB2	6:F:344:LEU:HD21	1.96	0.48
3:C:1003:THR:OG1	3:C:1007:LYS:HD2	2.14	0.48
3:C:1104:PRO:HG2	4:D:725:MET:SD	2.54	0.48
3:C:1242:LYS:HD2	4:D:465:GLN:HE22	1.79	0.48
4:D:105:ILE:HD13	4:D:273:ILE:HG12	1.94	0.48
4:D:185:ILE:O	4:D:189:LEU:HD12	2.14	0.48
4:D:197:GLU:O	4:D:201:LEU:HG	2.14	0.48
4:D:1109:LEU:HB3	4:D:1113:VAL:CG2	2.44	0.48
1:H:42:DG:H4'	1:H:43:DG:O5'	2.13	0.48
2:B:43:LEU:O	2:B:47:LEU:HG	2.13	0.48
2:B:106:GLY:H	2:B:138:ALA:CB	2.27	0.48
2:B:190:ALA:O	2:B:198:LEU:HB2	2.14	0.48
3:C:1031:ALA:HA	3:C:1034:ARG:NH1	2.27	0.48
4:D:559:ALA:HB3	4:D:562:GLU:CG	2.37	0.48
4:D:738:ARG:NH1	4:D:738:ARG:HB3	2.29	0.48
4:D:1109:LEU:HB3	4:D:1113:VAL:HG21	1.95	0.48
5:E:30:MET:HB2	5:E:46:THR:CG2	2.41	0.48
5:E:41:GLU:HG3	5:E:41:GLU:O	2.13	0.48
6:F:465:ARG:HA	6:F:468:ARG:HH12	1.78	0.48
3:C:424:ASP:O	3:C:428:VAL:HG23	2.13	0.48
4:D:194:LEU:HD23	4:D:224:LEU:HD22	1.94	0.48
4:D:377:PHE:O	4:D:381:ILE:HG13	2.13	0.48
4:D:548:VAL:HG21	4:D:574:VAL:HG22	1.94	0.48
4:D:1106:ILE:H	4:D:1122:ALA:HB1	1.78	0.48
4:D:1280:VAL:HG11	4:D:1304:ARG:NH2	2.11	0.48
6:F:140:ALA:CB	6:F:269:LEU:HD22	2.44	0.48
1:H:38:DT:H2''	1:H:39:DA:C5'	2.41	0.48
3:C:367:TYR:CD1	3:C:384:LEU:HD13	2.49	0.48
4:D:449:LEU:HD13	4:D:466:MET:HE1	1.95	0.48
4:D:665:GLN:O	4:D:669:GLN:HG2	2.13	0.48
2:A:14:VAL:HG13	2:A:15:ASP:OD1	2.14	0.47
2:A:111:THR:OG1	2:A:112:ALA:N	2.47	0.47
3:C:160:ASP:O	3:C:164:THR:OG1	2.26	0.47
3:C:966:ILE:O	3:C:969:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1295:SER:HB2	4:D:346:ARG:O	2.14	0.47
4:D:611:ILE:HG22	4:D:612:LEU:HD12	1.95	0.47
4:D:749:LYS:NZ	4:D:751:ASP:OD2	2.47	0.47
4:D:785:ASP:O	4:D:789:LYS:HG2	2.14	0.47
4:D:986:ASP:OD2	4:D:990:ARG:HB3	2.13	0.47
4:D:1052:GLU:HG3	4:D:1053:LEU:H	1.77	0.47
3:C:149:LEU:CD1	3:C:453:ILE:HG12	2.44	0.47
3:C:296:VAL:HA	3:C:315:MET:O	2.13	0.47
3:C:979:LEU:CD1	3:C:1002:LEU:HD22	2.44	0.47
3:C:1105:SER:HB2	4:D:731:ARG:HG3	1.96	0.47
4:D:506:VAL:O	4:D:510:LEU:HD22	2.14	0.47
4:D:822:MET:CE	4:D:838:ARG:HB3	2.44	0.47
1:H:6:DA:H2''	1:H:7:DA:C5'	2.43	0.47
2:A:211:ILE:CG2	2:A:216:ALA:HB2	2.44	0.47
2:A:211:ILE:HG23	2:A:216:ALA:HB2	1.95	0.47
3:C:229:ILE:HG23	3:C:240:GLU:HB2	1.95	0.47
3:C:629:PHE:HE2	3:C:650:VAL:HG21	1.80	0.47
3:C:1008:GLN:CA	3:C:1011:LEU:HD12	2.38	0.47
4:D:536:LEU:CD1	4:D:541:LEU:HD12	2.44	0.47
6:F:310:GLU:O	6:F:344:LEU:HD11	2.14	0.47
3:C:77:GLU:OE1	3:C:77:GLU:N	2.46	0.47
3:C:106:GLU:HB2	3:C:114:VAL:CG2	2.45	0.47
3:C:685:MET:HE1	3:C:1073:LYS:HE2	1.95	0.47
3:C:1101:LEU:HD23	4:D:725:MET:SD	2.54	0.47
4:D:523:GLU:OE1	4:D:547:ARG:N	2.47	0.47
4:D:1025:MET:HB3	4:D:1124:ILE:HG22	1.96	0.47
4:D:1314:LEU:HD23	4:D:1326:GLN:OE1	2.14	0.47
6:F:289:LYS:O	6:F:293:GLU:HB2	2.14	0.47
3:C:18:ARG:HB2	3:C:1188:ASP:OD2	2.14	0.47
3:C:681:MET:HB3	3:C:685:MET:HE3	1.96	0.47
3:C:841:ARG:HG3	3:C:842:ASP:H	1.79	0.47
3:C:1276:TRP:HH2	4:D:798:ARG:HG2	1.78	0.47
4:D:38:VAL:HG11	4:D:56:LEU:HD12	1.96	0.47
4:D:1009:GLU:N	4:D:1009:GLU:OE1	2.48	0.47
5:E:30:MET:HE3	5:E:49:ILE:CG2	2.37	0.47
1:H:22:DG:H22	7:G:41:DC:C1'	2.25	0.47
2:A:62:ASP:OD1	2:A:63:GLY:N	2.48	0.47
3:C:38:PHE:HD2	3:C:39:ILE:HG23	1.79	0.47
3:C:78:PRO:HB3	3:C:93:SER:O	2.14	0.47
3:C:803:ALA:HB2	3:C:1227:VAL:HG12	1.96	0.47
3:C:905:ILE:O	6:F:599:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:872:LEU:O	4:D:877:VAL:HG12	2.15	0.47
6:F:548:LEU:HD11	6:F:560:ARG:HG3	1.96	0.47
1:H:6:DA:H2''	1:H:7:DA:O4'	2.15	0.47
2:A:19:VAL:HB	2:A:23:HIS:HB3	1.97	0.47
3:C:145:ILE:HD13	3:C:512:SER:HA	1.97	0.47
3:C:262:TYR:CE1	3:C:276:GLN:HB3	2.49	0.47
3:C:742:TYR:HB3	3:C:743:PRO:HD2	1.95	0.47
3:C:979:LEU:HD12	3:C:1002:LEU:HD22	1.95	0.47
3:C:1122:LYS:HD2	3:C:1178:LYS:O	2.15	0.47
3:C:1283:ALA:HA	4:D:479:GLU:OE1	2.13	0.47
4:D:233:LYS:HB3	4:D:235:GLU:OE1	2.15	0.47
4:D:647:PRO:HG2	4:D:650:LYS:HB2	1.96	0.47
4:D:720:ASN:ND2	4:D:722:ILE:HG22	2.30	0.47
4:D:980:THR:O	4:D:997:VAL:HG23	2.14	0.47
4:D:1136:GLY:HA2	4:D:1140:ARG:CB	2.44	0.47
6:F:122:ARG:O	6:F:126:GLY:N	2.43	0.47
6:F:150:ARG:CG	6:F:155:GLU:HB3	2.44	0.47
2:B:61:ILE:CD1	2:B:142:MET:HE2	2.44	0.47
3:C:287:VAL:HB	3:C:288:PRO:HD2	1.97	0.47
3:C:654:ASP:N	3:C:654:ASP:OD1	2.46	0.47
3:C:845:LEU:HD12	3:C:845:LEU:H	1.79	0.47
3:C:1103:VAL:HG22	3:C:1111:GLN:HE21	1.79	0.47
4:D:269:TYR:O	4:D:273:ILE:HG13	2.15	0.47
4:D:948:SER:OG	4:D:1022:PRO:HD3	2.14	0.47
6:F:271:ASN:O	6:F:275:VAL:HG23	2.15	0.47
2:A:98:VAL:HG11	2:A:121:VAL:CG2	2.45	0.47
3:C:38:PHE:O	3:C:49:LEU:HB2	2.14	0.47
3:C:179:TYR:OH	3:C:462:ASN:ND2	2.45	0.47
4:D:208:THR:CG2	4:D:213:LYS:HE3	2.45	0.47
4:D:1030:GLU:CD	4:D:1090:ILE:HG23	2.40	0.47
6:F:227:GLN:HE21	6:F:231:THR:CG2	2.28	0.47
2:A:175:ALA:HB1	2:A:177:TYR:CE1	2.50	0.47
2:B:205:MET:HE3	2:B:213:PRO:HB3	1.97	0.47
3:C:320:ASP:O	3:C:324:LYS:N	2.46	0.47
3:C:974:ARG:O	3:C:978:VAL:HG23	2.15	0.47
3:C:1005:GLU:HB3	3:C:1006:GLU:OE1	2.15	0.47
3:C:1155:VAL:HG12	3:C:1156:ARG:H	1.80	0.47
6:F:150:ARG:HG2	6:F:155:GLU:HB3	1.97	0.47
6:F:234:THR:HG23	6:F:245:ALA:O	2.14	0.47
1:H:40:DA:H5'	1:H:41:DT:C7	2.45	0.46
3:C:221:LEU:CD1	3:C:313:ALA:HB1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:CYS:SG	4:D:59:ALA:N	2.88	0.46
4:D:441:LEU:HD22	4:D:441:LEU:H	1.80	0.46
4:D:548:VAL:HG12	4:D:549:LYS:H	1.80	0.46
4:D:721:SER:O	4:D:725:MET:HE3	2.15	0.46
4:D:930:LEU:HD22	4:D:1244:GLN:OE1	2.14	0.46
4:D:978:ARG:HD2	4:D:978:ARG:N	2.30	0.46
4:D:1037:PHE:CE2	4:D:1111:ASP:HB2	2.50	0.46
6:F:134:VAL:HG13	6:F:273:MET:CE	2.42	0.46
6:F:282:THR:HA	6:F:285:ARG:HB2	1.96	0.46
2:A:166:ARG:HB2	2:A:167:PRO:HD3	1.96	0.46
2:B:27:THR:OG1	2:B:28:LEU:N	2.48	0.46
3:C:132:ASP:OD1	3:C:132:ASP:N	2.48	0.46
4:D:39:LYS:O	4:D:40:LYS:HG3	2.15	0.46
4:D:62:PHE:CD1	4:D:247:PRO:HD3	2.50	0.46
4:D:186:GLN:O	4:D:190:LYS:HB3	2.15	0.46
4:D:254:PRO:HB3	4:D:260:PHE:CE1	2.50	0.46
4:D:848:VAL:HG11	4:D:880:VAL:HG13	1.97	0.46
4:D:1040:MET:SD	4:D:1078:LEU:HG	2.56	0.46
4:D:1196:LEU:HG	4:D:1198:VAL:HG12	1.96	0.46
6:F:383:ASN:OD1	6:F:383:ASN:N	2.45	0.46
3:C:217:THR:HG23	3:C:351:LEU:CD2	2.45	0.46
3:C:690:VAL:HG11	3:C:830:THR:HG21	1.96	0.46
3:C:1128:ILE:O	3:C:1132:LEU:HB3	2.16	0.46
4:D:743:MET:CG	4:D:760:THR:HA	2.45	0.46
4:D:850:LYS:HZ2	4:D:855:ASP:HB3	1.79	0.46
4:D:949:SER:HA	4:D:1019:ASN:OD1	2.16	0.46
4:D:959:LYS:HB2	4:D:985:ILE:CG1	2.45	0.46
6:F:137:TYR:HB2	6:F:361:ILE:HD13	1.97	0.46
6:F:585:GLU:CD	6:F:588:ARG:HD2	2.41	0.46
2:A:194:GLN:O	2:A:195:ARG:HG2	2.14	0.46
2:B:201:LEU:HD21	2:B:203:ILE:HD11	1.97	0.46
3:C:215:TYR:CB	3:C:220:ILE:HD11	2.44	0.46
4:D:122:SER:OG	4:D:125:GLY:HA3	2.14	0.46
4:D:1167:LYS:HE3	4:D:1170:LYS:CD	2.34	0.46
6:F:570:ASP:OD1	6:F:570:ASP:N	2.49	0.46
6:F:593:LYS:HA	6:F:596:ARG:NH1	2.29	0.46
1:H:5:DC:H1'	1:H:6:DA:N7	2.31	0.46
2:A:14:VAL:HG12	2:A:27:THR:HB	1.97	0.46
3:C:252:SER:CA	3:C:265:LYS:HG3	2.42	0.46
3:C:454:ARG:HG2	3:C:458:GLU:CD	2.40	0.46
3:C:697:LYS:HA	3:C:795:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:294:ASN:ND2	6:F:406:GLN:HE21	2.14	0.46
4:D:485:MET:HG3	4:D:486:SER:H	1.80	0.46
4:D:1101:LEU:HD22	4:D:1107:VAL:HG12	1.96	0.46
5:E:41:GLU:HB2	5:E:49:ILE:HD11	1.97	0.46
1:H:48:DT:H2"	3:C:183:TRP:CZ3	2.51	0.46
2:B:89:ALA:O	2:B:124:VAL:HG22	2.15	0.46
3:C:360:LEU:HD22	3:C:378:ARG:HE	1.79	0.46
3:C:953:LEU:CD1	3:C:1033:ARG:HG3	2.46	0.46
4:D:848:VAL:HG22	4:D:858:VAL:CG2	2.38	0.46
4:D:952:VAL:HG11	4:D:984:LEU:HD22	1.96	0.46
4:D:959:LYS:HB2	4:D:985:ILE:HG12	1.97	0.46
4:D:1027:VAL:CG2	4:D:1122:ALA:HB3	2.46	0.46
6:F:503:GLU:HB2	6:F:504:PRO:HD2	1.97	0.46
3:C:672:GLU:HB3	3:C:1187:PHE:CE1	2.51	0.46
3:C:993:PRO:HG2	3:C:996:ARG:HB3	1.97	0.46
3:C:1304:MET:CE	3:C:1308:ILE:HD11	2.45	0.46
4:D:1025:MET:HE3	4:D:1124:ILE:HG22	1.98	0.46
6:F:165:PHE:HD1	6:F:259:PHE:HA	1.80	0.46
6:F:519:LEU:O	6:F:519:LEU:HD23	2.15	0.46
2:A:191:ARG:HD3	2:A:191:ARG:HA	1.70	0.46
3:C:521:LEU:O	3:C:525:THR:HG22	2.16	0.46
3:C:975:ILE:O	3:C:979:LEU:HD13	2.16	0.46
4:D:21:LYS:HG2	4:D:22:ILE:N	2.31	0.46
4:D:74:LYS:HD3	4:D:87:LYS:NZ	2.30	0.46
4:D:500:ILE:HG22	4:D:500:ILE:O	2.16	0.46
4:D:1314:LEU:HD21	4:D:1331:VAL:CG2	2.45	0.46
4:D:1314:LEU:HD23	4:D:1326:GLN:CB	2.45	0.46
3:C:109:ALA:HB1	3:C:110:PRO:HD2	1.98	0.46
3:C:205:PRO:O	3:C:208:ILE:HG22	2.16	0.46
3:C:232:ILE:HG23	3:C:237:LEU:HD23	1.97	0.46
3:C:296:VAL:CG2	3:C:314:ASN:HA	2.46	0.46
3:C:1242:LYS:HD2	4:D:465:GLN:NE2	2.30	0.46
4:D:41:PRO:HB2	4:D:270:ARG:HG2	1.98	0.46
4:D:288:PRO:HB3	6:F:377:LYS:HG2	1.97	0.46
6:F:573:LEU:HD12	6:F:574:GLU:H	1.80	0.46
2:A:155:ALA:N	2:A:174:ASP:OD1	2.45	0.46
3:C:724:VAL:HG22	3:C:734:ILE:CD1	2.46	0.46
4:D:536:LEU:HD12	4:D:541:LEU:HD12	1.98	0.46
4:D:664:ILE:CG2	4:D:681:LYS:HD2	2.46	0.46
4:D:1045:THR:HG21	4:D:1076:PRO:CB	2.45	0.46
4:D:1057:SER:HB2	4:D:1059:LEU:CD1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1174:ARG:HA	4:D:1189:MET:HA	1.97	0.46
6:F:102:MET:SD	6:F:388:ILE:HD13	2.56	0.46
6:F:295:CYS:SG	6:F:330:LEU:HD23	2.56	0.46
7:G:52:DC:H2"	7:G:53:DA:C8	2.51	0.46
3:C:243:PRO:O	3:C:246:LEU:HD12	2.15	0.45
3:C:836:LEU:CD1	3:C:1054:LEU:HD13	2.46	0.45
3:C:1010:GLN:HA	3:C:1013:GLN:HB2	1.97	0.45
3:C:1211:ARG:O	3:C:1211:ARG:HD3	2.16	0.45
4:D:411:ILE:O	4:D:415:VAL:HG23	2.16	0.45
6:F:234:THR:HB	6:F:248:GLU:CD	2.40	0.45
2:B:162:GLU:OE2	2:B:165:GLU:HA	2.16	0.45
3:C:34:SER:O	3:C:457:GLY:HA3	2.16	0.45
3:C:812:PHE:CE2	3:C:813:GLU:HG2	2.51	0.45
3:C:1079:ILE:O	3:C:1079:ILE:HG13	2.16	0.45
4:D:452:LEU:HD13	4:D:500:ILE:HG22	1.97	0.45
4:D:616:PRO:HA	4:D:619:ILE:HG22	1.98	0.45
4:D:1074:LEU:O	4:D:1075:ARG:HD3	2.16	0.45
3:C:255:ILE:O	3:C:262:TYR:N	2.49	0.45
3:C:646:SER:OG	3:C:649:GLN:HG3	2.16	0.45
3:C:1072:ASN:OD1	3:C:1072:ASN:N	2.48	0.45
4:D:644:MET:HE2	4:D:722:ILE:HD12	1.97	0.45
4:D:872:LEU:HB3	4:D:877:VAL:CG1	2.46	0.45
4:D:967:VAL:HG13	4:D:972:LYS:N	2.32	0.45
4:D:1235:ASN:O	4:D:1239:ASP:HB2	2.16	0.45
4:D:1268:ASN:O	4:D:1300:ALA:HB1	2.17	0.45
6:F:247:GLU:HG2	6:F:250:LEU:HD12	1.97	0.45
6:F:277:MET:HE3	6:F:281:ARG:HB2	1.97	0.45
2:A:15:ASP:OD1	2:A:15:ASP:N	2.49	0.45
2:B:20:SER:O	2:B:23:HIS:N	2.28	0.45
2:B:205:MET:HG2	2:B:206:GLU:O	2.16	0.45
2:B:205:MET:CE	2:B:217:ILE:HG13	2.45	0.45
3:C:106:GLU:CB	3:C:114:VAL:HG21	2.47	0.45
4:D:681:LYS:O	4:D:685:ILE:HG22	2.16	0.45
4:D:843:VAL:HG23	4:D:883:ARG:HD3	1.98	0.45
6:F:353:LEU:HB3	6:F:357:GLN:HB2	1.98	0.45
6:F:387:VAL:HG22	6:F:435:ILE:HD13	1.98	0.45
6:F:544:THR:O	6:F:548:LEU:HB3	2.16	0.45
2:A:69:SER:OG	2:A:70:THR:N	2.49	0.45
2:B:158:ARG:HD2	2:B:172:LEU:HD21	1.98	0.45
4:D:264:ASP:HB2	4:D:324:LEU:HD22	1.99	0.45
4:D:548:VAL:HG21	4:D:574:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:895:CYS:SG	4:D:897:HIS:N	2.89	0.45
4:D:1034:PHE:HB2	4:D:1081:VAL:CG2	2.47	0.45
6:F:90:GLU:OE1	6:F:90:GLU:N	2.49	0.45
6:F:312:SER:OG	6:F:314:THR:HG23	2.17	0.45
2:A:14:VAL:HG12	2:A:27:THR:O	2.17	0.45
3:C:788:SER:O	3:C:789:THR:HG23	2.16	0.45
3:C:1028:LYS:HE2	3:C:1028:LYS:HB3	1.78	0.45
4:D:130:MET:HE2	4:D:135:ILE:CG1	2.47	0.45
4:D:800:LEU:HD22	4:D:1256:ILE:CD1	2.38	0.45
4:D:844:THR:O	4:D:861:ASN:HB3	2.16	0.45
4:D:865:HIS:CE1	4:D:867:GLN:HG2	2.51	0.45
4:D:999:TYR:HE2	4:D:1027:VAL:HG13	1.81	0.45
6:F:335:GLU:O	6:F:339:ARG:HG2	2.17	0.45
6:F:436:ARG:O	6:F:440:THR:HG22	2.16	0.45
1:H:42:DG:C6	6:F:106:GLY:HA3	2.52	0.45
3:C:106:GLU:OE1	3:C:106:GLU:HA	2.16	0.45
3:C:979:LEU:HD11	3:C:1011:LEU:CD2	2.41	0.45
3:C:1132:LEU:HD11	3:C:1174:GLU:HG2	1.98	0.45
3:C:1293:VAL:CG2	3:C:1315:MET:HE3	2.46	0.45
3:C:1307:ASN:HB3	3:C:1312:ASN:O	2.17	0.45
4:D:490:ILE:O	4:D:490:ILE:HG12	2.17	0.45
4:D:925:GLU:HG3	4:D:926:PRO:HD3	1.98	0.45
4:D:974:VAL:HG21	4:D:1030:GLU:CB	2.46	0.45
3:C:228:VAL:HB	3:C:335:THR:CG2	2.47	0.45
3:C:347:ILE:HD13	3:C:347:ILE:HA	1.75	0.45
3:C:1211:ARG:H	3:C:1211:ARG:HG3	1.56	0.45
4:D:17:PHE:HE2	4:D:20:ILE:HD11	1.81	0.45
4:D:80:HIS:HB3	4:D:83:VAL:HG12	1.99	0.45
4:D:133:ARG:NH2	6:F:93:ARG:HA	2.32	0.45
4:D:1026:PRO:HA	4:D:1122:ALA:O	2.17	0.45
4:D:1038:THR:HG21	4:D:1079:LYS:CB	2.47	0.45
4:D:1059:LEU:CB	4:D:1107:VAL:HG23	2.46	0.45
4:D:1101:LEU:HD13	4:D:1107:VAL:CG1	2.46	0.45
3:C:101:ARG:HD3	3:C:118:LYS:HZ3	1.82	0.45
3:C:936:ARG:HH21	3:C:1047:LEU:CD2	2.30	0.45
3:C:953:LEU:HD21	3:C:1033:ARG:HD2	1.99	0.45
3:C:1214:ASP:OD1	3:C:1215:GLY:N	2.48	0.45
3:C:1337:ILE:HG13	4:D:21:LYS:O	2.17	0.45
4:D:841:GLY:O	4:D:842:ARG:HG3	2.16	0.45
4:D:850:LYS:HB3	4:D:851:PRO:HD2	1.99	0.45
4:D:1038:THR:HG21	4:D:1079:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:228:TYR:HA	6:F:252:LEU:HD22	1.99	0.45
3:C:677:ASN:OD1	4:D:779:ALA:HB1	2.17	0.45
3:C:1103:VAL:CG2	3:C:1111:GLN:HE21	2.31	0.45
3:C:1341:ASP:OD1	3:C:1341:ASP:N	2.41	0.45
4:D:929:GLN:OE1	4:D:930:LEU:HG	2.17	0.45
4:D:1027:VAL:CG2	4:D:1102:PRO:HD2	2.33	0.45
6:F:227:GLN:CG	6:F:252:LEU:HD13	2.46	0.45
6:F:337:VAL:O	6:F:341:LEU:HD23	2.17	0.45
7:G:26:DT:H6	7:G:26:DT:H2'	1.64	0.45
3:C:12:ARG:NH1	3:C:1182:ILE:O	2.50	0.44
3:C:128:PRO:O	3:C:129:LEU:HD23	2.17	0.44
3:C:413:GLU:OE1	3:C:413:GLU:N	2.36	0.44
3:C:810:TYR:CE1	4:D:359:PRO:HD2	2.51	0.44
4:D:17:PHE:O	4:D:17:PHE:CD1	2.70	0.44
4:D:294:ASN:HD22	6:F:406:GLN:HE21	1.65	0.44
4:D:807:LEU:HD12	4:D:1259:GLN:OE1	2.17	0.44
4:D:1058:SER:O	4:D:1060:VAL:HG23	2.17	0.44
7:G:57:DT:H2''	7:G:58:DG:O5'	2.17	0.44
3:C:210:LEU:HD21	3:C:429:MET:CE	2.48	0.44
3:C:492:MET:HE2	3:C:492:MET:HB3	1.91	0.44
4:D:967:VAL:CG1	4:D:971:GLY:HA2	2.47	0.44
4:D:1208:ASP:OD1	4:D:1209:VAL:N	2.50	0.44
5:E:30:MET:HE2	5:E:49:ILE:HG22	1.98	0.44
1:H:17:DC:O2	7:G:46:DG:N2	2.49	0.44
1:H:40:DA:H8	6:F:428:SER:HB3	1.81	0.44
2:A:26:VAL:HG22	2:A:203:ILE:HB	2.00	0.44
2:B:39:LEU:HA	2:B:39:LEU:HD23	1.70	0.44
3:C:242:VAL:HG22	3:C:245:ARG:HE	1.82	0.44
3:C:468:LEU:O	3:C:468:LEU:HD23	2.18	0.44
3:C:900:LYS:HG2	6:F:563:PHE:CD1	2.53	0.44
3:C:906:PHE:CD2	6:F:611:LEU:HD11	2.53	0.44
4:D:650:LYS:HG3	4:D:693:VAL:HG21	1.99	0.44
4:D:967:VAL:CG2	4:D:973:LEU:HG	2.47	0.44
4:D:1045:THR:CG2	4:D:1076:PRO:HB3	2.46	0.44
4:D:1260:MET:HG3	4:D:1307:LEU:O	2.18	0.44
6:F:291:CYS:HB3	6:F:297:MET:CE	2.47	0.44
2:B:59:VAL:HG22	2:B:171:LEU:HB2	1.99	0.44
3:C:320:ASP:OD1	3:C:320:ASP:N	2.49	0.44
4:D:1024:THR:C	4:D:1026:PRO:HD3	2.42	0.44
4:D:1081:VAL:HB	4:D:1085:GLY:C	2.43	0.44
4:D:1153:PRO:O	4:D:1194:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:MET:H	5:E:30:MET:HG2	1.54	0.44
6:F:235:ILE:HD13	6:F:245:ALA:O	2.17	0.44
6:F:585:GLU:OE2	6:F:588:ARG:HD2	2.17	0.44
7:G:2:DC:H2''	7:G:3:DT:H6	1.83	0.44
7:G:56:DT:H2''	7:G:57:DT:C5	2.53	0.44
3:C:319:LEU:HA	3:C:322:LEU:HD12	1.98	0.44
3:C:988:LYS:HA	3:C:991:LYS:CG	2.42	0.44
3:C:1004:ASP:HA	3:C:1008:GLN:HG2	2.00	0.44
3:C:1339:LEU:HD22	4:D:17:PHE:CD2	2.52	0.44
4:D:294:ASN:HB3	6:F:406:GLN:NE2	2.32	0.44
6:F:342:GLN:O	6:F:346:GLN:HG3	2.17	0.44
6:F:515:GLU:HG2	6:F:516:ASP:OD1	2.18	0.44
2:A:42:ALA:O	2:A:46:ILE:HG12	2.18	0.44
2:B:62:ASP:OD1	2:B:62:ASP:N	2.40	0.44
2:B:105:SER:HA	2:B:138:ALA:C	2.42	0.44
3:C:316:GLU:O	3:C:317:LEU:HD23	2.18	0.44
4:D:552:ILE:HD11	4:D:570:LYS:HB2	1.99	0.44
4:D:615:LYS:HB2	4:D:616:PRO:HD3	2.00	0.44
4:D:1087:ASP:HB2	4:D:1096:PRO:HB3	1.98	0.44
6:F:217:ALA:O	6:F:221:PHE:HB2	2.18	0.44
6:F:250:LEU:HB3	6:F:254:GLU:OE2	2.17	0.44
6:F:343:LYS:O	6:F:347:ILE:HG13	2.17	0.44
2:A:90:VAL:HG23	2:A:123:ILE:HD13	2.00	0.44
2:B:96:ASP:O	2:B:147:GLN:HA	2.18	0.44
3:C:96:LEU:HB3	3:C:125:GLY:O	2.17	0.44
3:C:367:TYR:OH	3:C:374:GLU:OE2	2.23	0.44
4:D:161:THR:CG2	4:D:164:GLN:HG3	2.37	0.44
4:D:678:ARG:HD2	4:D:678:ARG:O	2.18	0.44
4:D:966:VAL:HG12	4:D:967:VAL:H	1.83	0.44
4:D:1095:MET:SD	4:D:1096:PRO:HD2	2.58	0.44
4:D:1282:TYR:O	4:D:1285:VAL:HG22	2.18	0.44
6:F:426:LYS:HG2	6:F:427:PHE:H	1.83	0.44
1:H:12:DA:H1'	1:H:13:DT:H5'	2.00	0.44
3:C:618:GLN:NE2	4:D:770:LEU:HB2	2.32	0.44
3:C:1115:THR:HG23	3:C:1228:GLY:HA3	2.00	0.44
4:D:426:ALA:HB3	4:D:427:PRO:CD	2.48	0.44
7:G:12:DG:H8	7:G:12:DG:H5''	1.82	0.44
2:A:225:ALA:CB	2:B:232:VAL:HG11	2.47	0.44
3:C:745:GLU:CG	3:C:1017:GLN:HG3	2.48	0.44
3:C:755:LYS:HA	3:C:766:ASN:HB2	1.99	0.44
3:C:1298:VAL:HG23	3:C:1321:GLU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:931:THR:O	4:D:931:THR:OG1	2.35	0.44
4:D:1341:ARG:HH11	4:D:1341:ARG:CG	2.14	0.44
7:G:0:DC:H2''	7:G:1:DC:C6	2.53	0.44
1:H:18:DA:H2''	1:H:19:DA:C8	2.53	0.43
1:H:43:DG:H1'	6:F:102:MET:HE1	2.00	0.43
2:A:71:LYS:HG3	2:A:72:GLU:N	2.33	0.43
3:C:135:THR:CG2	3:C:527:LYS:HE2	2.48	0.43
3:C:1001:GLY:O	3:C:1002:LEU:HD12	2.18	0.43
3:C:1014:LEU:HA	3:C:1017:GLN:HB2	1.99	0.43
3:C:1131:MET:HE2	3:C:1141:LEU:CD1	2.42	0.43
4:D:949:SER:HB3	4:D:1016:THR:CB	2.47	0.43
4:D:1021:ASP:HB3	4:D:1024:THR:O	2.18	0.43
4:D:1048:ARG:HH21	4:D:1059:LEU:HD21	1.83	0.43
1:H:63:DG:OP1	4:D:1170:LYS:HG3	2.18	0.43
2:A:73:GLY:O	2:A:134:THR:HG22	2.18	0.43
2:A:226:GLU:O	2:B:10:LYS:NZ	2.51	0.43
2:B:14:VAL:HB	2:B:28:LEU:HD13	1.99	0.43
3:C:818:VAL:O	3:C:1079:ILE:HA	2.18	0.43
3:C:1289:GLU:OE1	4:D:473:THR:HG22	2.18	0.43
3:C:1335:ILE:HD12	4:D:1336:ALA:CB	2.48	0.43
4:D:581:MET:C	4:D:582:ILE:HD13	2.43	0.43
4:D:1099:TYR:HD1	4:D:1099:TYR:HA	1.67	0.43
4:D:1167:LYS:O	4:D:1167:LYS:HD2	2.18	0.43
6:F:163:THR:HG21	6:F:262:VAL:HG13	2.00	0.43
6:F:329:LYS:NZ	6:F:332:ASP:HB2	2.33	0.43
6:F:582:VAL:HG23	6:F:584:ARG:HH12	1.82	0.43
7:G:36:DT:H2''	7:G:37:DA:C8	2.53	0.43
7:G:42:DT:H6	7:G:42:DT:H2'	1.63	0.43
1:H:52:DA:H2''	1:H:53:DC:H5'	1.99	0.43
3:C:8:LYS:HD3	3:C:1168:GLU:OE1	2.17	0.43
3:C:272:ARG:HA	3:C:275:ARG:CG	2.48	0.43
3:C:839:VAL:HG21	3:C:841:ARG:NH2	2.33	0.43
4:D:133:ARG:CZ	6:F:93:ARG:HG2	2.47	0.43
4:D:949:SER:O	4:D:951:GLN:HG2	2.18	0.43
4:D:1063:ASP:OD1	4:D:1066:GLU:N	2.51	0.43
3:C:219:GLN:HA	3:C:222:ASP:HB3	2.01	0.43
3:C:624:ASP:OD2	3:C:628:HIS:HB2	2.18	0.43
4:D:555:TYR:HE1	4:D:565:ALA:HB2	1.83	0.43
4:D:683:ILE:HA	4:D:683:ILE:HD13	1.79	0.43
4:D:1034:PHE:O	4:D:1080:ILE:HG23	2.19	0.43
4:D:1061:VAL:HG23	4:D:1107:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:316:PHE:O	6:F:320:ILE:HD12	2.18	0.43
7:G:27:DA:H1'	7:G:28:DG:H5'	1.99	0.43
1:H:22:DG:N2	7:G:41:DC:H1'	2.27	0.43
1:H:47:DC:H6	1:H:47:DC:H5''	1.84	0.43
3:C:818:VAL:HG12	3:C:819:SER:O	2.18	0.43
4:D:208:THR:HG21	4:D:213:LYS:CB	2.48	0.43
4:D:645:VAL:O	4:D:741:ALA:HB1	2.17	0.43
4:D:1004:ALA:N	4:D:1017:VAL:O	2.50	0.43
4:D:1062:LEU:HB3	4:D:1066:GLU:O	2.17	0.43
6:F:108:VAL:HG21	6:F:382:ALA:HA	1.99	0.43
6:F:248:GLU:CA	6:F:251:LYS:HE2	2.45	0.43
7:G:43:DT:H2''	7:G:44:DT:C5'	2.48	0.43
2:A:193:GLU:HG3	2:A:194:GLN:N	2.33	0.43
2:B:211:ILE:HD13	2:B:211:ILE:HA	1.88	0.43
3:C:79:VAL:HG13	3:C:80:PHE:H	1.83	0.43
3:C:797:GLY:N	3:C:1231:TYR:OH	2.50	0.43
3:C:867:GLU:OE2	3:C:943:LYS:HD2	2.19	0.43
3:C:887:VAL:HB	3:C:913:VAL:HG22	2.00	0.43
3:C:905:ILE:HG22	3:C:906:PHE:CE1	2.54	0.43
3:C:1002:LEU:CD2	3:C:1007:LYS:HB2	2.27	0.43
4:D:646:ILE:HD12	4:D:762:ASN:ND2	2.33	0.43
4:D:1328:THR:HG23	4:D:1332:LEU:HD23	2.00	0.43
4:D:1355:ARG:NH1	4:D:1369:ARG:HH12	2.17	0.43
6:F:102:MET:HA	6:F:105:MET:CE	2.46	0.43
6:F:219:GLU:HG3	6:F:220:LYS:HG2	2.00	0.43
6:F:269:LEU:O	6:F:273:MET:HG2	2.18	0.43
6:F:452:ILE:HD11	6:F:457:ILE:HD11	2.00	0.43
7:G:3:DT:H2''	7:G:4:DG:C8	2.54	0.43
3:C:35:PHE:CE2	3:C:39:ILE:HG12	2.53	0.43
3:C:805:MET:HE1	3:C:1221:PHE:CZ	2.54	0.43
3:C:979:LEU:HG	3:C:1002:LEU:HD13	2.00	0.43
3:C:988:LYS:HE3	3:C:988:LYS:HB2	1.72	0.43
4:D:848:VAL:HG13	4:D:858:VAL:HG21	2.00	0.43
6:F:261:LEU:HD21	6:F:266:PHE:HA	2.00	0.43
7:G:30:DA:H2''	7:G:31:DC:O5'	2.19	0.43
7:G:32:DA:H2''	7:G:33:DA:C5'	2.48	0.43
3:C:138:ILE:HB	3:C:143:ARG:HD2	2.01	0.43
3:C:303:ASP:OD1	3:C:305:SER:N	2.47	0.43
3:C:632:ASP:OD1	3:C:633:LEU:HD23	2.18	0.43
3:C:1075:VAL:HG11	4:D:356:THR:HG22	2.00	0.43
3:C:1103:VAL:HB	3:C:1104:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1294:LYS:O	4:D:348:ASP:HB2	2.18	0.43
4:D:641:ILE:HD12	4:D:641:ILE:HA	1.87	0.43
4:D:678:ARG:HD2	4:D:678:ARG:C	2.44	0.43
6:F:324:LYS:HG3	6:F:326:TRP:CZ2	2.53	0.43
6:F:364:ARG:O	6:F:367:ILE:HB	2.18	0.43
7:G:6:DA:H5'	7:G:6:DA:H8	1.82	0.43
2:A:225:ALA:HB3	2:B:232:VAL:HG11	2.01	0.43
2:B:20:SER:HG	2:B:23:HIS:HB3	1.84	0.43
3:C:1146:GLN:O	3:C:1146:GLN:NE2	2.48	0.43
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.68	0.43
4:D:1016:THR:O	4:D:1016:THR:OG1	2.33	0.43
4:D:1107:VAL:HG12	4:D:1121:LEU:O	2.19	0.43
5:E:19:LEU:HD11	5:E:51:LEU:CD2	2.48	0.43
6:F:261:LEU:CD2	6:F:266:PHE:HA	2.49	0.43
6:F:298:PRO:HD3	6:F:326:TRP:CD2	2.53	0.43
6:F:354:THR:HG22	6:F:357:GLN:OE1	2.18	0.43
6:F:574:GLU:OE1	6:F:583:THR:HB	2.18	0.43
2:A:61:ILE:HG22	2:A:62:ASP:H	1.84	0.43
3:C:887:VAL:HB	3:C:913:VAL:HG21	2.01	0.43
3:C:1007:LYS:HE3	3:C:1007:LYS:HB3	1.83	0.43
3:C:1292:THR:HG21	3:C:1317:PRO:HB2	2.01	0.43
4:D:79:LYS:HE2	6:F:569:THR:HB	2.01	0.43
4:D:94:GLN:O	4:D:97:VAL:HG12	2.19	0.43
4:D:694:SER:HB3	4:D:738:ARG:NH2	2.34	0.43
4:D:1027:VAL:HB	4:D:1121:LEU:H	1.84	0.43
1:H:58:DG:H2''	1:H:59:DC:C6	2.54	0.42
2:A:135:ASP:OD1	2:A:136:GLU:N	2.52	0.42
2:B:61:ILE:HG22	2:B:64:VAL:N	2.33	0.42
3:C:1340:GLU:CD	4:D:1341:ARG:HE	2.26	0.42
4:D:491:LEU:HD12	4:D:904:ALA:O	2.19	0.42
4:D:527:LEU:HB2	4:D:550:VAL:HG12	2.00	0.42
4:D:820:ILE:HG22	4:D:1227:HIS:ND1	2.34	0.42
4:D:1196:LEU:HD12	4:D:1196:LEU:HA	1.83	0.42
4:D:1269:ALA:HB3	4:D:1274:PHE:HD1	1.83	0.42
6:F:147:GLN:HG2	6:F:150:ARG:NH2	2.33	0.42
6:F:147:GLN:HG2	6:F:150:ARG:HH21	1.84	0.42
6:F:287:ILE:HD12	6:F:310:GLU:OE1	2.19	0.42
6:F:294:GLN:NE2	6:F:333:VAL:HG21	2.34	0.42
6:F:548:LEU:HD22	6:F:560:ARG:HH21	1.84	0.42
2:B:162:GLU:HG3	2:B:166:ARG:NH1	2.34	0.42
3:C:148:GLN:O	3:C:453:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:441:GLU:OE2	3:C:441:GLU:HA	2.19	0.42
3:C:629:PHE:CE2	3:C:650:VAL:HG21	2.54	0.42
3:C:1120:ALA:HB2	3:C:1199:LEU:HD21	2.01	0.42
4:D:572:THR:OG1	4:D:576:ARG:HB2	2.19	0.42
4:D:1042:ASP:CB	4:D:1048:ARG:HB2	2.37	0.42
4:D:1221:LEU:HD22	4:D:1306:LEU:HB2	2.01	0.42
6:F:389:SER:HA	6:F:392:LYS:HE3	2.02	0.42
2:B:34:GLY:O	2:B:38:THR:HG22	2.20	0.42
3:C:510:GLN:OE1	3:C:510:GLN:N	2.47	0.42
3:C:636:CYS:HB2	3:C:645:PHE:CD2	2.54	0.42
3:C:981:ALA:HB3	3:C:1007:LYS:HE3	2.02	0.42
4:D:116:PHE:O	4:D:124:ILE:HG13	2.19	0.42
4:D:162:GLU:H	4:D:162:GLU:HG3	1.59	0.42
4:D:423:LEU:CG	4:D:466:MET:HE3	2.49	0.42
4:D:846:GLU:HA	4:D:860:ARG:NH1	2.35	0.42
4:D:1156:LEU:HD13	4:D:1208:ASP:C	2.44	0.42
6:F:354:THR:O	6:F:358:VAL:HG23	2.20	0.42
2:B:188:GLU:OE2	2:B:202:VAL:HG21	2.20	0.42
3:C:231:GLU:CG	3:C:233:ARG:HG3	2.50	0.42
3:C:724:VAL:HG11	3:C:727:VAL:CG2	2.49	0.42
3:C:972:PHE:HD2	3:C:975:ILE:HD11	1.85	0.42
3:C:1083:GLU:OE1	3:C:1083:GLU:N	2.52	0.42
3:C:1240:ASP:OD1	3:C:1240:ASP:N	2.52	0.42
3:C:1264:GLN:OE1	3:C:1264:GLN:HA	2.20	0.42
4:D:982:LEU:O	4:D:994:SER:HA	2.18	0.42
6:F:267:ASP:O	6:F:271:ASN:HB2	2.19	0.42
6:F:347:ILE:O	6:F:350:GLU:HB2	2.19	0.42
6:F:572:THR:CB	6:F:575:GLU:HB3	2.48	0.42
7:G:32:DA:H2''	7:G:33:DA:H5'	2.01	0.42
1:H:15:DG:O6	6:F:585:GLU:HG3	2.20	0.42
2:A:13:LEU:HD12	2:A:14:VAL:H	1.84	0.42
3:C:12:ARG:CD	3:C:1183:ALA:HB2	2.48	0.42
3:C:17:LYS:N	3:C:17:LYS:HD2	2.35	0.42
3:C:158:ASP:OD1	3:C:159:SER:N	2.47	0.42
3:C:227:LYS:HD2	3:C:334:GLU:CG	2.49	0.42
3:C:1164:PHE:CD1	3:C:1168:GLU:HB2	2.52	0.42
4:D:24:LEU:HD12	4:D:24:LEU:HA	1.85	0.42
4:D:903:LEU:HD21	4:D:909:ILE:HD13	2.01	0.42
4:D:1172:LYS:HE2	4:D:1189:MET:HE1	2.01	0.42
4:D:1266:ILE:HD11	4:D:1278:GLU:HG3	2.02	0.42
2:A:27:THR:C	2:A:28:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:71:LYS:HZ3	2:A:140:ILE:HG22	1.84	0.42
3:C:260:LYS:HD3	3:C:262:TYR:CE1	2.55	0.42
4:D:78:LEU:O	4:D:78:LEU:HD23	2.19	0.42
4:D:151:MET:HE2	4:D:175:GLU:OE2	2.20	0.42
4:D:395:LYS:HE2	4:D:395:LYS:HB3	1.87	0.42
4:D:549:LYS:HE3	4:D:549:LYS:HB2	1.85	0.42
4:D:1038:THR:HG21	4:D:1079:LYS:HB2	2.02	0.42
6:F:157:ARG:CD	6:F:160:ASP:HB2	2.49	0.42
6:F:262:VAL:HG12	6:F:263:PRO:CD	2.50	0.42
6:F:562:ARG:HG2	6:F:591:GLU:OE1	2.19	0.42
3:C:1327:LEU:O	3:C:1331:ARG:HG3	2.19	0.42
4:D:117:LEU:HB2	4:D:124:ILE:HD12	2.02	0.42
4:D:552:ILE:HG13	4:D:570:LYS:HG3	2.02	0.42
4:D:658:GLU:O	4:D:661:VAL:HG12	2.19	0.42
4:D:848:VAL:HG13	4:D:858:VAL:CG2	2.50	0.42
4:D:1168:GLU:HG2	4:D:1173:ARG:HG3	2.02	0.42
5:E:76:GLU:HA	5:E:79:GLU:HB2	2.01	0.42
6:F:248:GLU:HA	6:F:251:LYS:HG3	2.01	0.42
6:F:262:VAL:HG12	6:F:263:PRO:HD2	2.02	0.42
6:F:511:ILE:HD13	6:F:522:PHE:CE2	2.55	0.42
2:B:64:VAL:HG21	2:B:78:ILE:HD11	2.01	0.42
3:C:622:ASN:HB2	3:C:630:VAL:HG22	2.00	0.42
3:C:736:VAL:HG23	3:C:737:ASN:O	2.20	0.42
3:C:1103:VAL:HG11	3:C:1112:ILE:HD11	2.01	0.42
3:C:1223:ARG:HH21	4:D:721:SER:HB3	1.85	0.42
4:D:218:THR:CA	4:D:221:ILE:HG22	2.41	0.42
4:D:733:SER:HB3	4:D:736:GLN:HE21	1.84	0.42
4:D:1024:THR:HG22	4:D:1026:PRO:CD	2.39	0.42
4:D:1108:GLN:HG2	4:D:1109:LEU:HD23	2.01	0.42
4:D:1306:LEU:HD23	4:D:1306:LEU:O	2.18	0.42
3:C:1222:GLU:OE1	4:D:512:TYR:OH	2.32	0.42
3:C:1292:THR:HG21	3:C:1317:PRO:CB	2.50	0.42
4:D:309:ASN:HB2	4:D:326:SER:HB3	2.01	0.42
4:D:416:ILE:HG22	4:D:416:ILE:O	2.19	0.42
4:D:416:ILE:HD12	4:D:416:ILE:HG23	1.84	0.42
4:D:766:GLY:O	4:D:767:LEU:HD12	2.20	0.42
4:D:1314:LEU:HD22	4:D:1314:LEU:HA	1.61	0.42
6:F:96:ASP:O	6:F:100:MET:HG3	2.20	0.42
2:A:13:LEU:HD12	2:A:14:VAL:N	2.35	0.42
2:A:51:MET:HE2	2:A:216:ALA:HB1	2.02	0.42
2:A:64:VAL:HG23	2:A:69:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:VAL:CG2	2:B:171:LEU:HD12	2.50	0.42
2:B:158:ARG:H	2:B:158:ARG:HG3	1.48	0.42
3:C:22:LEU:HB3	3:C:655:VAL:HG11	2.01	0.42
3:C:231:GLU:HG3	3:C:233:ARG:HG3	2.01	0.42
3:C:550:VAL:HG11	4:D:776:THR:HG22	2.02	0.42
3:C:696:ASP:O	3:C:697:LYS:HB3	2.20	0.42
3:C:1043:ALA:HB1	3:C:1044:PRO:HD2	2.01	0.42
3:C:1297:ASP:O	3:C:1301:ARG:HG2	2.20	0.42
4:D:130:MET:HE2	4:D:135:ILE:HG12	2.02	0.42
4:D:450:HIS:NE2	4:D:625:MET:HE1	2.35	0.42
4:D:816:THR:OG1	4:D:889:ASP:HB2	2.20	0.42
4:D:1142:ALA:O	4:D:1146:GLU:HG2	2.19	0.42
4:D:1194:ARG:HD2	4:D:1211:SER:OG	2.20	0.42
6:F:136:GLU:O	6:F:138:PRO:HD3	2.20	0.42
6:F:286:LEU:O	6:F:290:LEU:HD22	2.20	0.42
2:B:12:ARG:NE	2:B:12:ARG:HA	2.35	0.41
2:B:98:VAL:HG21	2:B:121:VAL:HG21	2.02	0.41
3:C:101:ARG:HD3	3:C:118:LYS:NZ	2.35	0.41
3:C:900:LYS:HG2	6:F:563:PHE:HD1	1.84	0.41
3:C:992:LEU:HD22	3:C:996:ARG:HH11	1.85	0.41
4:D:211:GLU:O	4:D:215:LYS:HB2	2.19	0.41
4:D:973:LEU:N	4:D:1003:LEU:HD12	2.32	0.41
5:E:15:ASN:HB3	5:E:18:ASP:OD1	2.19	0.41
6:F:234:THR:HB	6:F:248:GLU:OE1	2.19	0.41
2:A:182:ARG:O	2:A:183:ILE:HD13	2.20	0.41
2:B:29:GLU:HB3	2:B:200:LYS:HG3	2.02	0.41
3:C:98:VAL:HG21	3:C:124:MET:SD	2.60	0.41
3:C:979:LEU:CG	3:C:1002:LEU:HD22	2.49	0.41
4:D:510:LEU:HD23	4:D:601:ILE:HD13	2.02	0.41
4:D:1238:GLN:OE1	4:D:1238:GLN:HA	2.20	0.41
4:D:1314:LEU:HD22	4:D:1322:ALA:HB1	2.01	0.41
6:F:144:LEU:HD12	6:F:147:GLN:CG	2.49	0.41
6:F:299:LYS:HA	6:F:302:PHE:HD2	1.85	0.41
6:F:383:ASN:O	6:F:386:LEU:HB3	2.20	0.41
1:H:13:DT:C2'	1:H:14:DT:H71	2.48	0.41
1:H:43:DG:H1'	6:F:102:MET:CE	2.50	0.41
2:A:95:LYS:NZ	2:A:120:ASP:OD2	2.53	0.41
2:A:219:ARG:O	2:A:223:ILE:HG13	2.20	0.41
3:C:50:GLU:OE2	3:C:70:TYR:OH	2.23	0.41
3:C:187:GLU:HG3	3:C:188:PHE:O	2.20	0.41
3:C:678:ARG:HA	3:C:678:ARG:HD2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:963:VAL:CG2	4:D:980:THR:HG23	2.50	0.41
6:F:585:GLU:HG2	6:F:588:ARG:NH1	2.33	0.41
2:A:75:GLN:O	2:A:76:GLU:HG3	2.20	0.41
2:B:62:ASP:OD1	2:B:141:SER:HB3	2.20	0.41
3:C:179:TYR:HB2	3:C:397:LEU:O	2.20	0.41
3:C:538:LEU:CD2	3:C:547:VAL:HG21	2.50	0.41
3:C:1010:GLN:NE2	3:C:1013:GLN:HB3	2.34	0.41
3:C:1210:ILE:HG22	3:C:1211:ARG:H	1.84	0.41
4:D:233:LYS:N	4:D:233:LYS:HD2	2.35	0.41
4:D:270:ARG:O	4:D:274:ASN:ND2	2.52	0.41
4:D:1037:PHE:HD1	4:D:1037:PHE:HA	1.70	0.41
4:D:1040:MET:HE2	4:D:1040:MET:HB3	1.98	0.41
6:F:452:ILE:HD11	6:F:457:ILE:CD1	2.50	0.41
1:H:61:DG:H4'	1:H:62:DG:OP1	2.20	0.41
2:B:36:GLY:HA3	2:B:187:VAL:CG2	2.50	0.41
2:B:203:ILE:HG22	2:B:204:GLU:H	1.86	0.41
3:C:634:VAL:O	3:C:644:LEU:HA	2.20	0.41
3:C:1287:LEU:O	3:C:1291:LEU:HG	2.20	0.41
4:D:15:GLU:OE2	4:D:15:GLU:HA	2.21	0.41
4:D:639:VAL:HG13	4:D:639:VAL:O	2.20	0.41
4:D:1191:PRO:HB3	4:D:1193:TRP:HZ3	1.82	0.41
3:C:660:VAL:HG21	4:D:769:VAL:CG1	2.50	0.41
3:C:930:ASP:O	3:C:931:VAL:HG23	2.20	0.41
4:D:846:GLU:HA	4:D:860:ARG:NH2	2.36	0.41
4:D:888:CYS:SG	4:D:889:ASP:N	2.93	0.41
4:D:1025:MET:HB3	4:D:1124:ILE:CB	2.49	0.41
2:A:32:GLU:HG3	2:A:33:ARG:H	1.86	0.41
2:A:179:PRO:HB2	2:A:211:ILE:HB	2.03	0.41
2:B:12:ARG:O	2:B:13:LEU:HB3	2.20	0.41
2:B:76:GLU:OE2	2:B:131:CYS:HA	2.21	0.41
2:B:212:ASP:OD1	2:B:212:ASP:N	2.53	0.41
3:C:18:ARG:HD3	3:C:1188:ASP:CG	2.46	0.41
3:C:298:ALA:HB3	3:C:334:GLU:CB	2.50	0.41
3:C:824:GLN:HE22	3:C:1082:ILE:HD11	1.86	0.41
3:C:1288:GLN:O	3:C:1288:GLN:HG2	2.20	0.41
4:D:1036:ARG:HH21	4:D:1081:VAL:HG11	1.85	0.41
4:D:1348:LYS:O	4:D:1348:LYS:HG2	2.20	0.41
6:F:471:LEU:HD12	6:F:477:GLU:HA	2.02	0.41
2:A:89:ALA:O	2:A:124:VAL:HG12	2.21	0.41
3:C:207:THR:HA	3:C:210:LEU:HD12	2.01	0.41
3:C:564:PRO:CD	3:C:572:ILE:HB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1248:THR:HG21	6:F:531:PRO:CG	2.51	0.41
3:C:1253:LEU:HA	6:F:525:ASP:HB3	2.03	0.41
4:D:654:ILE:O	4:D:658:GLU:HB2	2.20	0.41
4:D:958:ILE:O	4:D:1008:GLY:N	2.39	0.41
4:D:983:LYS:CE	4:D:991:THR:HB	2.50	0.41
6:F:295:CYS:SG	6:F:329:LYS:HD3	2.61	0.41
6:F:346:GLN:O	6:F:350:GLU:HG3	2.19	0.41
2:K:269:CYS:O	2:K:273:GLU:N	2.53	0.41
2:B:28:LEU:HD12	2:B:29:GLU:N	2.35	0.41
2:B:61:ILE:HD11	2:B:142:MET:HE2	2.03	0.41
3:C:67:GLU:O	3:C:102:LEU:HD12	2.21	0.41
3:C:78:PRO:HG3	3:C:92:TYR:HE1	1.86	0.41
3:C:86:GLN:HA	3:C:140:GLY:HA2	2.01	0.41
3:C:242:VAL:CG2	3:C:245:ARG:HB2	2.50	0.41
3:C:854:ILE:CG2	3:C:855:PRO:HD2	2.49	0.41
3:C:1012:GLU:O	3:C:1015:ALA:HB3	2.20	0.41
3:C:1339:LEU:HB3	4:D:17:PHE:HB2	2.02	0.41
4:D:265:LEU:HD23	4:D:265:LEU:HA	1.91	0.41
4:D:664:ILE:HD13	4:D:681:LYS:CG	2.48	0.41
4:D:682:VAL:HA	4:D:685:ILE:CG2	2.50	0.41
4:D:918:ILE:O	4:D:918:ILE:HG13	2.21	0.41
4:D:1059:LEU:HB3	4:D:1107:VAL:CG2	2.50	0.41
4:D:1144:LEU:HD23	4:D:1237:VAL:HG23	2.03	0.41
6:F:165:PHE:CE2	6:F:220:LYS:HB2	2.56	0.41
6:F:476:ARG:O	6:F:477:GLU:HB3	2.20	0.41
6:F:479:THR:HG22	6:F:482:GLU:CD	2.46	0.41
6:F:511:ILE:HD13	6:F:522:PHE:HE2	1.85	0.41
1:H:58:DG:H1	7:G:5:DC:H42	1.68	0.41
2:A:100:LEU:HD21	2:A:121:VAL:CG1	2.40	0.41
3:C:296:VAL:HG21	3:C:314:ASN:HA	2.03	0.41
3:C:557:ARG:O	3:C:575:LEU:HD12	2.21	0.41
3:C:972:PHE:HD1	3:C:994:ARG:HH21	1.69	0.41
3:C:1065:LYS:HE2	3:C:1235:LEU:CD1	2.42	0.41
4:D:21:LYS:HG3	4:D:22:ILE:H	1.86	0.41
4:D:422:LEU:HA	4:D:422:LEU:HD12	1.86	0.41
4:D:949:SER:CB	4:D:1016:THR:HB	2.51	0.41
4:D:1027:VAL:O	4:D:1120:THR:HA	2.21	0.41
4:D:1211:SER:OG	4:D:1212:ASP:N	2.53	0.41
1:H:45:DA:H8	1:H:45:DA:O5'	2.04	0.40
2:B:11:PRO:HB2	2:B:28:LEU:CD1	2.47	0.40
3:C:26:TYR:HE2	3:C:32:LEU:HD12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:839:VAL:HG12	3:C:1049:ILE:HG12	2.02	0.40
3:C:1077:SER:OG	4:D:357:VAL:HG23	2.21	0.40
4:D:963:VAL:CG1	4:D:980:THR:HG23	2.51	0.40
4:D:967:VAL:HA	4:D:973:LEU:HA	2.03	0.40
4:D:1197:ASN:HB2	4:D:1210:ILE:O	2.21	0.40
5:E:21:LEU:HA	5:E:21:LEU:HD23	1.87	0.40
6:F:516:ASP:OD1	6:F:516:ASP:N	2.49	0.40
2:B:24:ALA:HB3	2:B:213:PRO:CB	2.51	0.40
2:B:102:LEU:HD12	2:B:103:ASN:H	1.87	0.40
3:C:471:VAL:HG21	3:C:498:ILE:HD11	2.03	0.40
3:C:715:THR:HG21	3:C:782:VAL:CG2	2.47	0.40
3:C:724:VAL:CG1	3:C:727:VAL:HG23	2.49	0.40
3:C:963:GLU:O	3:C:967:LEU:HB3	2.21	0.40
3:C:985:GLU:C	3:C:989:LEU:HB2	2.46	0.40
4:D:999:TYR:HE2	4:D:1027:VAL:HA	1.84	0.40
6:F:336:GLU:HA	6:F:339:ARG:CG	2.45	0.40
1:H:12:DA:H2''	1:H:13:DT:O5'	2.21	0.40
2:B:61:ILE:HG21	2:B:64:VAL:HB	2.03	0.40
3:C:230:PHE:CE1	3:C:239:MET:HG3	2.57	0.40
3:C:367:TYR:CE1	3:C:384:LEU:HD13	2.56	0.40
3:C:633:LEU:HD12	3:C:644:LEU:HB3	2.04	0.40
3:C:1019:ASP:HA	3:C:1022:LYS:HB3	2.03	0.40
3:C:1024:GLU:O	3:C:1028:LYS:HG3	2.21	0.40
3:C:1247:SER:O	3:C:1248:THR:OG1	2.31	0.40
4:D:905:ARG:NH2	4:D:907:HIS:HB2	2.21	0.40
4:D:996:LYS:HG3	4:D:997:VAL:H	1.86	0.40
4:D:1174:ARG:HG3	4:D:1189:MET:HB3	2.03	0.40
4:D:1261:LEU:O	4:D:1261:LEU:HD12	2.22	0.40
6:F:246:GLN:N	6:F:246:GLN:OE1	2.53	0.40
6:F:281:ARG:HB3	6:F:281:ARG:CZ	2.51	0.40
6:F:303:ILE:HG13	6:F:304:THR:H	1.86	0.40
1:H:17:DC:H2''	1:H:18:DA:O5'	2.20	0.40
2:B:91:ARG:HD3	2:B:124:VAL:HG13	2.02	0.40
3:C:59:ILE:HD12	3:C:475:VAL:HG11	2.04	0.40
3:C:114:VAL:HG12	3:C:115:LYS:CE	2.52	0.40
3:C:272:ARG:HG2	3:C:276:GLN:HG3	2.02	0.40
3:C:292:ILE:HG23	3:C:295:LYS:HG3	2.03	0.40
3:C:320:ASP:O	3:C:324:LYS:HG3	2.21	0.40
3:C:419:ILE:HD13	3:C:419:ILE:H	1.86	0.40
4:D:88:CYS:O	4:D:90:VAL:N	2.46	0.40
4:D:120:LEU:CB	4:D:121:PRO:HD3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:398:LYS:HD3	6:F:532:LEU:HD21	2.04	0.40
4:D:1273:ASP:OD2	4:D:1276:GLU:HB2	2.22	0.40
6:F:163:THR:HG23	6:F:262:VAL:HG22	2.03	0.40
7:G:41:DC:C3'	7:G:42:DT:H5''	2.52	0.40
2:A:231:PHE:HE1	2:B:39:LEU:HD13	1.87	0.40
3:C:626:GLU:HB2	3:C:628:HIS:HD2	1.85	0.40
3:C:1014:LEU:HD12	3:C:1017:GLN:HB2	2.03	0.40
4:D:593:ASN:O	4:D:593:ASN:ND2	2.55	0.40
4:D:703:THR:CG2	4:D:715:LYS:HD3	2.49	0.40
4:D:865:HIS:HE1	4:D:867:GLN:HG2	1.87	0.40
4:D:923:ILE:HD11	4:D:1252:HIS:O	2.22	0.40
4:D:1307:LEU:N	4:D:1307:LEU:HD23	2.36	0.40
6:F:96:ASP:HA	6:F:97:PRO:HD3	1.86	0.40
6:F:224:LEU:HG	6:F:225:ARG:HD3	2.03	0.40
6:F:273:MET:HE2	6:F:273:MET:HB3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
2	A	228/329 (69%)	207 (91%)	21 (9%)	0	100	100
2	B	226/329 (69%)	199 (88%)	26 (12%)	1 (0%)	30	60
2	K	63/329 (19%)	56 (89%)	7 (11%)	0	100	100
3	C	1335/1342 (100%)	1165 (87%)	167 (12%)	3 (0%)	43	72
4	D	1331/1407 (95%)	1179 (89%)	152 (11%)	0	100	100
5	E	71/91 (78%)	65 (92%)	6 (8%)	0	100	100
6	F	466/613 (76%)	440 (94%)	26 (6%)	0	100	100
All	All	3720/4440 (84%)	3311 (89%)	405 (11%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1164	PHE
2	B	21	SER
3	C	1159	VAL
3	C	1224	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	198/286 (69%)	180 (91%)	18 (9%)	9	33
2	B	196/286 (68%)	173 (88%)	23 (12%)	5	25
2	K	57/286 (20%)	44 (77%)	13 (23%)	1	6
3	C	1154/1157 (100%)	1024 (89%)	130 (11%)	5	26
4	D	1103/1168 (94%)	970 (88%)	133 (12%)	5	24
5	E	64/75 (85%)	54 (84%)	10 (16%)	2	16
6	F	420/540 (78%)	376 (90%)	44 (10%)	6	29
All	All	3192/3798 (84%)	2821 (88%)	371 (12%)	7	25

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	254	LEU
2	K	257	VAL
2	K	261	GLU
2	K	263	THR
2	K	270	LEU
2	K	277	TYR
2	K	303	ILE
2	K	306	VAL
2	K	307	LEU
2	K	313	SER
2	K	314	LEU
2	K	318	LEU

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Mol	Chain	Res	Type
2	K	319	GLU
2	A	54	CYS
2	A	71	LYS
2	A	77	ASP
2	A	96	ASP
2	A	98	VAL
2	A	111	THR
2	A	124	VAL
2	A	150	ARG
2	A	157	THR
2	A	163	GLU
2	A	176	CYS
2	A	177	TYR
2	A	187	VAL
2	A	191	ARG
2	A	193	GLU
2	A	211	ILE
2	A	229	GLU
2	A	233	ASP
2	B	12	ARG
2	B	14	VAL
2	B	16	ILE
2	B	17	GLU
2	B	27	THR
2	B	29	GLU
2	B	38	THR
2	B	56	VAL
2	B	70	THR
2	B	91	ARG
2	B	98	VAL
2	B	137	ASN
2	B	141	SER
2	B	146	VAL
2	B	158	ARG
2	B	164	ASP
2	B	172	LEU
2	B	183	ILE
2	B	187	VAL
2	B	207	THR
2	B	210	THR
2	B	212	ASP
2	B	222	THR

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Mol	Chain	Res	Type
3	C	11	ILE
3	C	21	VAL
3	C	39	ILE
3	C	46	GLN
3	C	49	LEU
3	C	60	GLN
3	C	79	VAL
3	C	81	ASP
3	C	91	THR
3	C	117	ILE
3	C	122	VAL
3	C	129	LEU
3	C	132	ASP
3	C	161	LYS
3	C	187	GLU
3	C	197	ARG
3	C	199	ASP
3	C	203	LYS
3	C	230	PHE
3	C	234	ASP
3	C	246	LEU
3	C	263	VAL
3	C	269	ILE
3	C	284	LEU
3	C	285	ILE
3	C	287	VAL
3	C	289	VAL
3	C	296	VAL
3	C	311	CYS
3	C	317	LEU
3	C	318	SER
3	C	327	GLN
3	C	347	ILE
3	C	350	THR
3	C	351	LEU
3	C	352	ARG
3	C	366	ILE
3	C	391	SER
3	C	414	ILE
3	C	419	ILE
3	C	444	ASP
3	C	448	LEU

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Mol	Chain	Res	Type
3	C	463	GLN
3	C	465	ARG
3	C	469	VAL
3	C	471	VAL
3	C	472	GLU
3	C	479	LEU
3	C	481	LEU
3	C	486	THR
3	C	504	GLU
3	C	524	ILE
3	C	531	SER
3	C	538	LEU
3	C	546	GLU
3	C	547	VAL
3	C	549	ASP
3	C	550	VAL
3	C	551	HIS
3	C	598	VAL
3	C	609	ILE
3	C	615	VAL
3	C	641	GLU
3	C	663	VAL
3	C	704	MET
3	C	717	VAL
3	C	750	ILE
3	C	754	THR
3	C	764	CYS
3	C	765	ILE
3	C	777	VAL
3	C	789	THR
3	C	791	LEU
3	C	802	VAL
3	C	819	SER
3	C	829	THR
3	C	834	GLN
3	C	845	LEU
3	C	851	THR
3	C	854	ILE
3	C	857	VAL
3	C	892	GLU
3	C	895	LEU
3	C	912	ASP

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Mol	Chain	Res	Type
3	C	915	ASP
3	C	922	ASN
3	C	942	ASP
3	C	963	GLU
3	C	966	ILE
3	C	972	PHE
3	C	973	SER
3	C	980	VAL
3	C	998	LEU
3	C	1002	LEU
3	C	1007	LYS
3	C	1013	GLN
3	C	1020	GLU
3	C	1023	HIS
3	C	1030	GLU
3	C	1056	VAL
3	C	1069	ARG
3	C	1075	VAL
3	C	1088	ASP
3	C	1106	ARG
3	C	1124	ILE
3	C	1132	LEU
3	C	1134	GLN
3	C	1138	VAL
3	C	1150	ASP
3	C	1151	LEU
3	C	1157	GLN
3	C	1158	LYS
3	C	1161	LEU
3	C	1162	SER
3	C	1174	GLU
3	C	1191	LYS
3	C	1201	LEU
3	C	1211	ARG
3	C	1217	THR
3	C	1225	VAL
3	C	1232	MET
3	C	1233	LEU
3	C	1243	MET
3	C	1246	ARG
3	C	1254	VAL
3	C	1287	LEU

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Mol	Chain	Res	Type
3	C	1292	THR
3	C	1293	VAL
3	C	1295	SER
3	C	1309	VAL
4	D	15	GLU
4	D	24	LEU
4	D	46	TYR
4	D	56	LEU
4	D	60	ARG
4	D	78	LEU
4	D	120	LEU
4	D	130	MET
4	D	136	GLU
4	D	152	THR
4	D	166	LEU
4	D	167	ASP
4	D	170	GLU
4	D	175	GLU
4	D	179	LYS
4	D	183	GLU
4	D	186	GLN
4	D	192	MET
4	D	208	THR
4	D	214	ARG
4	D	217	LEU
4	D	227	PHE
4	D	232	ASN
4	D	233	LYS
4	D	235	GLU
4	D	244	VAL
4	D	255	LEU
4	D	262	THR
4	D	297	ARG
4	D	300	GLN
4	D	303	VAL
4	D	306	LEU
4	D	316	ILE
4	D	332	LYS
4	D	347	VAL
4	D	352	ARG
4	D	393	THR
4	D	395	LYS

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Mol	Chain	Res	Type
4	D	402	GLU
4	D	407	VAL
4	D	408	VAL
4	D	413	ASP
4	D	422	LEU
4	D	423	LEU
4	D	424	ASN
4	D	431	ARG
4	D	434	ILE
4	D	440	VAL
4	D	460	ASP
4	D	468	VAL
4	D	473	THR
4	D	487	THR
4	D	490	ILE
4	D	506	VAL
4	D	510	LEU
4	D	517	CYS
4	D	527	LEU
4	D	545	HIS
4	D	548	VAL
4	D	552	ILE
4	D	569	LEU
4	D	591	ILE
4	D	592	VAL
4	D	602	SER
4	D	624	ILE
4	D	642	ASP
4	D	648	GLU
4	D	652	GLU
4	D	678	ARG
4	D	682	VAL
4	D	685	ILE
4	D	708	ASN
4	D	710	ASP
4	D	717	VAL
4	D	738	ARG
4	D	753	SER
4	D	762	ASN
4	D	775	SER
4	D	776	THR
4	D	780	ARG

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Mol	Chain	Res	Type
4	D	786	THR
4	D	797	THR
4	D	805	GLN
4	D	806	ASP
4	D	817	HIS
4	D	825	VAL
4	D	847	ASP
4	D	848	VAL
4	D	849	LEU
4	D	863	LEU
4	D	869	CYS
4	D	874	GLU
4	D	894	VAL
4	D	895	CYS
4	D	902	ASP
4	D	905	ARG
4	D	908	ILE
4	D	913	GLU
4	D	918	ILE
4	D	925	GLU
4	D	928	THR
4	D	929	GLN
4	D	931	THR
4	D	952	VAL
4	D	972	LYS
4	D	979	ASN
4	D	990	ARG
4	D	991	THR
4	D	1016	THR
4	D	1028	ILE
4	D	1037	PHE
4	D	1041	ILE
4	D	1099	TYR
4	D	1143	ASP
4	D	1155	ILE
4	D	1167	LYS
4	D	1193	TRP
4	D	1210	ILE
4	D	1226	VAL
4	D	1249	ASN
4	D	1255	VAL
4	D	1266	ILE

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Mol	Chain	Res	Type
4	D	1275	LEU
4	D	1307	LEU
4	D	1314	LEU
4	D	1327	GLU
4	D	1329	THR
4	D	1341	ARG
4	D	1342	ASP
4	D	1344	LEU
4	D	1345	ARG
4	D	1351	VAL
4	D	1366	HIS
5	E	3	ARG
5	E	4	VAL
5	E	16	ARG
5	E	19	LEU
5	E	28	ARG
5	E	30	MET
5	E	31	GLN
5	E	36	ASP
5	E	46	THR
5	E	55	GLU
6	F	98	VAL
6	F	105	MET
6	F	108	VAL
6	F	121	LYS
6	F	146	GLU
6	F	151	VAL
6	F	162	ILE
6	F	216	LEU
6	F	247	GLU
6	F	262	VAL
6	F	265	GLN
6	F	279	ARG
6	F	281	ARG
6	F	286	LEU
6	F	289	LYS
6	F	290	LEU
6	F	293	GLU
6	F	295	CYS
6	F	296	LYS
6	F	299	LYS
6	F	302	PHE

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Mol	Chain	Res	Type
6	F	306	PHE
6	F	328	GLU
6	F	329	LYS
6	F	360	ASP
6	F	383	ASN
6	F	392	LYS
6	F	400	GLN
6	F	454	VAL
6	F	459	THR
6	F	465	ARG
6	F	483	LEU
6	F	500	ILE
6	F	505	ILE
6	F	540	LEU
6	F	546	ASP
6	F	547	VAL
6	F	552	THR
6	F	559	LEU
6	F	566	ASP
6	F	573	LEU
6	F	582	VAL
6	F	587	ILE
6	F	590	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	HIS
2	A	66	HIS
2	B	93	GLN
2	B	147	GLN
2	B	227	GLN
3	C	31	GLN
3	C	60	GLN
3	C	69	GLN
3	C	120	GLN
3	C	139	ASN
3	C	463	GLN
3	C	526	HIS
3	C	618	GLN
3	C	628	HIS
3	C	760	ASN

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Mol	Chain	Res	Type
3	C	1013	GLN
3	C	1072	ASN
3	C	1108	ASN
3	C	1111	GLN
3	C	1157	GLN
3	C	1257	GLN
3	C	1268	GLN
4	D	157	GLN
4	D	186	GLN
4	D	196	GLN
4	D	277	ASN
4	D	488	ASN
4	D	593	ASN
4	D	702	GLN
4	D	712	GLN
4	D	736	GLN
4	D	865	HIS
4	D	1197	ASN
4	D	1235	ASN
5	E	29	GLN
6	F	227	GLN
6	F	294	GLN
6	F	400	GLN
6	F	406	GLN
6	F	455	HIS
6	F	464	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

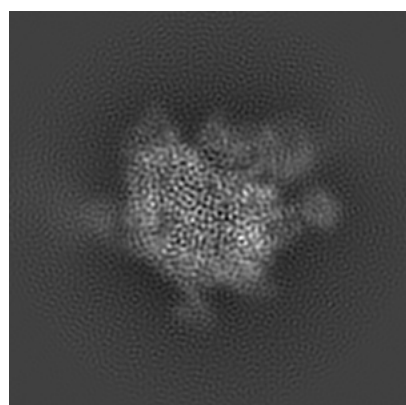
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30376. These allow visual inspection of the internal detail of the map and identification of artifacts.

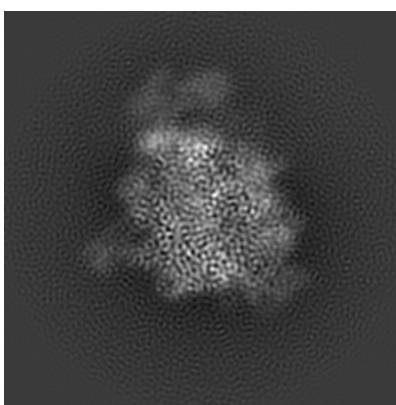
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

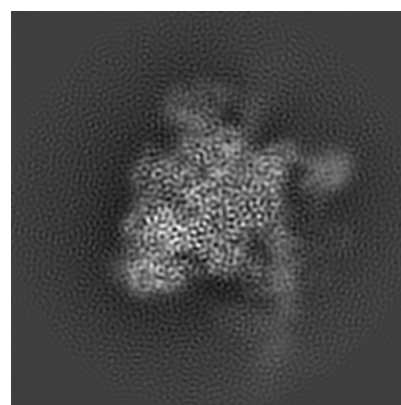
6.1.1 Primary map



X



Y

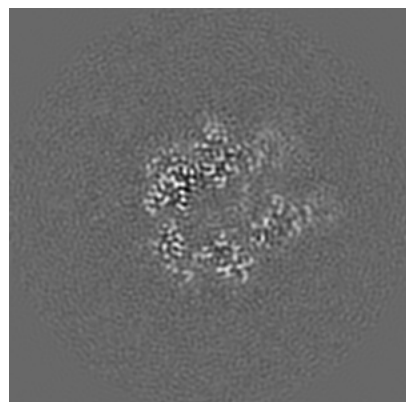


Z

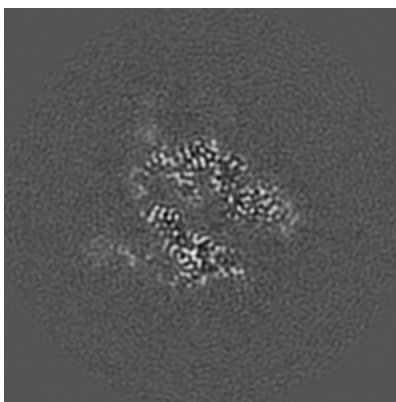
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

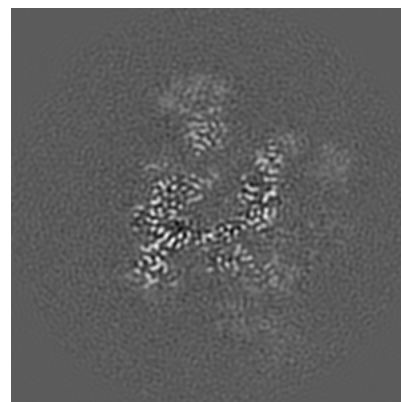
6.2.1 Primary map



X Index: 100



Y Index: 100

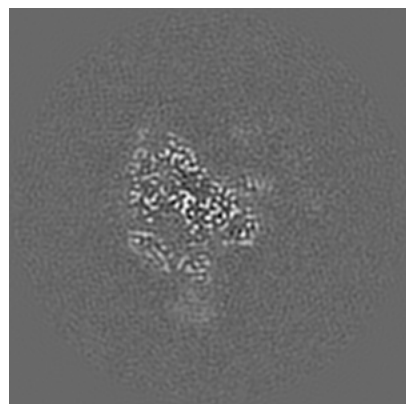


Z Index: 100

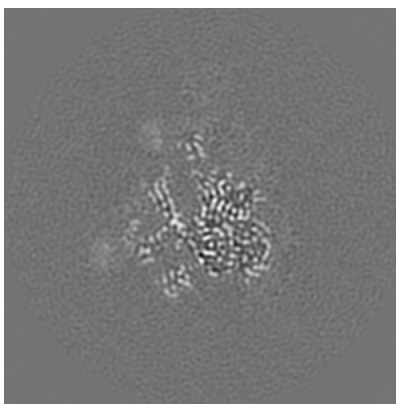
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

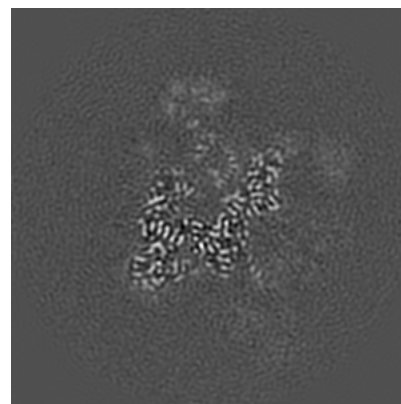
6.3.1 Primary map



X Index: 74



Y Index: 86

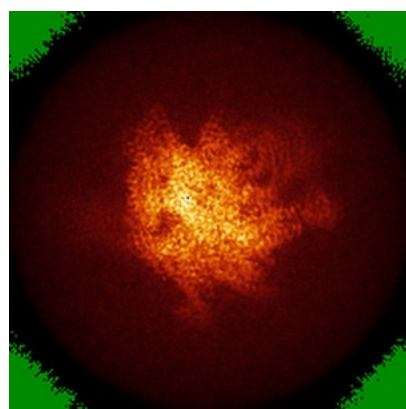


Z Index: 104

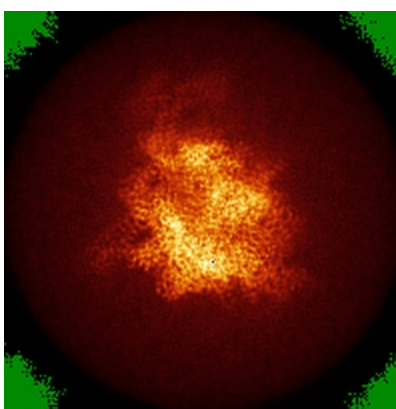
The images above show the largest variance slices of the map in three orthogonal directions.

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

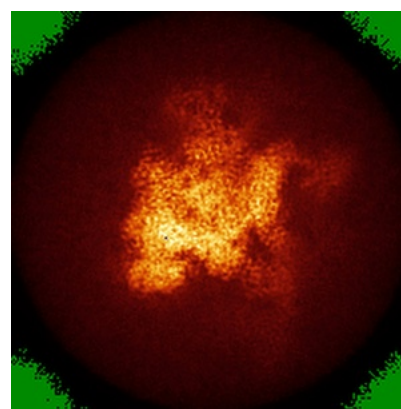
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0259. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

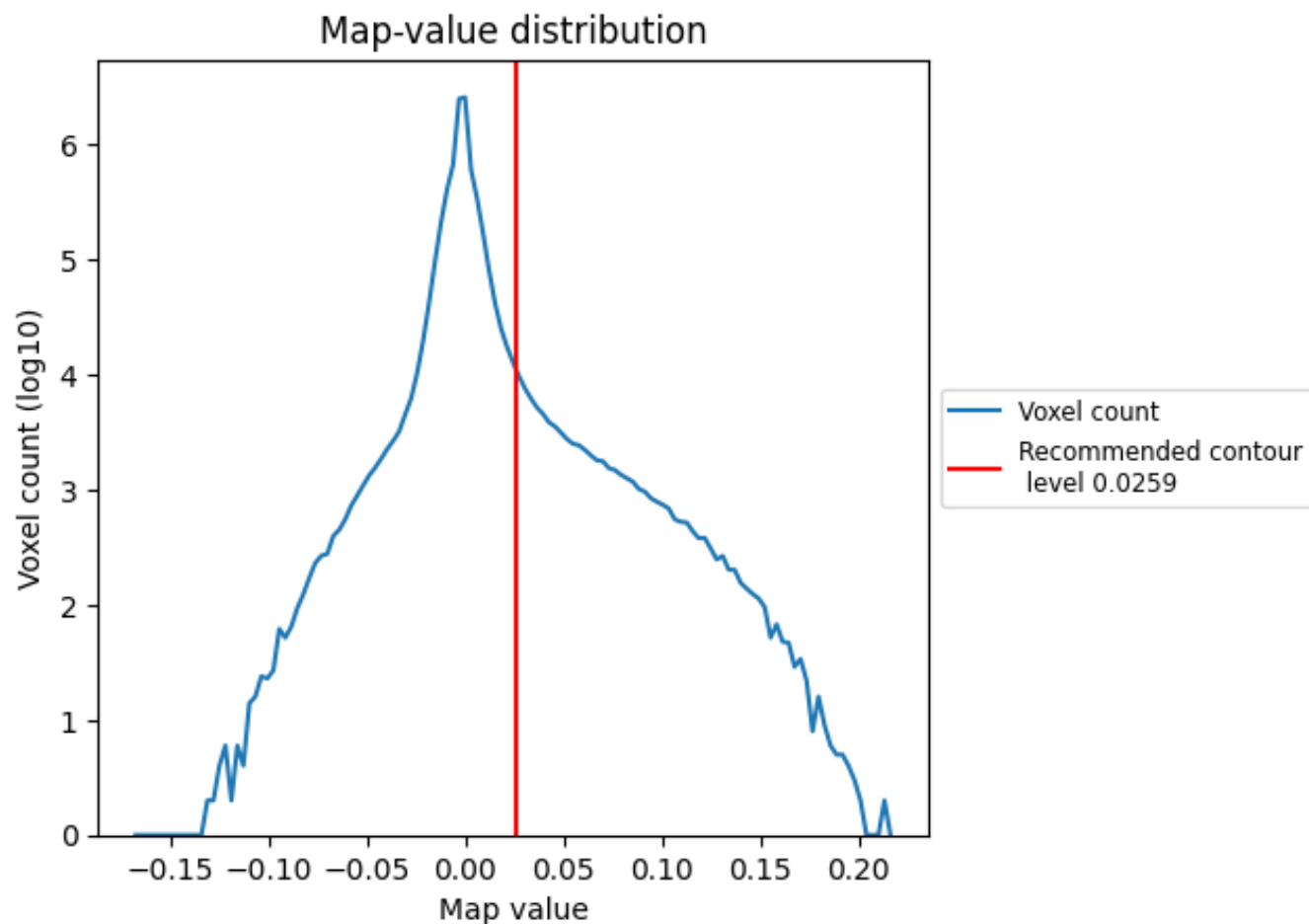
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

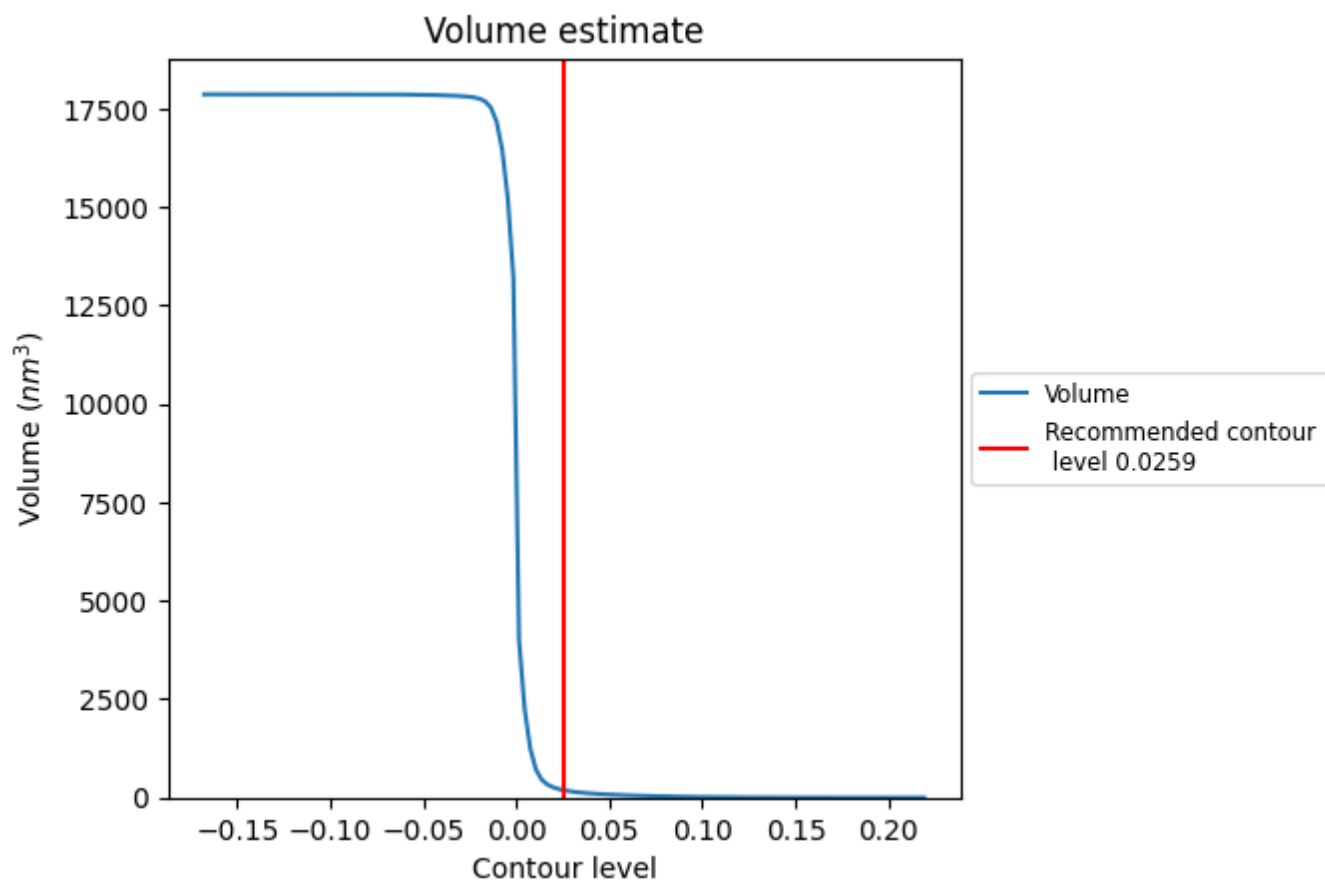
This section contains the results of statistical analysis of the map.

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.

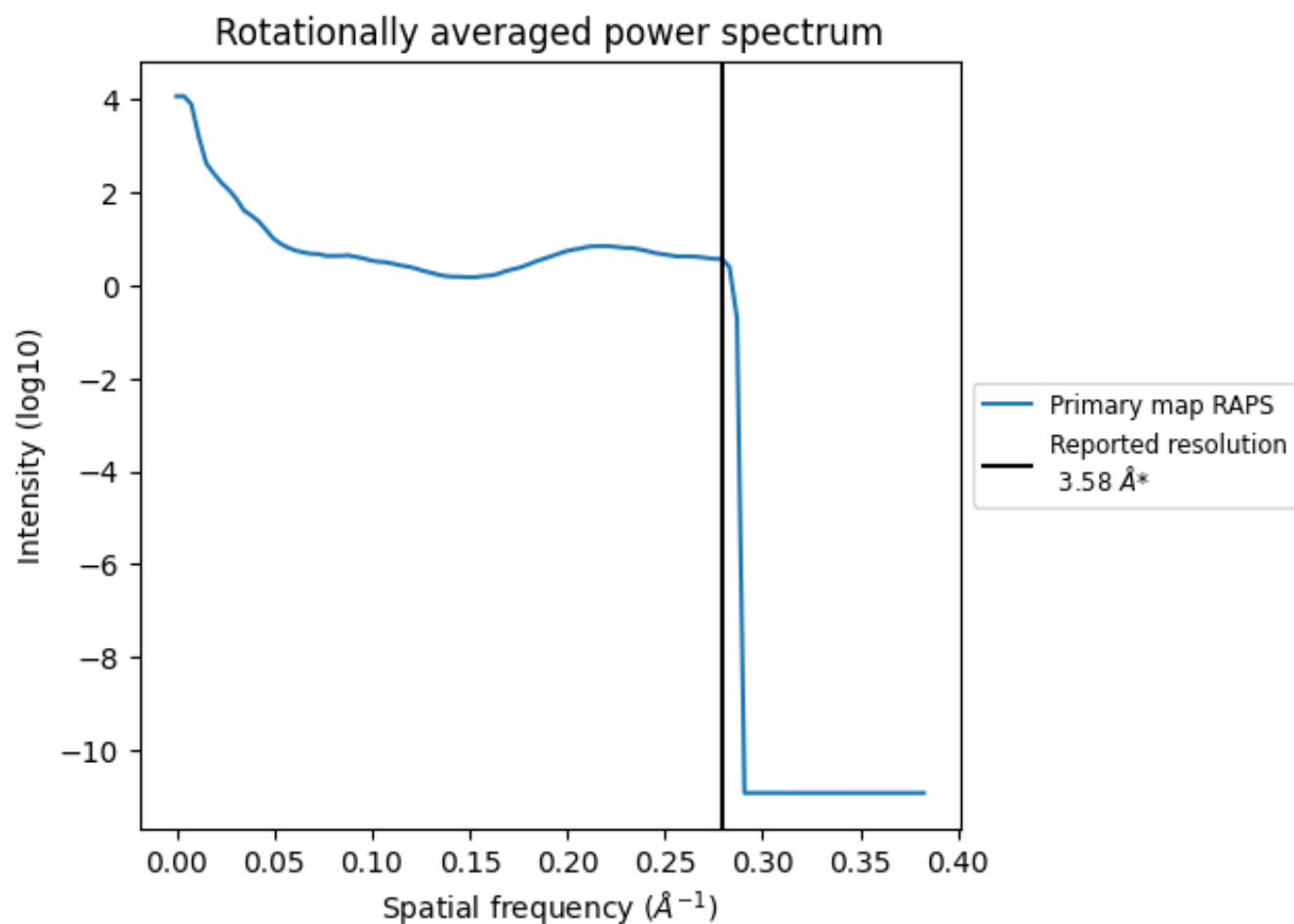
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm³; this corresponds to an approximate mass of 165 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 0.279 $\text{\AA}^{-1}$

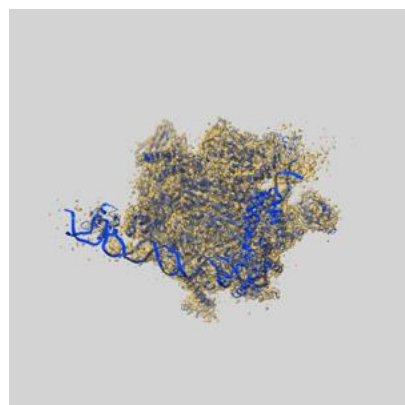
8 Fourier-Shell correlation ⓘ

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

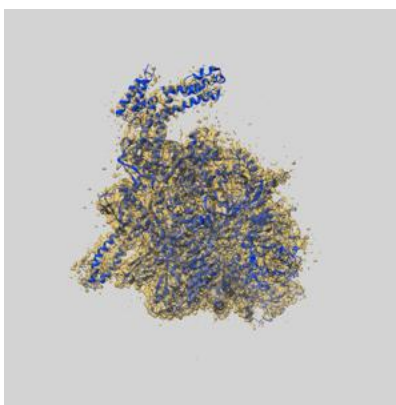
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30376 and PDB model 7CHW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

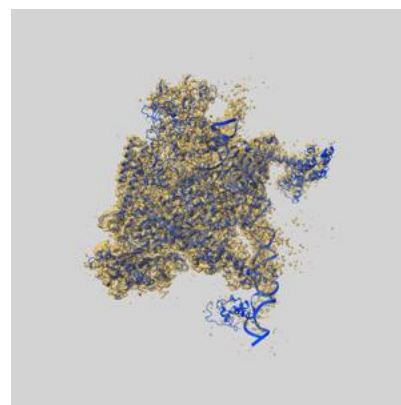
9.1 Map-model overlay [i](#)



X



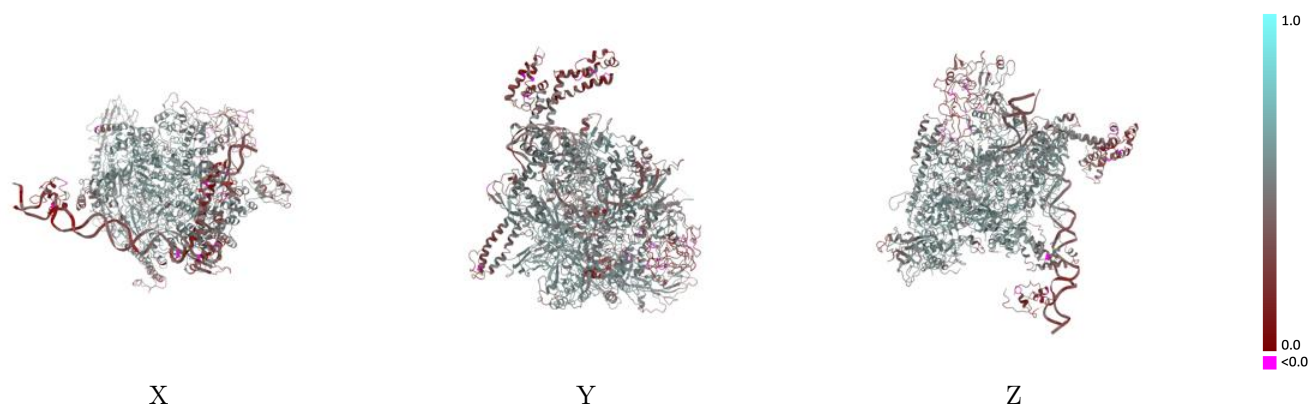
Y



Z

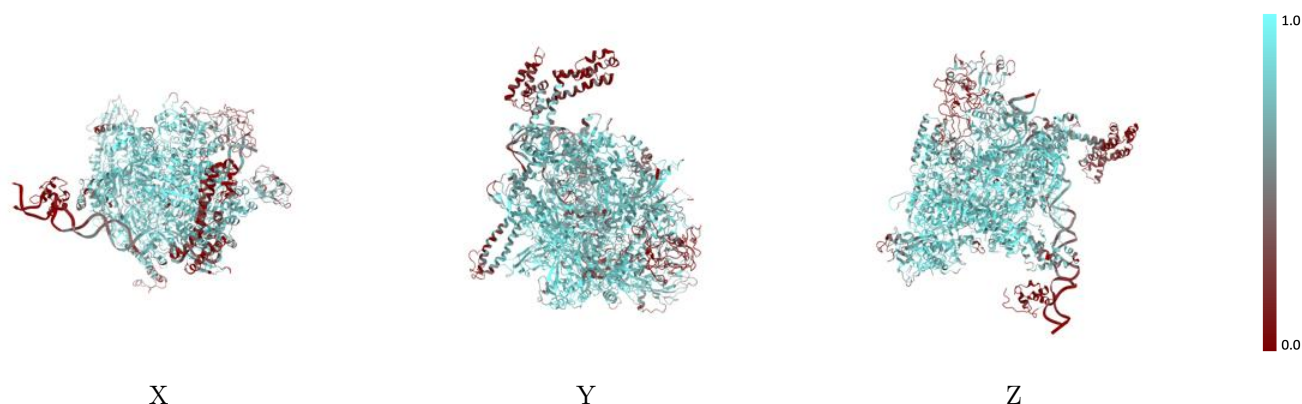
The images above show the 3D surface view of the map at the recommended contour level 0.0259 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



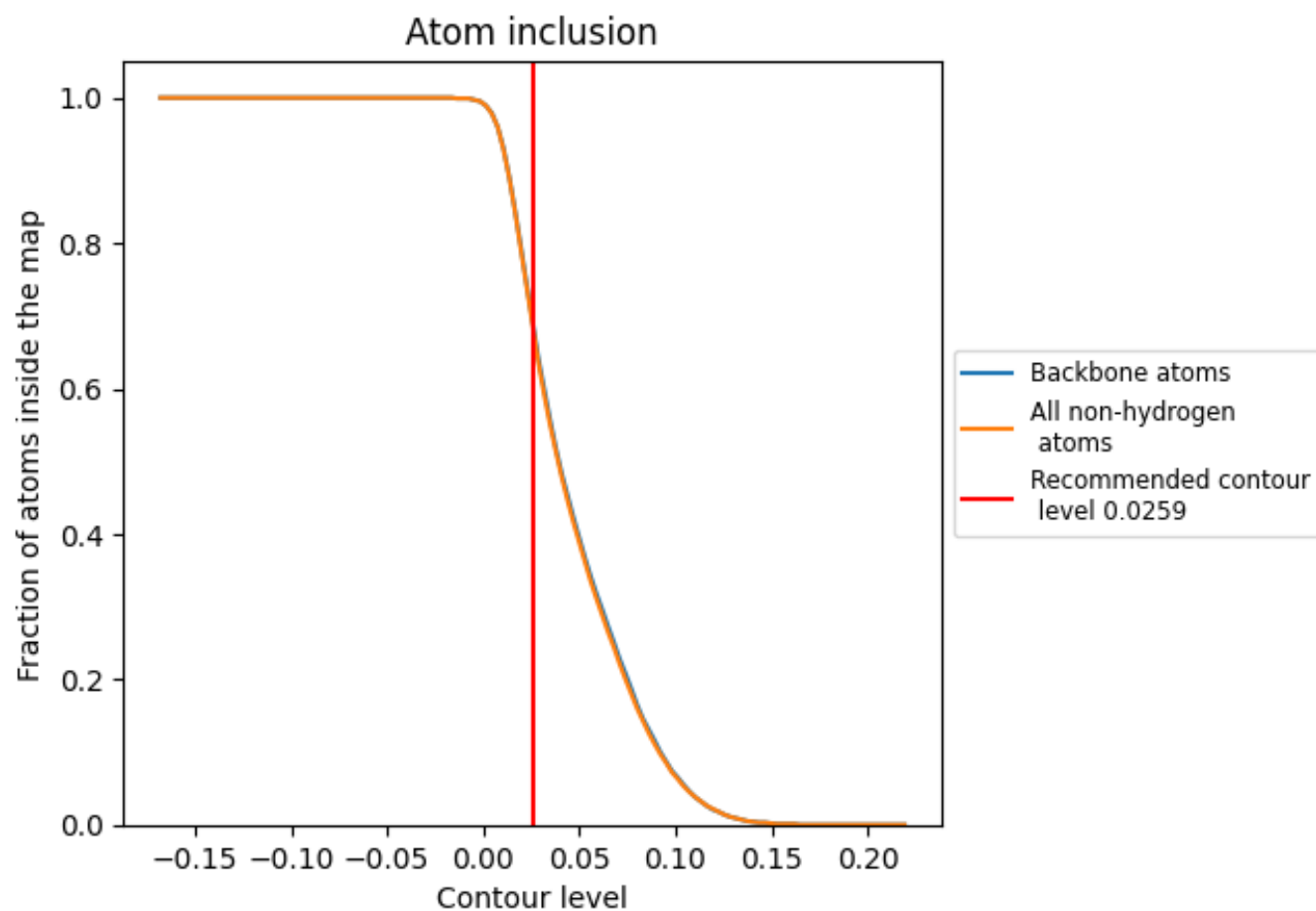
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0259).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 68% 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 (0.0259) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.4700
A	0.7950	0.5300
B	0.7040	0.4860
C	0.7760	0.5100
D	0.7170	0.4880
E	0.7660	0.5040
F	0.4970	0.3890
G	0.4570	0.3200
H	0.4590	0.3370
K	0.0240	0.2210

1.0

0.0

<0.0