



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:03 AM EST

PDB ID : 6WMU
EMDB ID : EMD-21853
Title : E. coli RNAPs70-SspA-gadA DNA complex
Authors : Travis, B.A.; Brennan, R.G.; Schumacher, M.A.
Deposited on : 2020-04-21
Resolution : 3.18 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

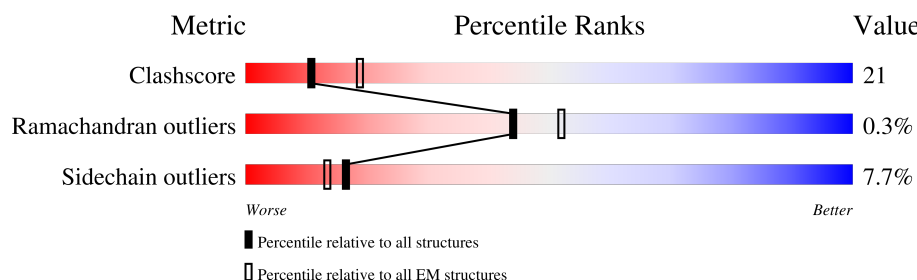
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1430	
4	E	91	
5	F	613	
6	G	37	
7	H	27	

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Mol	Chain	Length	Quality of chain
8	I	11	<div><div></div><div>36%64%</div></div>
9	J	11	<div><div></div><div>27%73%</div></div>
10	K	232	<div><div></div><div>50%34%14%</div></div>
10	L	232	<div><div></div><div>47%36%5%12%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 34094 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1787	1112	317	352	6		
1	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1339	Total	C	N	O	S	0	0
			10556	6624	1840	2049	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1363	Total	C	N	O	S	0	0
			10504	6594	1872	1988	50		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7
D	1410	ARG	-	expression tag	UNP P0A8T7
D	1411	ARG	-	expression tag	UNP P0A8T7
D	1412	ALA	-	expression tag	UNP P0A8T7
D	1413	SER	-	expression tag	UNP P0A8T7
D	1414	GLU	-	expression tag	UNP P0A8T7
D	1415	ASN	-	expression tag	UNP P0A8T7
D	1416	LEU	-	expression tag	UNP P0A8T7
D	1417	TYR	-	expression tag	UNP P0A8T7
D	1418	PHE	-	expression tag	UNP P0A8T7
D	1419	GLN	-	expression tag	UNP P0A8T7
D	1420	GLY	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1421	HIS	-	expression tag	UNP P0A8T7
D	1422	HIS	-	expression tag	UNP P0A8T7
D	1423	HIS	-	expression tag	UNP P0A8T7
D	1424	HIS	-	expression tag	UNP P0A8T7
D	1425	HIS	-	expression tag	UNP P0A8T7
D	1426	HIS	-	expression tag	UNP P0A8T7
D	1427	HIS	-	expression tag	UNP P0A8T7
D	1428	HIS	-	expression tag	UNP P0A8T7
D	1429	HIS	-	expression tag	UNP P0A8T7
D	1430	HIS	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	87	Total	C	N	O	S	0	0
			660	401	126	132	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	471	Total	C	N	O	S	0	0
			3836	2403	684	726	23		

- Molecule 6 is a DNA chain called DNA NT-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	37	Total	C	N	O	P	0	0
			746	361	116	232	37		

- Molecule 7 is a DNA chain called DNA T-strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	27	Total	C	N	O	P	0	0
			561	266	109	159	27		

- Molecule 8 is a DNA chain called DNA NT-strand downstream.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	11	Total	C	N	O	P	0	0
			225	106	41	67	11		

- Molecule 9 is a DNA chain called DNA T-strand downstream.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	11	Total	C	N	O	P	0	0
			226	106	44	65	11		

- Molecule 10 is a protein called Stringent starvation protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	199	Total	C	N	O	S	0	0
			1592	1024	262	298	8		
10	L	204	Total	C	N	O	S	0	0
			1631	1049	274	300	8		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-19	MET	-	initiating methionine	UNP A0A1X3LEF3
K	-18	GLY	-	expression tag	UNP A0A1X3LEF3
K	-17	SER	-	expression tag	UNP A0A1X3LEF3
K	-16	SER	-	expression tag	UNP A0A1X3LEF3
K	-15	HIS	-	expression tag	UNP A0A1X3LEF3
K	-14	HIS	-	expression tag	UNP A0A1X3LEF3
K	-13	HIS	-	expression tag	UNP A0A1X3LEF3
K	-12	HIS	-	expression tag	UNP A0A1X3LEF3
K	-11	HIS	-	expression tag	UNP A0A1X3LEF3
K	-10	HIS	-	expression tag	UNP A0A1X3LEF3
K	-9	SER	-	expression tag	UNP A0A1X3LEF3
K	-8	SER	-	expression tag	UNP A0A1X3LEF3
K	-7	GLY	-	expression tag	UNP A0A1X3LEF3
K	-6	LEU	-	expression tag	UNP A0A1X3LEF3
K	-5	VAL	-	expression tag	UNP A0A1X3LEF3
K	-4	PRO	-	expression tag	UNP A0A1X3LEF3
K	-3	ARG	-	expression tag	UNP A0A1X3LEF3
K	-2	GLY	-	expression tag	UNP A0A1X3LEF3
K	-1	SER	-	expression tag	UNP A0A1X3LEF3
K	0	HIS	-	expression tag	UNP A0A1X3LEF3
L	-19	MET	-	initiating methionine	UNP A0A1X3LEF3
L	-18	GLY	-	expression tag	UNP A0A1X3LEF3
L	-17	SER	-	expression tag	UNP A0A1X3LEF3
L	-16	SER	-	expression tag	UNP A0A1X3LEF3
L	-15	HIS	-	expression tag	UNP A0A1X3LEF3
L	-14	HIS	-	expression tag	UNP A0A1X3LEF3
L	-13	HIS	-	expression tag	UNP A0A1X3LEF3
L	-12	HIS	-	expression tag	UNP A0A1X3LEF3
L	-11	HIS	-	expression tag	UNP A0A1X3LEF3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-10	HIS	-	expression tag	UNP A0A1X3LEF3
L	-9	SER	-	expression tag	UNP A0A1X3LEF3
L	-8	SER	-	expression tag	UNP A0A1X3LEF3
L	-7	GLY	-	expression tag	UNP A0A1X3LEF3
L	-6	LEU	-	expression tag	UNP A0A1X3LEF3
L	-5	VAL	-	expression tag	UNP A0A1X3LEF3
L	-4	PRO	-	expression tag	UNP A0A1X3LEF3
L	-3	ARG	-	expression tag	UNP A0A1X3LEF3
L	-2	GLY	-	expression tag	UNP A0A1X3LEF3
L	-1	SER	-	expression tag	UNP A0A1X3LEF3
L	0	HIS	-	expression tag	UNP A0A1X3LEF3

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

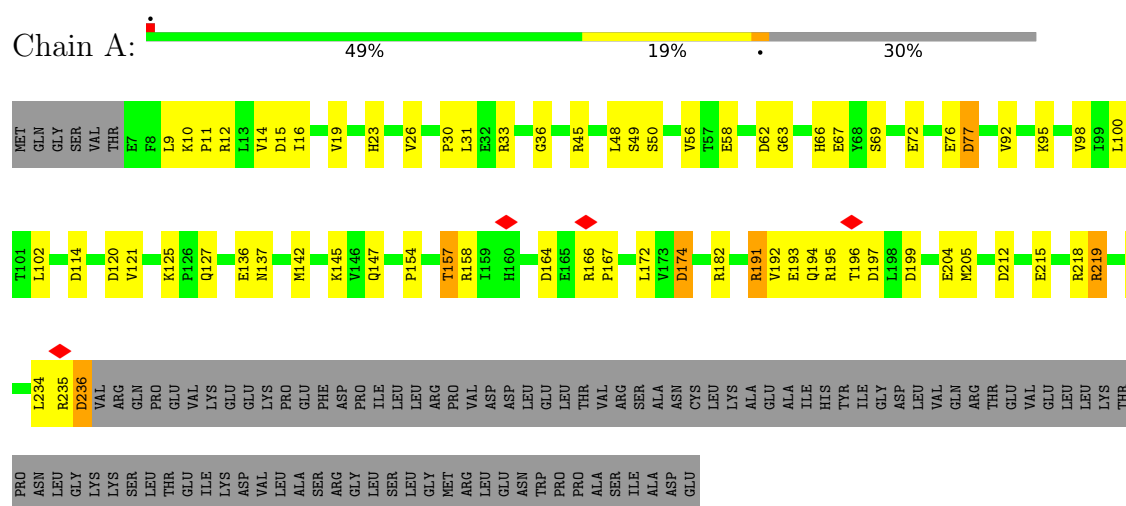
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

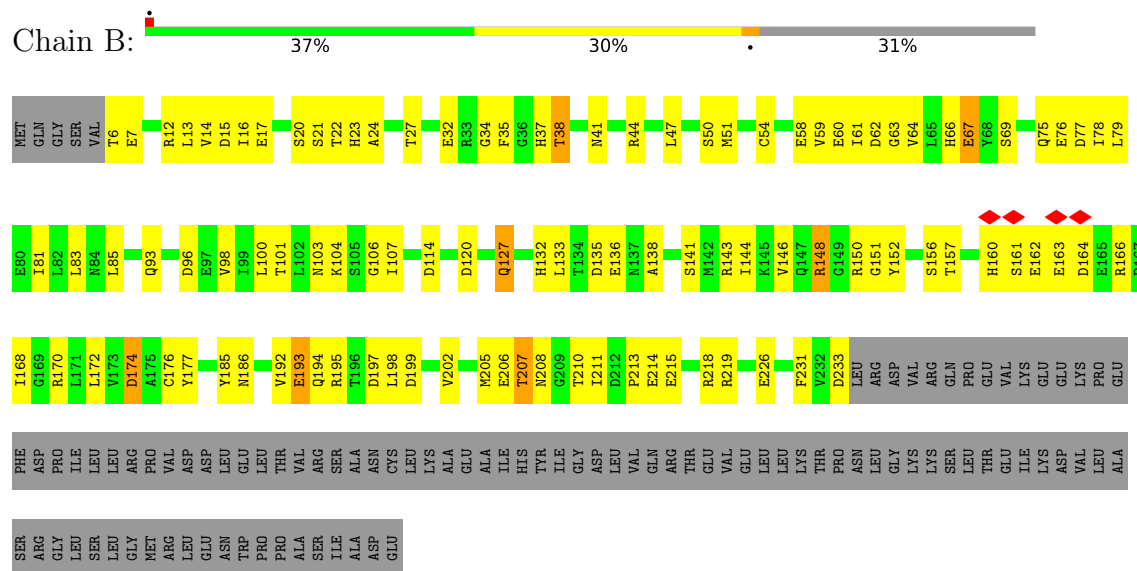
3 Residue-property plots

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.

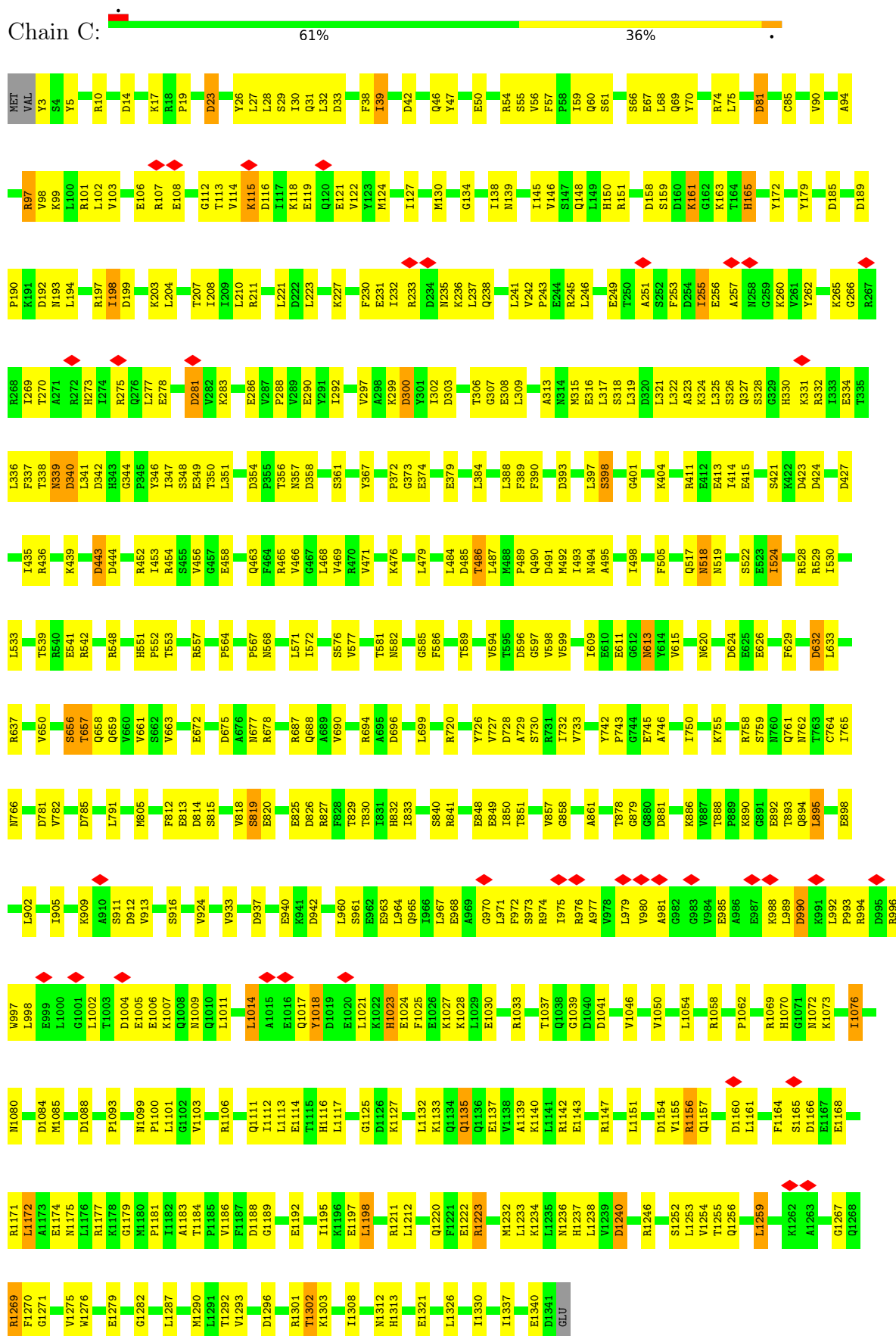
• Molecule 1: DNA-directed RNA polymerase subunit alpha



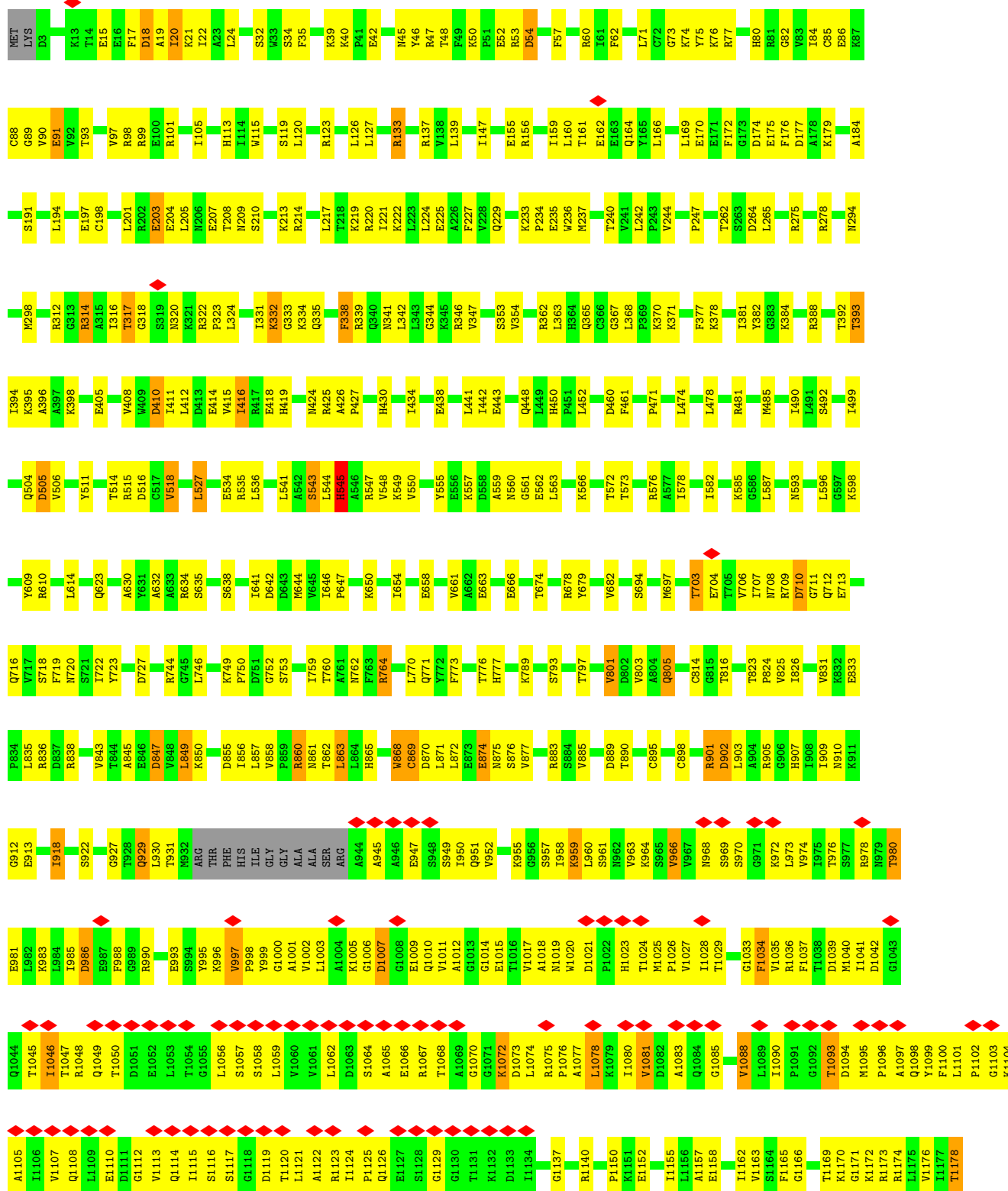
• Molecule 1: DNA-directed RNA polymerase subunit alpha



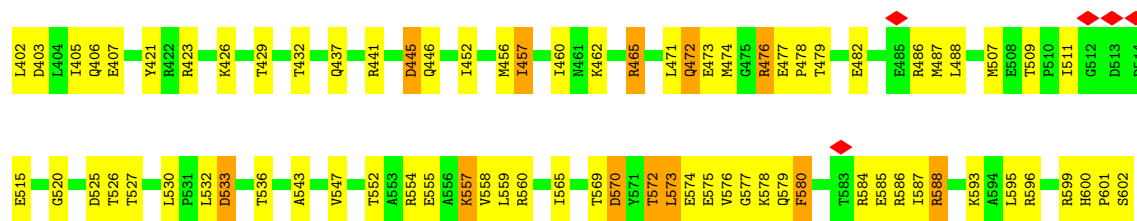
• Molecule 2: DNA-directed RNA polymerase subunit beta



• Molecule 3: DNA-directed RNA polymerase subunit beta'



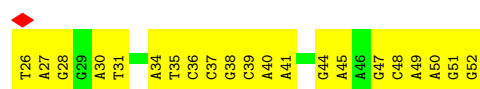
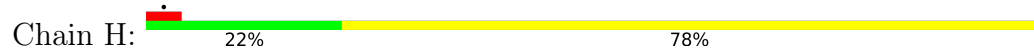




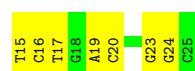
- Molecule 6: DNA NT-strand



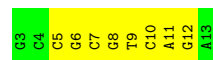
- Molecule 7: DNA T-strand



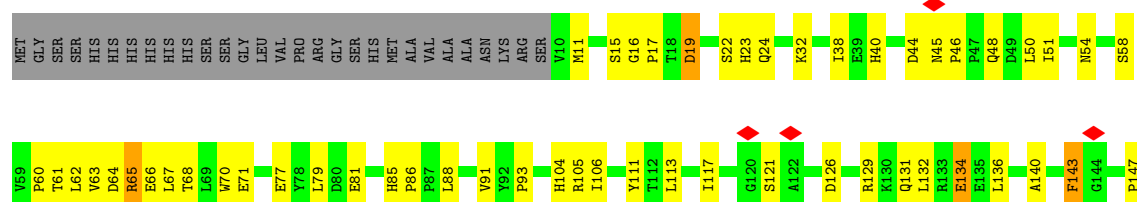
- Molecule 8: DNA NT-strand downstream

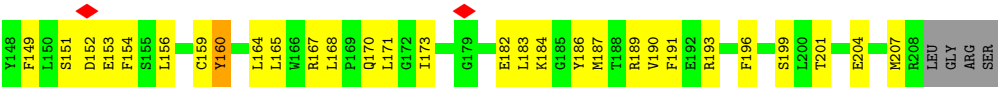


- Molecule 9: DNA T-strand downstream

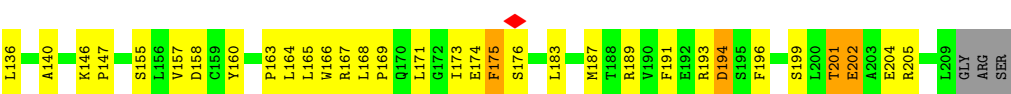
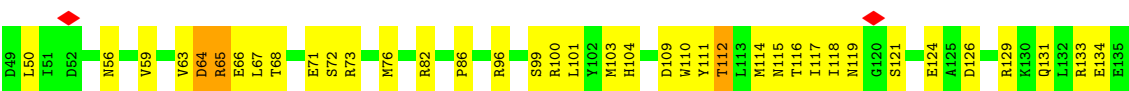
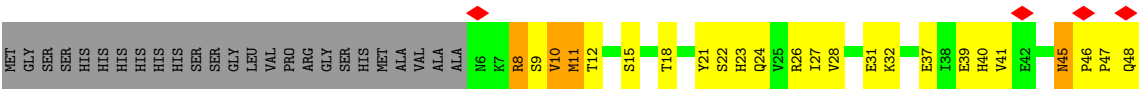


- Molecule 10: Stringent starvation protein A





• Molecule 10: Stringent starvation protein A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49560	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	1/1809 (0.1%)	0.63	0/2451
1	B	0.64	0/1789	0.60	0/2425
2	C	0.83	1/10725 (0.0%)	0.60	0/14472
3	D	0.77	1/10662 (0.0%)	0.62	0/14404
4	E	0.57	0/662	0.53	0/894
5	F	0.53	0/3887	0.51	0/5224
6	G	1.10	0/830	1.13	1/1277 (0.1%)
7	H	0.99	0/631	0.96	0/973
8	I	1.44	0/251	0.99	0/385
9	J	1.23	0/253	0.88	0/388
10	K	0.54	0/1633	0.50	0/2222
10	L	0.58	0/1672	0.53	0/2272
All	All	0.77	3/34804 (0.0%)	0.63	1/47387 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	4
10	L	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	SER	C-N	-5.80	1.20	1.34
3	D	545	HIS	CA-CB	-5.61	1.41	1.53
2	C	517	GLN	CA-CB	-5.03	1.42	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	43	DT	O4'-C4'-C3'	-5.00	102.50	104.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	198	ILE	Peptide
3	D	1184	ASP	Peptide
3	D	119	SER	Peptide
3	D	1344	LEU	Peptide
3	D	860	ARG	Peptide
10	L	8	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1810	52	0
1	B	1767	0	1789	85	0
2	C	10556	0	10572	382	0
3	D	10504	0	10644	481	0
4	E	660	0	646	15	0
5	F	3836	0	3907	226	0
6	G	746	0	425	51	0
7	H	561	0	304	28	0
8	I	225	0	124	11	0
9	J	226	0	123	13	0
10	K	1592	0	1550	60	0
10	L	1631	0	1601	74	0
11	D	1	0	0	0	0
12	D	2	0	0	0	0
All	All	34094	0	33495	1393	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1393) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:607:LEU:HA	5:F:610:PHE:HB2	1.51	0.89
8:I:23:DG:N1	9:J:5:DC:N3	2.21	0.89
6:G:12:DC:H2''	6:G:13:DT:H5'	1.55	0.89
5:F:604:SER:O	5:F:607:LEU:N	2.07	0.87
10:L:41:VAL:HG11	10:L:59:VAL:HG11	1.58	0.86
3:D:998:PRO:HG2	3:D:1001:ALA:HB2	1.56	0.85
3:D:1027:VAL:HG21	3:D:1102:PRO:HD2	1.60	0.84
8:I:20:DC:O2	9:J:8:DG:N2	2.08	0.83
10:K:113:LEU:HD23	10:K:132:LEU:HB2	1.59	0.83
8:I:23:DG:N2	9:J:5:DC:O2	2.11	0.82
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.62	0.81
3:D:42:GLU:HB3	3:D:52:GLU:HG3	1.62	0.81
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.12	0.81
4:E:4:VAL:HG23	4:E:5:THR:HG23	1.61	0.81
3:D:1039:ASP:HA	3:D:1074:LEU:HG	1.64	0.80
10:L:187:MET:O	10:L:191:PHE:HB2	1.82	0.79
6:G:44:DT:H2''	6:G:45:DA:C8	2.18	0.79
2:C:528:ARG:NH2	2:C:576:SER:O	2.16	0.78
5:F:402:LEU:HD23	5:F:405:ILE:HD11	1.65	0.78
5:F:476:ARG:NH1	5:F:477:GLU:O	2.16	0.78
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.63	0.78
5:F:576:VAL:O	5:F:580:PHE:HB2	1.83	0.78
3:D:845:ALA:O	3:D:860:ARG:NH1	2.17	0.78
5:F:304:THR:HG23	5:F:305:LEU:HD22	1.65	0.78
3:D:334:LYS:HA	3:D:339:ARG:HD2	1.66	0.78
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.65	0.78
3:D:950:ILE:HG12	3:D:1020:TRP:HH2	1.50	0.77
5:F:602:SER:H	5:F:605:GLU:HG2	1.50	0.77
2:C:519:ASN:HB2	2:C:522:SER:H	1.50	0.77
5:F:584:ARG:NH1	6:G:15:DG:OP2	2.19	0.76
2:C:1005:GLU:OE1	2:C:1007:LYS:NZ	2.17	0.76
2:C:1161:LEU:HD23	2:C:1161:LEU:O	1.86	0.75
3:D:1314:LEU:HB2	3:D:1326:GLN:HE22	1.51	0.75
10:L:133:ARG:NH2	10:L:174:GLU:O	2.19	0.75
5:F:162:ILE:HA	5:F:261:LEU:HA	1.69	0.74
10:L:194:ASP:OD1	10:L:194:ASP:N	2.20	0.74
3:D:903:LEU:HD11	3:D:909:ILE:HD12	1.70	0.74
10:K:24:GLN:NE2	10:K:111:TYR:OH	2.21	0.74
8:I:20:DC:N3	9:J:8:DG:N1	2.32	0.73
10:L:133:ARG:HH22	10:L:176:SER:H	1.35	0.73
2:C:548:ARG:NH2	2:C:567:PRO:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:552:THR:N	5:F:555:GLU:OE1	2.21	0.73
6:G:47:DT:H5"	6:G:47:DT:H6	1.54	0.73
8:I:23:DG:O6	9:J:5:DC:N4	2.20	0.73
1:B:78:ILE:HA	1:B:81:ILE:HD12	1.70	0.73
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.54	0.73
3:D:1157:ALA:O	3:D:1207:GLY:N	2.21	0.73
3:D:1158:GLU:N	3:D:1158:GLU:OE2	2.21	0.73
10:L:166:TRP:NE1	10:L:204:GLU:O	2.21	0.73
2:C:251:ALA:HB3	2:C:266:GLY:H	1.53	0.73
3:D:197:GLU:OE1	3:D:220:ARG:NH2	2.22	0.73
3:D:294:ASN:OD1	5:F:406:GLN:NE2	2.22	0.73
5:F:311:THR:HB	5:F:345:GLN:HG2	1.71	0.73
3:D:1024:THR:HG23	3:D:1123:ARG:HB3	1.70	0.73
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.21	0.72
2:C:1240:ASP:N	2:C:1240:ASP:OD1	2.22	0.72
2:C:675:ASP:OD2	2:C:677:ASN:ND2	2.22	0.72
5:F:586:ARG:NH1	6:G:14:DT:OP2	2.23	0.72
2:C:69:GLN:OE1	2:C:101:ARG:NH2	2.22	0.72
5:F:348:GLU:OE2	5:F:355:ILE:N	2.16	0.72
3:D:661:VAL:HG23	3:D:682:VAL:HG22	1.71	0.72
5:F:601:PRO:HA	5:F:605:GLU:HG2	1.72	0.71
3:D:1025:MET:N	3:D:1124:ILE:O	2.20	0.71
3:D:836:ARG:NE	3:D:869:CYS:SG	2.63	0.71
1:B:106:GLY:H	1:B:138:ALA:HB1	1.54	0.71
2:C:1151:LEU:HD11	2:C:1197:GLU:HB3	1.73	0.71
1:A:158:ARG:HH12	1:A:172:LEU:HD22	1.54	0.71
1:B:156:SER:O	1:B:160:HIS:ND1	2.21	0.71
2:C:421:SER:OG	2:C:423:ASP:OD1	2.09	0.71
3:D:1287:ILE:HD11	3:D:1300:ALA:HB1	1.72	0.71
3:D:209:ASN:HA	3:D:214:ARG:HD2	1.73	0.71
3:D:77:ARG:NH2	5:F:570:ASP:OD2	2.24	0.70
5:F:572:THR:OG1	5:F:575:GLU:OE1	2.08	0.70
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.19	0.70
3:D:1023:HIS:HA	3:D:1126:GLN:H	1.55	0.70
1:B:61:ILE:HB	1:B:64:VAL:HG12	1.74	0.70
3:D:978:ARG:HB2	3:D:1197:ASN:HD21	1.56	0.70
2:C:119:GLU:OE2	2:C:490:GLN:NE2	2.24	0.70
3:D:1036:ARG:CZ	3:D:1081:VAL:HG11	2.22	0.70
2:C:1151:LEU:O	2:C:1151:LEU:HG	1.91	0.70
10:K:187:MET:O	10:K:191:PHE:N	2.15	0.70
3:D:1046:ILE:HD12	3:D:1059:LEU:HD23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:599:ARG:HA	5:F:604:SER:HB3	1.74	0.69
2:C:413:GLU:OE2	2:C:413:GLU:N	2.23	0.69
3:D:1081:VAL:HA	3:D:1088:VAL:H	1.56	0.69
3:D:1002:VAL:HB	3:D:1019:ASN:HB2	1.74	0.69
5:F:145:LEU:HD23	5:F:221:PHE:HD1	1.56	0.69
5:F:600:HIS:ND1	5:F:601:PRO:O	2.25	0.69
1:B:166:ARG:HB3	1:B:170:ARG:HG3	1.73	0.69
2:C:235:ASN:ND2	2:C:286:GLU:OE2	2.25	0.69
3:D:514:THR:HG21	3:D:596:LEU:HB3	1.72	0.69
3:D:1344:LEU:O	3:D:1346:GLY:N	2.26	0.69
5:F:354:THR:HG22	5:F:356:GLU:H	1.57	0.69
3:D:909:ILE:HD11	3:D:913:GLU:HG2	1.73	0.69
5:F:593:LYS:HA	5:F:596:ARG:HD3	1.73	0.69
1:A:136:GLU:OE1	1:A:137:ASN:ND2	2.24	0.69
2:C:303:ASP:O	2:C:307:GLY:N	2.20	0.69
2:C:998:LEU:HD11	2:C:1018:TYR:HD2	1.57	0.69
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.24	0.69
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.73	0.69
6:G:44:DT:H2"	6:G:45:DA:N7	2.08	0.69
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.25	0.68
1:B:107:ILE:HD11	1:B:136:GLU:H	1.59	0.68
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.75	0.68
1:A:234:LEU:H	1:B:218:ARG:HD3	1.58	0.68
3:D:1035:VAL:HG23	3:D:1078:LEU:HD21	1.75	0.68
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.59	0.68
5:F:348:GLU:O	5:F:352:GLY:N	2.27	0.68
5:F:574:GLU:HB3	5:F:578:LYS:HE2	1.74	0.68
10:L:47:PRO:HD2	10:L:50:LEU:HD23	1.76	0.68
5:F:607:LEU:O	5:F:611:LEU:N	2.27	0.68
2:C:961:SER:O	2:C:965:GLN:HB2	1.92	0.68
3:D:959:LYS:O	3:D:959:LYS:NZ	2.24	0.68
2:C:23:ASP:N	2:C:23:ASP:OD1	2.22	0.67
2:C:398:SER:HB2	2:C:401:GLY:H	1.59	0.67
3:D:959:LYS:HZ1	3:D:983:LYS:HD2	1.58	0.67
3:D:966:VAL:H	3:D:974:VAL:HG22	1.60	0.67
5:F:130:VAL:HG23	5:F:365:MET:HG2	1.76	0.67
5:F:288:MET:O	5:F:292:VAL:HG22	1.94	0.67
2:C:963:GLU:O	2:C:967:LEU:HB2	1.93	0.67
5:F:145:LEU:HD22	5:F:225:ARG:HE	1.59	0.67
10:L:22:SER:HG	10:L:26:ARG:HH21	1.43	0.67
1:B:176:CYS:SG	3:D:535:ARG:NH2	2.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:18:ASP:N	3:D:18:ASP:OD1	2.28	0.67
3:D:1029:THR:OG1	3:D:1119:ASP:O	2.13	0.67
3:D:1166:GLY:HA3	3:D:1174:ARG:HE	1.59	0.67
5:F:437:GLN:OE1	6:G:35:DC:N4	2.28	0.67
2:C:340:ASP:OD1	2:C:340:ASP:N	2.27	0.66
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.75	0.66
2:C:993:PRO:HG2	2:C:996:ARG:HG2	1.77	0.66
3:D:370:LYS:HG3	3:D:441:LEU:HD12	1.77	0.66
2:C:106:GLU:N	2:C:112:GLY:O	2.25	0.66
3:D:1002:VAL:O	3:D:1019:ASN:N	2.26	0.66
3:D:1239:ASP:OD1	3:D:1242:ARG:NH1	2.27	0.66
3:D:74:LYS:NZ	3:D:86:GLU:OE2	2.27	0.66
4:E:32:VAL:O	4:E:34:GLY:N	2.29	0.66
5:F:150:ARG:HB3	5:F:155:GLU:HB2	1.77	0.66
5:F:532:LEU:O	5:F:536:THR:HG23	1.95	0.66
1:A:191:ARG:NH2	1:A:196:THR:O	2.29	0.66
3:D:71:LEU:HB2	3:D:90:VAL:HG21	1.77	0.65
1:B:77:ASP:OD1	1:B:78:ILE:N	2.29	0.65
5:F:584:ARG:O	5:F:588:ARG:NH2	2.30	0.65
10:L:45:ASN:OD1	10:L:45:ASN:N	2.30	0.65
3:D:993:GLU:OE1	3:D:995:TYR:OH	2.09	0.65
3:D:1219:ASP:OD2	3:D:1222:ARG:NH2	2.29	0.65
2:C:746:ALA:HB2	2:C:974:ARG:HD2	1.77	0.65
3:D:1042:ASP:HA	3:D:1046:ILE:HG13	1.79	0.65
3:D:1098:GLN:NE2	3:D:1200:GLU:OE1	2.30	0.65
10:K:201:THR:N	10:K:204:GLU:OE1	2.26	0.65
3:D:91:GLU:OE1	10:L:82:ARG:NH2	2.30	0.65
5:F:507:MET:HG2	5:F:520:GLY:HA2	1.78	0.65
3:D:978:ARG:HE	3:D:999:TYR:HB3	1.61	0.64
2:C:672:GLU:OE1	2:C:672:GLU:N	2.27	0.64
2:C:1321:GLU:OE2	3:D:99:ARG:NE	2.26	0.64
3:D:872:LEU:HB3	3:D:877:VAL:HG21	1.78	0.64
3:D:930:LEU:HD13	3:D:1244:GLN:HB3	1.80	0.64
3:D:1327:GLU:OE1	3:D:1330:ARG:NH1	2.31	0.64
3:D:156:ARG:NH2	3:D:191:SER:OG	2.27	0.64
3:D:895:CYS:SG	3:D:898:CYS:N	2.65	0.64
10:K:48:GLN:O	10:K:48:GLN:NE2	2.31	0.64
2:C:745:GLU:OE1	2:C:1017:GLN:NE2	2.31	0.64
3:D:950:ILE:HG12	3:D:1020:TRP:CH2	2.33	0.64
5:F:554:ARG:HD2	5:F:580:PHE:HE1	1.63	0.64
3:D:644:MET:O	3:D:764:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.23	0.63
2:C:576:SER:OG	2:C:577:VAL:N	2.31	0.63
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.81	0.63
3:D:1357:ILE:HG22	3:D:1359:ALA:H	1.62	0.63
5:F:585:GLU:OE2	5:F:588:ARG:NH1	2.31	0.63
10:K:170:GLN:HB2	10:K:207:MET:HB3	1.79	0.63
2:C:960:LEU:HB3	2:C:1025:PHE:CE1	2.33	0.63
3:D:709:ARG:O	3:D:711:GLY:N	2.31	0.63
3:D:1036:ARG:NH2	3:D:1085:GLY:O	2.31	0.63
2:C:199:ASP:N	2:C:199:ASP:OD1	2.29	0.63
3:D:847:ASP:N	3:D:847:ASP:OD1	2.30	0.63
5:F:91:ILE:HG22	5:F:93:ARG:H	1.63	0.63
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.80	0.63
2:C:841:ARG:N	2:C:848:GLU:OE1	2.32	0.63
2:C:1143:GLU:OE2	2:C:1147:ARG:NH1	2.22	0.63
3:D:1034:PHE:HB2	3:D:1081:VAL:HG22	1.81	0.63
5:F:283:GLN:NE2	5:F:340:ALA:O	2.25	0.63
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.72	0.63
2:C:138:ILE:O	2:C:139:ASN:ND2	2.31	0.63
5:F:147:GLN:OE1	5:F:150:ARG:NH1	2.31	0.63
5:F:585:GLU:HA	5:F:588:ARG:NE	2.13	0.63
1:B:98:VAL:HG12	1:B:146:VAL:HG22	1.81	0.63
5:F:605:GLU:O	5:F:609:SER:OG	2.08	0.63
2:C:231:GLU:OE1	2:C:332:ARG:NH2	2.31	0.62
2:C:1006:GLU:HA	2:C:1009:ASN:HB2	1.81	0.62
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.82	0.62
3:D:1115:ILE:HD12	3:D:1119:ASP:HB2	1.81	0.62
5:F:124:GLU:O	5:F:128:ASN:ND2	2.32	0.62
5:F:348:GLU:HG3	5:F:355:ILE:HG12	1.81	0.62
1:A:67:GLU:OE1	1:A:67:GLU:N	2.26	0.62
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.82	0.62
3:D:969:SER:H	3:D:1117:SER:HB2	1.63	0.62
1:B:20:SER:O	1:B:20:SER:OG	2.15	0.62
3:D:1274:PHE:HB3	3:D:1275:LEU:HD12	1.82	0.62
1:B:66:HIS:O	1:B:69:SER:OG	2.16	0.62
3:D:1314:LEU:HB2	3:D:1326:GLN:NE2	2.15	0.62
3:D:762:ASN:OD1	3:D:762:ASN:N	2.29	0.62
2:C:300:ASP:OD1	2:C:313:ALA:N	2.32	0.62
2:C:620:ASN:O	2:C:620:ASN:ND2	2.32	0.62
5:F:141:ILE:HD11	5:F:224:LEU:HD11	1.82	0.62
5:F:145:LEU:HD13	5:F:225:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:251:LYS:HA	5:F:254:GLU:HG3	1.80	0.62
2:C:981:ALA:HB1	2:C:1007:LYS:HE2	1.82	0.62
5:F:602:SER:OG	5:F:603:ARG:NH1	2.32	0.62
10:K:46:PRO:HG2	10:K:51:ILE:HD11	1.80	0.62
1:A:154:PRO:HG2	1:A:157:THR:HG23	1.81	0.62
5:F:145:LEU:HD21	5:F:224:LEU:HB3	1.81	0.62
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.33	0.62
5:F:606:VAL:O	5:F:610:PHE:N	2.31	0.62
3:D:905:ARG:HH12	3:D:907:HIS:HB2	1.65	0.61
2:C:165:HIS:CE1	2:C:190:PRO:HG3	2.35	0.61
2:C:568:ASN:N	2:C:568:ASN:OD1	2.32	0.61
3:D:73:GLY:O	3:D:76:LYS:NZ	2.30	0.61
3:D:709:ARG:C	3:D:711:GLY:H	2.04	0.61
5:F:295:CYS:HA	5:F:329:LYS:HB3	1.81	0.61
2:C:238:GLN:HG3	2:C:286:GLU:HG3	1.83	0.61
2:C:324:LYS:O	2:C:327:GLN:NE2	2.30	0.61
3:D:885:VAL:HG21	3:D:1255:VAL:HG12	1.82	0.61
5:F:525:ASP:OD1	5:F:526:THR:N	2.32	0.61
6:G:43:DT:H2''	6:G:44:DT:O5'	1.99	0.61
10:L:111:TYR:OH	10:L:160:TYR:O	2.18	0.61
5:F:268:TYR:HD2	5:F:269:LEU:HD22	1.65	0.61
10:K:32:LYS:NZ	10:K:86:PRO:O	2.28	0.61
2:C:179:TYR:HB2	2:C:397:LEU:O	2.01	0.61
6:G:43:DT:C6	6:G:44:DT:H72	2.36	0.61
3:D:557:LYS:HB3	3:D:563:LEU:HD23	1.82	0.61
3:D:850:LYS:NZ	3:D:855:ASP:O	2.33	0.61
10:L:47:PRO:HD2	10:L:50:LEU:CD2	2.31	0.61
5:F:607:LEU:HD13	5:F:610:PHE:HB2	1.83	0.61
1:B:60:GLU:OE1	1:B:143:ARG:NH1	2.33	0.61
2:C:758:ARG:NH1	2:C:762:ASN:OD1	2.34	0.61
3:D:901:ARG:HG3	3:D:902:ASP:N	2.16	0.61
3:D:1029:THR:HG23	3:D:1121:LEU:HG	1.83	0.61
10:K:44:ASP:OD1	10:K:45:ASN:N	2.33	0.61
10:K:151:SER:OG	10:K:152:ASP:N	2.34	0.61
1:B:62:ASP:OD1	1:B:63:GLY:N	2.33	0.60
2:C:785:ASP:OD2	2:C:791:LEU:N	2.29	0.60
3:D:1027:VAL:CG2	3:D:1102:PRO:HD2	2.31	0.60
1:A:14:VAL:HG22	1:A:15:ASP:H	1.66	0.60
1:B:135:ASP:N	1:B:135:ASP:OD1	2.35	0.60
1:B:148:ARG:HH11	1:B:148:ARG:HB3	1.66	0.60
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.83	0.60
3:D:1026:PRO:HG2	3:D:1028:ILE:HD11	1.82	0.60
1:A:174:ASP:OD1	1:A:174:ASP:N	2.34	0.60
2:C:979:LEU:HD22	2:C:989:LEU:HD21	1.82	0.60
3:D:518:VAL:HG12	3:D:707:ILE:HD11	1.83	0.60
2:C:1160:ASP:O	2:C:1161:LEU:HB3	2.01	0.60
3:D:902:ASP:H	3:D:1251:LYS:NZ	1.99	0.60
2:C:974:ARG:HH11	2:C:974:ARG:HB2	1.65	0.60
3:D:45:ASN:ND2	3:D:45:ASN:O	2.35	0.60
3:D:1057:SER:HB2	3:D:1059:LEU:HD13	1.83	0.60
3:D:1116:SER:OG	3:D:1117:SER:N	2.34	0.60
2:C:75:LEU:HD11	2:C:127:ILE:HD11	1.83	0.60
3:D:74:LYS:NZ	3:D:75:TYR:OH	2.31	0.60
3:D:1041:ILE:HB	3:D:1074:LEU:HD21	1.84	0.60
5:F:141:ILE:HG21	5:F:252:LEU:HD21	1.83	0.60
10:K:17:PRO:HA	10:K:40:HIS:CE1	2.37	0.60
2:C:379:GLU:OE1	2:C:379:GLU:N	2.34	0.60
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.31	0.60
3:D:720:ASN:HD22	3:D:723:TYR:H	1.48	0.60
1:A:66:HIS:O	1:A:69:SER:OG	2.18	0.59
5:F:472:GLN:NE2	5:F:473:GLU:OE2	2.35	0.59
1:B:58:GLU:HG2	1:B:172:LEU:HD12	1.83	0.59
2:C:1023:HIS:CD2	2:C:1027:LYS:HE2	2.37	0.59
5:F:426:LYS:NZ	6:G:40:DT:OP1	2.34	0.59
3:D:559:ALA:HB3	3:D:562:GLU:HB2	1.85	0.59
10:K:64:ASP:O	10:K:66:GLU:N	2.33	0.59
2:C:50:GLU:OE2	2:C:54:ARG:NE	2.35	0.59
3:D:1078:LEU:HD13	3:D:1121:LEU:HD22	1.85	0.59
8:I:16:DC:H2'	8:I:17:DT:H71	1.83	0.59
2:C:998:LEU:HD11	2:C:1018:TYR:CD2	2.37	0.59
3:D:1090:ILE:HD11	3:D:1099:TYR:HE1	1.67	0.59
3:D:405:GLU:O	3:D:408:VAL:HG22	2.03	0.59
10:L:112:THR:O	10:L:116:THR:HG23	2.03	0.59
1:B:75:GLN:HG2	1:B:132:HIS:HB2	1.84	0.59
2:C:826:ASP:OD1	2:C:829:THR:OG1	2.16	0.59
2:C:898:GLU:OE1	2:C:898:GLU:N	2.34	0.59
2:C:992:LEU:HD11	2:C:997:TRP:CE2	2.36	0.59
5:F:297:MET:HG3	5:F:326:TRP:CD2	2.37	0.59
2:C:204:LEU:HB3	2:C:208:ILE:HD12	1.84	0.59
3:D:1062:LEU:HD23	3:D:1066:GLU:HB3	1.85	0.59
5:F:281:ARG:O	5:F:285:ARG:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.36	0.59
2:C:59:ILE:HG23	2:C:476:LYS:HE3	1.83	0.58
2:C:624:ASP:O	2:C:626:GLU:N	2.36	0.58
4:E:67:ARG:NH2	4:E:71:GLU:OE2	2.35	0.58
5:F:465:ARG:HH12	7:H:26:DT:H3'	1.68	0.58
5:F:557:LYS:HG2	5:F:580:PHE:HE2	1.67	0.58
10:K:77:GLU:OE1	10:L:100:ARG:NE	2.35	0.58
2:C:316:GLU:CD	2:C:316:GLU:H	2.06	0.58
3:D:1162:ILE:O	3:D:1178:THR:N	2.29	0.58
10:L:121:SER:N	10:L:124:GLU:OE1	2.36	0.58
3:D:1034:PHE:N	3:D:1081:VAL:O	2.34	0.58
3:D:1165:PHE:HB3	3:D:1173:ARG:HD2	1.85	0.58
1:B:106:GLY:N	1:B:138:ALA:HB1	2.18	0.58
3:D:353:SER:OG	3:D:354:VAL:N	2.36	0.58
3:D:1269:ALA:HB3	3:D:1274:PHE:HD1	1.68	0.58
5:F:327:SER:HA	5:F:330:LEU:HD12	1.86	0.58
1:A:33:ARG:NH2	1:A:199:ASP:OD1	2.36	0.58
2:C:1164:PHE:HB3	2:C:1168:GLU:HB2	1.86	0.58
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.85	0.58
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.85	0.58
2:C:1014:LEU:HD12	2:C:1017:GLN:HG3	1.86	0.58
3:D:278:ARG:NH1	5:F:407:GLU:OE2	2.37	0.58
3:D:555:TYR:HB3	3:D:563:LEU:HB3	1.86	0.57
3:D:1093:THR:OG1	3:D:1094:ASP:N	2.37	0.57
1:B:101:THR:HG22	1:B:143:ARG:HG2	1.87	0.57
2:C:858:GLY:O	2:C:861:ALA:N	2.32	0.57
3:D:194:LEU:O	3:D:198:CYS:HB2	2.05	0.57
5:F:355:ILE:HA	5:F:358:VAL:HG12	1.86	0.57
10:L:136:LEU:HB3	10:L:175:PHE:HZ	1.69	0.57
2:C:979:LEU:HB3	2:C:989:LEU:HD21	1.86	0.57
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.84	0.57
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.31	0.57
3:D:48:THR:O	3:D:50:LYS:N	2.38	0.57
3:D:1080:ILE:HD11	3:D:1121:LEU:HD11	1.84	0.57
5:F:386:LEU:O	5:F:389:SER:OG	2.19	0.57
3:D:952:VAL:O	3:D:1014:GLY:N	2.37	0.57
3:D:1021:ASP:HB2	3:D:1024:THR:HB	1.85	0.57
3:D:1068:THR:HG23	3:D:1070:GLY:H	1.70	0.57
5:F:557:LYS:HD3	10:K:85:HIS:CD2	2.39	0.57
2:C:830:THR:OG1	2:C:832:HIS:NE2	2.34	0.57
5:F:262:VAL:HG23	5:F:265:GLN:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:10:VAL:O	10:L:11:MET:HB3	2.05	0.57
2:C:960:LEU:HB3	2:C:1025:PHE:HE1	1.70	0.57
3:D:342:LEU:HB3	3:D:1352:ILE:HG23	1.87	0.57
2:C:1211:ARG:HD3	2:C:1220:GLN:OE1	2.05	0.56
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.70	0.56
10:L:196:PHE:O	10:L:199:SER:OG	2.16	0.56
3:D:384:LYS:HG3	3:D:415:VAL:HG12	1.87	0.56
3:D:874:GLU:OE1	3:D:875:ASN:ND2	2.39	0.56
5:F:347:ILE:O	5:F:351:THR:HG23	2.04	0.56
1:A:92:VAL:HG12	1:A:121:VAL:HG22	1.88	0.56
2:C:198:ILE:HG21	2:C:388:LEU:HD21	1.87	0.56
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.85	0.56
2:C:970:GLY:O	2:C:973:SER:OG	2.18	0.56
3:D:1083:ALA:N	3:D:1114:GLN:HE22	2.03	0.56
5:F:279:ARG:CZ	5:F:347:ILE:HG12	2.36	0.56
5:F:344:LEU:HD21	5:F:355:ILE:HG13	1.87	0.56
5:F:385:ARG:HE	6:G:42:DT:H5'	1.70	0.56
6:G:20:DC:O2	7:H:44:DG:N2	2.38	0.56
10:L:63:VAL:HG12	10:L:68:THR:HG22	1.87	0.56
1:B:174:ASP:OD1	1:B:174:ASP:N	2.38	0.56
6:G:25:DC:H2''	6:G:26:DG:H8	1.70	0.56
5:F:543:ALA:O	5:F:547:VAL:HG23	2.04	0.56
10:K:182:GLU:H	10:K:182:GLU:CD	2.09	0.56
2:C:161:LYS:HD2	2:C:161:LYS:H	1.71	0.56
2:C:270:THR:HG23	2:C:273:HIS:CE1	2.41	0.56
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.39	0.56
3:D:1037:PHE:HB3	3:D:1041:ILE:HD13	1.88	0.56
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.86	0.56
3:D:1263:LYS:HE2	3:D:1279:GLN:NE2	2.20	0.56
3:D:53:ARG:HH22	3:D:89:GLY:H	1.54	0.56
3:D:516:ASP:HA	3:D:545:HIS:HB3	1.87	0.56
5:F:287:ILE:HG22	5:F:302:PHE:HZ	1.69	0.56
10:K:151:SER:OG	10:K:153:GLU:N	2.38	0.56
10:L:64:ASP:N	10:L:64:ASP:OD1	2.38	0.56
2:C:273:HIS:O	2:C:277:LEU:HG	2.06	0.56
2:C:581:THR:HG23	2:C:585:GLY:HA2	1.88	0.56
2:C:1337:ILE:HD11	3:D:20:ILE:HD11	1.86	0.56
3:D:17:PHE:HZ	3:D:1353:VAL:HG21	1.70	0.56
2:C:485:ASP:OD1	2:C:486:THR:N	2.39	0.55
3:D:709:ARG:C	3:D:711:GLY:N	2.60	0.55
2:C:114:VAL:HG22	2:C:115:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.88	0.55
3:D:341:ASN:O	3:D:342:LEU:HB2	2.04	0.55
2:C:323:ALA:O	2:C:326:SER:OG	2.20	0.55
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.53	0.55
10:L:131:GLN:O	10:L:134:GLU:HG2	2.06	0.55
2:C:211:ARG:NH1	2:C:357:ASN:O	2.39	0.55
3:D:833:GLU:OE1	3:D:1247:LYS:NZ	2.39	0.55
3:D:1158:GLU:OE1	3:D:1186:TYR:OH	2.21	0.55
3:D:19:ALA:HA	3:D:1342:ASP:O	2.06	0.55
5:F:140:ALA:HA	5:F:269:LEU:HD11	1.89	0.55
7:H:51:DG:N3	7:H:52:DG:H5''	2.21	0.55
10:L:64:ASP:O	10:L:66:GLU:N	2.36	0.55
3:D:505:ASP:OD2	3:D:505:ASP:N	2.36	0.55
10:L:46:PRO:HB2	10:L:50:LEU:HD21	1.89	0.55
2:C:319:LEU:HA	2:C:322:LEU:HD12	1.88	0.55
3:D:789:LYS:HZ3	3:D:931:THR:HG21	1.72	0.55
5:F:267:ASP:O	5:F:271:ASN:ND2	2.39	0.55
5:F:256:PHE:HA	5:F:259:PHE:CE2	2.41	0.55
5:F:486:ARG:HA	5:F:486:ARG:NE	2.22	0.55
5:F:607:LEU:HD22	5:F:610:PHE:HD2	1.72	0.55
10:L:26:ARG:NH1	10:L:204:GLU:OE2	2.37	0.55
3:D:342:LEU:HD23	3:D:1352:ILE:CG2	2.37	0.55
4:E:41:GLU:OE1	4:E:43:ASN:N	2.38	0.55
2:C:102:LEU:HB3	2:C:489:PRO:HG3	1.88	0.54
2:C:972:PHE:HA	2:C:975:ILE:HB	1.89	0.54
2:C:1156:ARG:HG3	2:C:1156:ARG:O	2.06	0.54
3:D:84:ILE:HG12	3:D:91:GLU:HB2	1.87	0.54
7:H:50:DA:H2''	7:H:51:DG:H8	1.72	0.54
3:D:316:ILE:HA	3:D:323:PRO:HA	1.88	0.54
3:D:1007:ASP:N	3:D:1009:GLU:OE2	2.39	0.54
3:D:1102:PRO:HG2	3:D:1124:ILE:HD11	1.88	0.54
3:D:1268:ASN:HA	3:D:1274:PHE:CE1	2.42	0.54
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.89	0.54
5:F:353:LEU:HD23	5:F:357:GLN:HB3	1.89	0.54
8:I:19:DA:H1'	8:I:20:DC:H5'	1.90	0.54
1:A:76:GLU:N	1:A:76:GLU:OE1	2.41	0.54
1:B:22:THR:OG1	1:B:207:THR:O	2.25	0.54
5:F:102:MET:HG3	6:G:43:DT:N3	2.21	0.54
5:F:452:ILE:HG13	5:F:457:ILE:HG13	1.89	0.54
6:G:25:DC:H2''	6:G:26:DG:C8	2.42	0.54
10:L:147:PRO:O	10:L:189:ARG:NE	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LYS:NZ	2:C:334:GLU:OE1	2.36	0.54
2:C:551:HIS:ND1	2:C:552:PRO:HD2	2.22	0.54
3:D:559:ALA:O	3:D:561:GLY:N	2.40	0.54
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.89	0.54
3:D:516:ASP:OD1	3:D:516:ASP:N	2.36	0.54
5:F:162:ILE:HD11	5:F:259:PHE:HB3	1.89	0.54
1:B:20:SER:O	1:B:22:THR:N	2.41	0.54
2:C:303:ASP:N	2:C:308:GLU:O	2.26	0.54
3:D:438:GLU:OE2	3:D:481:ARG:NH2	2.37	0.54
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.29	0.54
6:G:47:DT:H5''	6:G:47:DT:C6	2.40	0.54
5:F:303:ILE:O	5:F:307:THR:OG1	2.12	0.54
3:D:1327:GLU:HA	9:J:12:DG:OP1	2.07	0.54
5:F:145:LEU:HD22	5:F:225:ARG:NE	2.22	0.54
10:K:54:ASN:ND2	10:K:58:SER:H	2.05	0.54
2:C:318:SER:O	2:C:322:LEU:HG	2.07	0.54
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.43	0.54
10:L:11:MET:HG3	10:L:64:ASP:OD1	2.07	0.54
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.89	0.53
2:C:253:PHE:N	2:C:265:LYS:HG3	2.23	0.53
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.73	0.53
3:D:947:GLU:O	3:D:1020:TRP:NE1	2.41	0.53
5:F:309:ASN:HD21	5:F:315:TRP:HD1	1.57	0.53
5:F:558:VAL:HG23	5:F:576:VAL:HG11	1.89	0.53
1:B:93:GLN:HB2	1:B:120:ASP:OD1	2.07	0.53
2:C:415:GLU:N	2:C:415:GLU:OE1	2.42	0.53
2:C:452:ARG:HH22	2:C:458:GLU:CD	2.11	0.53
3:D:1325:PHE:CE1	3:D:1326:GLN:HG3	2.43	0.53
10:L:9:SER:HA	10:L:65:ARG:HH12	1.73	0.53
2:C:192:ASP:OD1	2:C:436:ARG:NH2	2.42	0.53
2:C:905:ILE:HG22	5:F:595:LEU:HD22	1.90	0.53
2:C:937:ASP:HB3	2:C:1039:GLY:HA3	1.91	0.53
2:C:985:GLU:HG2	2:C:988:LYS:HE2	1.91	0.53
3:D:978:ARG:HB2	3:D:1197:ASN:ND2	2.23	0.53
5:F:267:ASP:HA	5:F:270:VAL:HG12	1.91	0.53
2:C:373:GLY:HA3	5:F:94:THR:HG21	1.90	0.53
2:C:727:VAL:HG23	2:C:732:ILE:HG12	1.89	0.53
3:D:980:THR:O	3:D:980:THR:OG1	2.27	0.53
3:D:1033:GLY:HA3	3:D:1080:ILE:HG22	1.90	0.53
4:E:8:ASP:N	4:E:8:ASP:OD1	2.40	0.53
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.42	0.53
5:F:530:LEU:O	5:F:533:ASP:N	2.42	0.53
6:G:44:DT:H1'	6:G:45:DA:O4'	2.09	0.53
9:J:11:DA:H2''	9:J:12:DG:C8	2.44	0.53
1:A:62:ASP:OD1	1:A:63:GLY:N	2.39	0.53
1:B:93:GLN:H	1:B:120:ASP:HB3	1.73	0.53
2:C:348:SER:OG	2:C:349:GLU:N	2.42	0.53
9:J:6:DG:C8	9:J:6:DG:H5'	2.44	0.53
2:C:242:VAL:HG12	2:C:245:ARG:HE	1.74	0.53
2:C:1017:GLN:O	2:C:1021:LEU:HB2	2.09	0.53
2:C:1088:ASP:OD1	2:C:1088:ASP:N	2.37	0.53
3:D:950:ILE:HB	3:D:1017:VAL:HG12	1.91	0.53
3:D:1042:ASP:CG	3:D:1048:ARG:HB2	2.29	0.53
2:C:909:LYS:NZ	2:C:911:SER:HA	2.23	0.53
3:D:207:GLU:HG3	3:D:208:THR:N	2.24	0.53
3:D:997:VAL:HG13	3:D:1001:ALA:HB3	1.90	0.53
10:L:11:MET:HA	10:L:63:VAL:O	2.09	0.53
2:C:942:ASP:OD2	2:C:942:ASP:N	2.28	0.52
1:B:20:SER:HG	1:B:23:HIS:HB3	1.74	0.52
3:D:393:THR:HG23	3:D:396:ALA:H	1.74	0.52
5:F:145:LEU:HD23	5:F:221:PHE:CD1	2.42	0.52
5:F:299:LYS:O	5:F:303:ILE:HG12	2.09	0.52
5:F:377:LYS:NZ	5:F:381:GLU:OE2	2.23	0.52
3:D:275:ARG:HD3	3:D:298:MET:HG3	1.90	0.52
3:D:1251:LYS:O	3:D:1255:VAL:HG13	2.10	0.52
1:B:207:THR:OG1	1:B:208:ASN:N	2.41	0.52
3:D:492:SER:HB2	3:D:499:ILE:HD13	1.91	0.52
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.09	0.52
6:G:26:DG:C2	7:H:38:DG:C2	2.97	0.52
3:D:82:GLY:HA3	10:K:93:PRO:HD2	1.90	0.52
3:D:1174:ARG:HB2	3:D:1189:MET:SD	2.49	0.52
5:F:112:THR:OG1	5:F:114:GLU:OE2	2.27	0.52
7:H:30:DA:H1'	7:H:31:DT:H5'	1.92	0.52
2:C:338:THR:O	2:C:338:THR:OG1	2.26	0.52
4:E:36:ASP:N	4:E:36:ASP:OD1	2.40	0.52
5:F:379:MET:O	5:F:383:ASN:ND2	2.36	0.52
1:B:100:LEU:HD12	1:B:144:ILE:HD11	1.90	0.52
2:C:1014:LEU:HA	2:C:1017:GLN:HG3	1.91	0.52
3:D:210:SER:O	3:D:213:LYS:N	2.42	0.52
5:F:248:GLU:HA	5:F:251:LYS:HZ2	1.74	0.52
5:F:273:MET:HE1	5:F:361:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.75	0.52
2:C:56:VAL:HG11	2:C:468:LEU:HD13	1.91	0.52
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.92	0.52
2:C:746:ALA:CB	2:C:974:ARG:HD2	2.40	0.52
3:D:1075:ARG:HB2	3:D:1100:PHE:HE1	1.73	0.52
5:F:397:ARG:HG2	7:H:26:DT:N3	2.25	0.52
10:K:129:ARG:NH2	10:K:171:LEU:O	2.34	0.52
10:L:63:VAL:HA	10:L:67:LEU:O	2.10	0.52
2:C:518:ASN:N	2:C:518:ASN:OD1	2.43	0.52
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.36	0.52
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.91	0.52
6:G:13:DT:H2"	6:G:14:DT:H71	1.91	0.52
1:B:12:ARG:O	1:B:13:LEU:HB3	2.10	0.51
2:C:1021:LEU:HA	2:C:1024:GLU:HB3	1.92	0.51
3:D:317:THR:HG23	3:D:320:ASN:O	2.10	0.51
3:D:789:LYS:NZ	3:D:931:THR:HG21	2.24	0.51
3:D:857:LEU:H	3:D:857:LEU:HD23	1.75	0.51
5:F:219:GLU:HG3	5:F:220:LYS:HD2	1.92	0.51
1:A:193:GLU:HG2	1:A:194:GLN:HG3	1.92	0.51
2:C:1005:GLU:HB2	2:C:1007:LYS:HD2	1.93	0.51
3:D:275:ARG:NH2	5:F:403:ASP:OD1	2.40	0.51
5:F:353:LEU:HB3	5:F:357:GLN:HB2	1.92	0.51
10:K:17:PRO:HA	10:K:40:HIS:HE1	1.75	0.51
1:B:6:THR:OG1	1:B:7:GLU:N	2.42	0.51
5:F:233:ASP:O	5:F:236:LYS:NZ	2.44	0.51
7:H:34:DA:C8	7:H:35:DT:H72	2.46	0.51
10:K:24:GLN:HG2	10:K:159:CYS:O	2.11	0.51
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.91	0.51
2:C:812:PHE:CD2	2:C:813:GLU:HG2	2.46	0.51
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.29	0.51
2:C:1161:LEU:O	2:C:1161:LEU:CD2	2.56	0.51
3:D:1107:VAL:HG22	3:D:1122:ALA:HB2	1.93	0.51
2:C:453:ILE:HD12	2:C:530:ILE:HD12	1.92	0.51
2:C:893:THR:OG1	2:C:894:GLN:N	2.44	0.51
3:D:1064:SER:OG	3:D:1195:GLN:N	2.43	0.51
3:D:1101:LEU:HD21	3:D:1121:LEU:HD12	1.91	0.51
5:F:277:MET:O	5:F:281:ARG:HG2	2.11	0.51
1:B:23:HIS:CG	1:B:206:GLU:HG2	2.45	0.51
2:C:5:TYR:OH	2:C:1171:ARG:NH2	2.34	0.51
2:C:443:ASP:OD1	2:C:443:ASP:N	2.43	0.51
5:F:93:ARG:CZ	5:F:93:ARG:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:140:ALA:HA	10:L:183:LEU:HD21	1.91	0.51
2:C:1326:LEU:HD13	3:D:342:LEU:HD22	1.93	0.51
3:D:555:TYR:CD2	3:D:585:LYS:HD2	2.46	0.51
5:F:331:HIS:O	5:F:334:SER:OG	2.26	0.51
6:G:15:DG:H2''	6:G:16:DC:C6	2.46	0.51
6:G:21:DA:H2''	6:G:22:DT:H5'	1.93	0.51
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.44	0.51
3:D:985:ILE:HG22	3:D:986:ASP:H	1.75	0.51
3:D:1067:ARG:CZ	3:D:1076:PRO:HG3	2.41	0.51
2:C:598:VAL:HG23	2:C:626:GLU:O	2.11	0.51
2:C:1222:GLU:OE1	2:C:1222:GLU:N	2.41	0.51
2:C:1287:LEU:HD21	3:D:1351:VAL:HG22	1.92	0.51
3:D:34:SER:OG	3:D:35:PHE:N	2.42	0.51
3:D:905:ARG:NH1	3:D:907:HIS:HB2	2.26	0.51
3:D:1176:VAL:HB	3:D:1187:GLU:HB3	1.92	0.51
5:F:606:VAL:HG22	5:F:610:PHE:CE2	2.46	0.51
3:D:654:ILE:HD13	3:D:760:THR:HB	1.93	0.50
3:D:718:SER:OG	3:D:719:PHE:N	2.40	0.50
3:D:918:ILE:O	3:D:922:SER:OG	2.28	0.50
5:F:229:VAL:HG13	5:F:232:ARG:HH21	1.76	0.50
5:F:277:MET:SD	5:F:362:ASN:HB2	2.51	0.50
5:F:584:ARG:HH21	6:G:15:DG:H8	1.58	0.50
5:F:601:PRO:CA	5:F:605:GLU:HG2	2.41	0.50
2:C:130:MET:SD	2:C:134:GLY:HA2	2.52	0.50
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.26	0.50
3:D:814:CYS:HB2	3:D:889:ASP:HB3	1.92	0.50
3:D:1105:ALA:HB1	3:D:1122:ALA:HB1	1.93	0.50
6:G:38:DC:H1'	6:G:39:DT:H5'	1.93	0.50
6:G:43:DT:N3	6:G:44:DT:C4	2.79	0.50
1:B:127:GLN:CD	1:B:127:GLN:H	2.14	0.50
2:C:297:VAL:HG12	2:C:315:MET:O	2.12	0.50
2:C:339:ASN:HD21	2:C:341:LEU:HB3	1.75	0.50
3:D:137:ARG:NH2	5:F:91:ILE:HD12	2.27	0.50
3:D:1090:ILE:HD11	3:D:1099:TYR:CE1	2.47	0.50
5:F:572:THR:HB	7:H:45:DA:OP1	2.11	0.50
6:G:43:DT:N3	6:G:44:DT:O4	2.44	0.50
10:L:99:SER:O	10:L:103:MET:HG3	2.10	0.50
10:L:109:ASP:HB3	10:L:110:TRP:CD1	2.47	0.50
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.93	0.50
3:D:536:LEU:HD22	3:D:541:LEU:HB2	1.94	0.50
3:D:861:ASN:OD1	3:D:861:ASN:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:117:ILE:HD11	10:K:129:ARG:HB2	1.93	0.50
10:L:96:ARG:HB3	10:L:100:ARG:HH12	1.76	0.50
2:C:59:ILE:N	2:C:68:LEU:O	2.33	0.50
6:G:43:DT:C2	6:G:44:DT:C5	2.98	0.50
7:H:38:DG:C2	7:H:39:DC:C4	2.99	0.50
10:K:111:TYR:CE1	10:K:164:LEU:HD12	2.46	0.50
10:L:24:GLN:O	10:L:28:VAL:HG23	2.12	0.50
2:C:325:LEU:HA	2:C:330:HIS:HD2	1.76	0.50
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.27	0.50
5:F:345:GLN:O	5:F:349:GLU:HG2	2.12	0.50
6:G:43:DT:C5	6:G:44:DT:H72	2.46	0.50
9:J:8:DG:H2'	9:J:9:DT:H71	1.94	0.50
1:A:45:ARG:NH1	2:C:1084:ASP:OD1	2.43	0.50
1:B:192:VAL:O	1:B:194:GLN:N	2.42	0.50
2:C:452:ARG:HH12	2:C:454:ARG:HG2	1.76	0.50
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.12	0.50
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.94	0.50
3:D:973:LEU:HD12	3:D:1006:GLY:HA2	1.94	0.50
3:D:1179:PRO:CD	3:D:1184:ASP:HA	2.42	0.50
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.12	0.50
3:D:1313:SER:O	3:D:1316:THR:OG1	2.29	0.50
1:B:192:VAL:O	1:B:192:VAL:HG13	2.11	0.50
2:C:728:ASP:OD1	2:C:729:ALA:N	2.45	0.50
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.47	0.50
3:D:1222:ARG:HG2	3:D:1223:LEU:HD23	1.94	0.50
5:F:344:LEU:HA	5:F:347:ILE:HD12	1.94	0.50
10:L:31:GLU:OE2	10:L:193:ARG:NH2	2.38	0.50
2:C:98:VAL:O	2:C:121:GLU:HA	2.11	0.50
10:L:41:VAL:HB	10:L:46:PRO:HA	1.93	0.50
1:B:164:ASP:O	1:B:166:ARG:NH1	2.45	0.49
2:C:624:ASP:C	2:C:626:GLU:H	2.15	0.49
2:C:1269:ARG:NE	3:D:344:GLY:O	2.45	0.49
3:D:1163:VAL:HG12	3:D:1202:GLU:O	2.12	0.49
5:F:127:ILE:O	5:F:130:VAL:HG12	2.11	0.49
10:K:19:ASP:OD2	10:K:60:PRO:HD3	2.12	0.49
1:B:162:GLU:HG3	1:B:166:ARG:HH22	1.77	0.49
3:D:1278:GLU:N	3:D:1278:GLU:OE1	2.45	0.49
5:F:397:ARG:HG2	7:H:26:DT:H3	1.77	0.49
6:G:33:DT:H1'	6:G:34:DC:H5'	1.94	0.49
2:C:59:ILE:O	2:C:68:LEU:N	2.26	0.49
2:C:60:GLN:O	2:C:476:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	1.93	0.49
3:D:793:SER:O	3:D:797:THR:HG22	2.12	0.49
3:D:945:ALA:HB3	3:D:1129:GLY:HA2	1.94	0.49
7:H:39:DC:H1'	7:H:40:DA:O4'	2.12	0.49
2:C:613:ASN:OD1	2:C:613:ASN:N	2.44	0.49
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.77	0.49
3:D:53:ARG:NH2	3:D:89:GLY:H	2.09	0.49
3:D:317:THR:HG22	3:D:322:ARG:O	2.12	0.49
6:G:15:DG:C2	7:H:49:DA:C2	3.00	0.49
2:C:241:LEU:N	2:C:283:LYS:O	2.44	0.49
2:C:444:ASP:N	2:C:444:ASP:OD1	2.38	0.49
2:C:611:GLU:OE2	2:C:637:ARG:NH2	2.45	0.49
2:C:1030:GLU:OE2	2:C:1033:ARG:NH2	2.44	0.49
3:D:749:LYS:O	3:D:752:GLY:N	2.43	0.49
3:D:1179:PRO:HD2	3:D:1184:ASP:O	2.12	0.49
5:F:476:ARG:NH2	5:F:477:GLU:HB3	2.27	0.49
2:C:977:ALA:O	2:C:980:VAL:HG22	2.12	0.49
2:C:990:ASP:O	2:C:994:ARG:NH1	2.43	0.49
5:F:309:ASN:ND2	5:F:312:SER:O	2.46	0.49
6:G:42:DT:H4'	6:G:43:DT:O5'	2.13	0.49
2:C:60:GLN:HA	2:C:67:GLU:HA	1.94	0.49
2:C:979:LEU:HD22	2:C:989:LEU:HD11	1.93	0.49
2:C:1002:LEU:HD23	2:C:1007:LYS:HB3	1.95	0.49
3:D:322:ARG:HG3	3:D:323:PRO:HD2	1.95	0.49
3:D:378:LYS:HE3	3:D:382:TYR:OH	2.13	0.49
3:D:630:ALA:O	3:D:634:ARG:HG2	2.13	0.49
5:F:225:ARG:O	5:F:229:VAL:HG23	2.13	0.49
5:F:585:GLU:O	5:F:588:ARG:HG2	2.11	0.49
6:G:43:DT:OP2	6:G:43:DT:H6	1.95	0.49
10:K:191:PHE:HA	10:K:196:PHE:CD2	2.47	0.49
3:D:54:ASP:CG	3:D:54:ASP:O	2.51	0.49
3:D:105:ILE:HD12	3:D:242:LEU:HD23	1.94	0.49
6:G:22:DT:H2''	6:G:23:DT:H71	1.95	0.49
2:C:596:ASP:OD1	2:C:597:GLY:N	2.41	0.49
2:C:1172:LEU:O	2:C:1175:ASN:N	2.45	0.49
2:C:1192:GLU:O	2:C:1195:ILE:N	2.45	0.49
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.12	0.49
3:D:235:GLU:CD	3:D:235:GLU:H	2.16	0.49
3:D:548:VAL:HG22	3:D:549:LYS:H	1.77	0.49
3:D:868:TRP:HA	3:D:868:TRP:CE3	2.47	0.49
3:D:959:LYS:HE3	3:D:959:LYS:HB3	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:105:MET:HE3	5:F:384:LEU:HB3	1.95	0.49
3:D:912:GLY:O	3:D:1360:GLY:N	2.36	0.48
3:D:970:SER:HB2	3:D:972:LYS:HZ3	1.77	0.48
5:F:295:CYS:SG	5:F:330:LEU:HA	2.52	0.48
5:F:395:THR:HG23	5:F:396:ASN:H	1.78	0.48
3:D:949:SER:OG	3:D:951:GLN:NE2	2.44	0.48
5:F:603:ARG:O	5:F:606:VAL:HG12	2.12	0.48
6:G:42:DT:H2''	6:G:43:DT:OP2	2.13	0.48
10:L:9:SER:OG	10:L:10:VAL:N	2.45	0.48
1:A:166:ARG:HG2	1:A:167:PRO:HD3	1.96	0.48
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.96	0.48
2:C:690:VAL:HG12	2:C:1234:LYS:O	2.13	0.48
2:C:696:ASP:OD2	2:C:696:ASP:N	2.31	0.48
3:D:45:ASN:O	3:D:47:ARG:N	2.45	0.48
3:D:582:ILE:HG13	3:D:623:GLN:HB3	1.95	0.48
3:D:1318:SER:HB2	3:D:1342:ASP:OD1	2.13	0.48
10:L:166:TRP:HE3	10:L:191:PHE:CE1	2.30	0.48
2:C:1155:VAL:HG12	2:C:1157:GLN:H	1.77	0.48
5:F:290:LEU:HD22	5:F:333:VAL:HG21	1.94	0.48
7:H:47:DG:C2	7:H:48:DC:C2	3.01	0.48
2:C:818:VAL:HG12	2:C:819:SER:O	2.14	0.48
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.47	0.48
3:D:298:MET:CE	5:F:402:LEU:HB3	2.43	0.48
3:D:514:THR:HG21	3:D:596:LEU:CB	2.43	0.48
3:D:961:SER:O	3:D:981:GLU:HB3	2.13	0.48
10:K:19:ASP:O	10:K:22:SER:OG	2.21	0.48
3:D:1318:SER:O	3:D:1318:SER:OG	2.29	0.48
5:F:287:ILE:HG21	5:F:306:PHE:CE1	2.48	0.48
5:F:487:MET:O	5:F:488:LEU:HD23	2.13	0.48
6:G:44:DT:OP2	6:G:44:DT:H2'	2.13	0.48
2:C:624:ASP:OD2	2:C:624:ASP:N	2.47	0.48
2:C:1270:PHE:O	3:D:344:GLY:HA2	2.14	0.48
3:D:338:PHE:HZ	3:D:1320:ILE:HG23	1.78	0.48
3:D:930:LEU:HB3	3:D:1244:GLN:HG3	1.96	0.48
6:G:21:DA:H2'	6:G:22:DT:H72	1.96	0.48
2:C:81:ASP:OD1	2:C:81:ASP:N	2.45	0.48
2:C:890:LYS:HB3	2:C:912:ASP:O	2.13	0.48
3:D:85:CYS:SG	3:D:86:GLU:N	2.86	0.48
3:D:703:THR:O	3:D:703:THR:OG1	2.26	0.48
3:D:960:LEU:HA	3:D:981:GLU:O	2.13	0.48
3:D:1026:PRO:HB3	3:D:1123:ARG:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:23:HIS:O	10:L:27:ILE:HG13	2.13	0.48
2:C:210:LEU:HA	2:C:210:LEU:HD23	1.51	0.48
2:C:974:ARG:HB2	2:C:974:ARG:NH1	2.29	0.48
3:D:410:ASP:OD1	3:D:410:ASP:N	2.46	0.48
3:D:1323:ALA:HB1	3:D:1328:THR:HG23	1.96	0.48
3:D:1367:GLN:O	3:D:1370:MET:HG3	2.14	0.48
5:F:278:ASP:O	5:F:282:THR:HG22	2.14	0.48
3:D:1194:ARG:HB3	3:D:1211:SER:HB3	1.96	0.48
5:F:327:SER:O	5:F:330:LEU:HB2	2.14	0.48
7:H:40:DA:H2"	7:H:41:DA:C8	2.49	0.48
2:C:658:GLN:HG2	2:C:1186:VAL:HG23	1.96	0.47
2:C:1290:MET:SD	3:D:347:VAL:HG11	2.53	0.47
3:D:398:LYS:HD2	5:F:532:LEU:HD21	1.94	0.47
3:D:902:ASP:H	3:D:1251:LYS:HZ1	1.62	0.47
3:D:957:SER:OG	3:D:958:ILE:N	2.47	0.47
3:D:1259:GLN:NE2	3:D:1262:ARG:HE	2.11	0.47
9:J:7:DC:H2"	9:J:8:DG:C8	2.48	0.47
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.30	0.47
3:D:610:ARG:HA	3:D:610:ARG:HD3	1.67	0.47
3:D:1056:LEU:HD22	3:D:1108:GLN:HE21	1.78	0.47
10:L:129:ARG:HG3	10:L:173:ILE:HD11	1.95	0.47
2:C:75:LEU:HD21	2:C:127:ILE:HD11	1.96	0.47
2:C:102:LEU:CB	2:C:489:PRO:HG3	2.44	0.47
2:C:256:GLU:HG3	2:C:260:LYS:C	2.34	0.47
2:C:1192:GLU:OE2	3:D:764:ARG:NE	2.28	0.47
2:C:1303:LYS:HD3	2:C:1303:LYS:HA	1.50	0.47
3:D:632:ALA:O	3:D:635:SER:OG	2.32	0.47
3:D:978:ARG:CZ	3:D:999:TYR:H	2.27	0.47
3:D:1184:ASP:N	3:D:1185:PRO:HD3	2.29	0.47
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.96	0.47
3:D:1266:ILE:H	3:D:1266:ILE:HG12	1.48	0.47
6:G:43:DT:C2	6:G:44:DT:C4	3.02	0.47
10:L:96:ARG:NH2	10:L:100:ARG:HH22	2.13	0.47
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.72	0.47
2:C:237:LEU:HD13	2:C:292:ILE:HG13	1.96	0.47
2:C:356:THR:OG1	2:C:357:ASN:N	2.47	0.47
2:C:494:ASN:OD1	2:C:495:ALA:N	2.48	0.47
2:C:629:PHE:HE2	2:C:650:VAL:HG21	1.79	0.47
2:C:1252:SER:OG	2:C:1253:LEU:N	2.48	0.47
3:D:1077:ALA:HB2	3:D:1100:PHE:CE1	2.49	0.47
10:K:147:PRO:HG2	10:K:152:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:HA	1:B:38:THR:CG2	2.45	0.47
2:C:257:ALA:HB3	2:C:262:TYR:HE2	1.79	0.47
3:D:21:LYS:HG2	3:D:22:ILE:N	2.29	0.47
3:D:930:LEU:CD1	3:D:1244:GLN:HB3	2.42	0.47
3:D:978:ARG:O	3:D:996:LYS:HD2	2.15	0.47
3:D:1045:THR:HB	3:D:1067:ARG:NH2	2.30	0.47
4:E:72:GLN:O	4:E:76:GLU:HG3	2.15	0.47
5:F:373:ARG:HB3	5:F:373:ARG:NH1	2.30	0.47
10:L:37:GLU:OE1	10:L:39:GLU:N	2.47	0.47
3:D:331:ILE:HG13	3:D:332:LYS:H	1.80	0.47
3:D:835:LEU:O	3:D:838:ARG:N	2.47	0.47
4:E:15:ASN:HB3	4:E:18:ASP:H	1.80	0.47
10:K:63:VAL:HA	10:K:67:LEU:O	2.14	0.47
2:C:42:ASP:OD2	2:C:46:GLN:HB3	2.14	0.47
2:C:61:SER:OG	2:C:66:SER:OG	2.31	0.47
2:C:231:GLU:O	2:C:238:GLN:N	2.47	0.47
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.97	0.47
3:D:133:ARG:NH2	8:I:23:DG:OP1	2.47	0.47
3:D:264:ASP:HB3	3:D:324:LEU:HD22	1.96	0.47
3:D:708:ASN:HA	3:D:713:GLU:HA	1.96	0.47
4:E:3:ARG:HH21	4:E:52:ARG:HG2	1.79	0.47
5:F:256:PHE:HD1	5:F:259:PHE:HD2	1.63	0.47
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.97	0.47
2:C:231:GLU:HA	2:C:331:LYS:O	2.15	0.47
3:D:1120:THR:HG22	3:D:1122:ALA:N	2.30	0.47
3:D:1166:GLY:HA3	3:D:1174:ARG:NE	2.27	0.47
3:D:1264:ALA:O	3:D:1277:GLY:HA2	2.15	0.47
10:L:15:SER:OG	10:L:26:ARG:NE	2.45	0.47
1:A:182:ARG:NH1	1:A:204:GLU:OE2	2.41	0.47
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.69	0.47
2:C:1275:VAL:O	2:C:1279:GLU:HG3	2.14	0.47
3:D:15:GLU:H	3:D:15:GLU:CD	2.16	0.47
3:D:371:LYS:HZ1	3:D:371:LYS:H	1.62	0.47
5:F:226:ALA:O	5:F:230:VAL:HG22	2.14	0.47
5:F:585:GLU:HA	5:F:588:ARG:CZ	2.45	0.47
5:F:602:SER:N	5:F:605:GLU:HG2	2.23	0.47
10:L:22:SER:OG	10:L:26:ARG:NH2	2.31	0.47
1:A:164:ASP:OD2	1:A:166:ARG:HD3	2.15	0.47
2:C:465:ARG:O	2:C:469:VAL:HG13	2.15	0.47
2:C:541:GLU:N	2:C:541:GLU:OE1	2.48	0.47
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:992:LEU:HD13	2:C:996:ARG:HB2	1.97	0.47
3:D:127:LEU:HD21	3:D:234:PRO:HB3	1.97	0.47
3:D:964:LYS:O	3:D:976:THR:HG21	2.15	0.47
5:F:292:VAL:HA	5:F:297:MET:H	1.79	0.47
3:D:1000:GLY:HA3	3:D:1026:PRO:O	2.14	0.46
1:A:11:PRO:HA	1:A:30:PRO:HD2	1.97	0.46
2:C:122:VAL:HG21	2:C:493:ILE:HG21	1.97	0.46
2:C:825:GLU:OE1	2:C:827:ARG:HD2	2.15	0.46
2:C:1137:GLU:OE2	2:C:1139:ALA:HB3	2.15	0.46
3:D:909:ILE:HG13	3:D:910:ASN:N	2.29	0.46
3:D:973:LEU:HB3	3:D:1003:LEU:HD23	1.97	0.46
3:D:1107:VAL:HG13	3:D:1121:LEU:O	2.15	0.46
5:F:324:LYS:HE3	5:F:325:PRO:HD2	1.97	0.46
7:H:36:DC:H2"	7:H:37:DC:C6	2.51	0.46
10:K:140:ALA:HA	10:K:143:PHE:CE2	2.50	0.46
1:A:95:LYS:H	1:A:95:LYS:HZ3	1.62	0.46
2:C:303:ASP:OD1	2:C:328:SER:OG	2.18	0.46
2:C:1137:GLU:HG3	2:C:1140:LYS:H	1.79	0.46
3:D:646:ILE:HD12	3:D:762:ASN:HD21	1.80	0.46
3:D:1002:VAL:N	3:D:1019:ASN:O	2.49	0.46
3:D:1171:GLY:O	3:D:1172:LYS:HG3	2.16	0.46
7:H:27:DA:C6	7:H:28:DG:C6	3.04	0.46
10:K:184:LYS:HA	10:K:187:MET:HE2	1.97	0.46
10:L:73:ARG:HA	10:L:76:MET:HE2	1.97	0.46
2:C:989:LEU:O	2:C:992:LEU:HG	2.15	0.46
3:D:377:PHE:CE2	3:D:416:ILE:HD11	2.50	0.46
3:D:1289:ASN:O	3:D:1292:LEU:N	2.48	0.46
6:G:44:DT:H2"	6:G:45:DA:C5	2.51	0.46
10:K:189:ARG:O	10:K:193:ARG:HG3	2.15	0.46
10:L:201:THR:HG23	10:L:204:GLU:HG3	1.97	0.46
1:B:47:LEU:HD23	1:B:51:MET:HE3	1.97	0.46
2:C:227:LYS:HA	2:C:227:LYS:HD3	1.75	0.46
2:C:245:ARG:HG3	2:C:337:PHE:CE2	2.51	0.46
2:C:421:SER:N	2:C:424:ASP:OD2	2.48	0.46
3:D:47:ARG:HH12	6:G:30:DA:H5"	1.81	0.46
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.50	0.46
3:D:773:PHE:O	3:D:776:THR:OG1	2.33	0.46
3:D:1078:LEU:HD12	3:D:1101:LEU:HD11	1.98	0.46
3:D:1090:ILE:HG13	3:D:1097:ALA:HB2	1.98	0.46
5:F:272:SER:O	5:F:276:MET:HG2	2.15	0.46
7:H:37:DC:H2"	7:H:38:DG:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:SER:OG	2:C:479:LEU:HB3	2.15	0.46
2:C:85:CYS:HB3	2:C:90:VAL:O	2.16	0.46
3:D:169:LEU:HD23	3:D:169:LEU:HA	1.67	0.46
3:D:1035:VAL:HG13	3:D:1112:GLY:H	1.80	0.46
3:D:1184:ASP:N	3:D:1184:ASP:OD2	2.45	0.46
5:F:143:TYR:HA	5:F:146:GLU:OE1	2.16	0.46
5:F:162:ILE:HG12	5:F:165:PHE:CE2	2.51	0.46
1:B:133:LEU:HD13	1:B:138:ALA:HA	1.96	0.46
2:C:367:TYR:OH	2:C:374:GLU:OE2	2.27	0.46
2:C:439:LYS:HE3	2:C:439:LYS:HB2	1.63	0.46
3:D:759:ILE:HG23	3:D:771:GLN:HB3	1.97	0.46
3:D:1050:THR:HG23	3:D:1110:GLU:OE1	2.15	0.46
1:A:45:ARG:O	1:A:49:SER:OG	2.21	0.46
1:B:162:GLU:HG3	1:B:166:ARG:HH12	1.81	0.46
2:C:230:PHE:CE1	2:C:292:ILE:HG23	2.51	0.46
2:C:357:ASN:OD1	2:C:358:ASP:N	2.49	0.46
2:C:389:PHE:HB2	2:C:390:PHE:CE2	2.50	0.46
3:D:1072:LYS:H	3:D:1072:LYS:HD3	1.80	0.46
3:D:1081:VAL:HA	3:D:1088:VAL:N	2.27	0.46
3:D:1158:GLU:O	3:D:1206:ARG:HB2	2.16	0.46
4:E:73:GLN:HA	4:E:76:GLU:CD	2.36	0.46
5:F:437:GLN:OE1	7:H:27:DA:N6	2.49	0.46
5:F:577:GLY:O	5:F:580:PHE:N	2.49	0.46
1:B:197:ASP:O	1:B:198:LEU:HD23	2.16	0.46
2:C:161:LYS:O	2:C:163:LYS:HG2	2.15	0.46
2:C:979:LEU:HD21	2:C:1011:LEU:HD11	1.98	0.46
3:D:318:GLY:C	3:D:320:ASN:H	2.19	0.46
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.98	0.46
5:F:111:LEU:HD22	5:F:382:ALA:HB1	1.97	0.46
5:F:456:MET:O	5:F:460:ILE:HG13	2.16	0.46
7:H:37:DC:H2"	7:H:38:DG:H8	1.80	0.46
10:K:196:PHE:O	10:K:199:SER:OG	2.32	0.46
1:A:145:LYS:HD3	1:A:147:GLN:HE21	1.80	0.46
2:C:189:ASP:OD1	2:C:193:ASN:N	2.37	0.46
2:C:564:PRO:HD2	2:C:572:ILE:HB	1.97	0.46
3:D:278:ARG:HH12	5:F:446:GLN:HE22	1.64	0.46
3:D:951:GLN:HB3	3:D:1014:GLY:HA2	1.98	0.46
5:F:279:ARG:NH2	5:F:347:ILE:HG12	2.31	0.46
5:F:358:VAL:O	5:F:362:ASN:ND2	2.49	0.46
10:K:64:ASP:C	10:K:66:GLU:H	2.18	0.46
10:L:15:SER:O	10:L:40:HIS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:HG3	1:B:231:PHE:O	2.15	0.45
2:C:813:GLU:O	2:C:815:SER:N	2.49	0.45
3:D:233:LYS:HB2	3:D:236:TRP:CE2	2.51	0.45
3:D:418:GLU:O	3:D:481:ARG:NH2	2.49	0.45
3:D:930:LEU:HA	3:D:930:LEU:HD23	1.75	0.45
3:D:1176:VAL:HA	3:D:1187:GLU:HA	1.97	0.45
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.71	0.45
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.52	0.45
2:C:733:VAL:HG22	2:C:750:ILE:HG12	1.98	0.45
2:C:996:ARG:HH11	2:C:996:ARG:HA	1.81	0.45
3:D:147:ILE:HD11	3:D:179:LYS:HG2	1.98	0.45
3:D:980:THR:HG1	3:D:997:VAL:H	1.64	0.45
3:D:1279:GLN:N	3:D:1279:GLN:OE1	2.48	0.45
3:D:1287:ILE:HD11	3:D:1300:ALA:CB	2.43	0.45
5:F:232:ARG:O	5:F:235:ILE:HG13	2.17	0.45
5:F:359:LYS:HA	5:F:362:ASN:HD21	1.80	0.45
1:B:23:HIS:HD2	1:B:24:ALA:N	2.14	0.45
1:B:104:LYS:NZ	1:B:114:ASP:OD2	2.30	0.45
2:C:281:ASP:OD1	2:C:281:ASP:N	2.49	0.45
3:D:77:ARG:HD2	3:D:77:ARG:HA	1.67	0.45
3:D:1029:THR:HG22	3:D:1099:TYR:HE2	1.81	0.45
5:F:140:ALA:HB1	5:F:256:PHE:HE2	1.81	0.45
5:F:300:LYS:HB3	5:F:300:LYS:HE3	1.66	0.45
6:G:32:DA:H1'	6:G:33:DT:H5'	1.98	0.45
1:B:205:MET:HE3	1:B:205:MET:HB3	1.69	0.45
2:C:99:LYS:HG2	2:C:121:GLU:HG2	1.99	0.45
2:C:221:LEU:HD13	2:C:336:LEU:HD11	1.98	0.45
2:C:996:ARG:HA	2:C:996:ARG:NH1	2.30	0.45
3:D:362:ARG:H	3:D:365:GLN:HE21	1.64	0.45
3:D:749:LYS:NZ	3:D:753:SER:OG	2.33	0.45
3:D:825:VAL:CG1	3:D:833:GLU:HB2	2.47	0.45
3:D:980:THR:O	3:D:996:LYS:HA	2.16	0.45
3:D:1266:ILE:HD11	3:D:1276:GLU:H	1.81	0.45
5:F:607:LEU:HD22	5:F:610:PHE:CD2	2.51	0.45
8:I:16:DC:H42	9:J:12:DG:H1	1.63	0.45
10:K:168:LEU:HD22	10:K:173:ILE:HB	1.98	0.45
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.99	0.45
1:B:114:ASP:N	1:B:114:ASP:OD1	2.50	0.45
2:C:158:ASP:OD1	2:C:159:SER:N	2.44	0.45
2:C:964:LEU:HD11	2:C:1021:LEU:HD13	1.99	0.45
3:D:614:LEU:HD12	3:D:614:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:986:ASP:CG	3:D:988:PHE:H	2.20	0.45
3:D:1023:HIS:C	3:D:1125:PRO:HA	2.36	0.45
3:D:1276:GLU:HB3	3:D:1278:GLU:OE2	2.16	0.45
5:F:304:THR:O	5:F:305:LEU:HD13	2.17	0.45
10:L:202:GLU:HA	10:L:205:ARG:HH11	1.82	0.45
1:A:9:LEU:HA	1:A:9:LEU:HD23	1.74	0.45
3:D:82:GLY:O	10:L:82:ARG:NH1	2.50	0.45
3:D:91:GLU:OE2	3:D:101:ARG:NH2	2.41	0.45
3:D:1040:MET:SD	3:D:1078:LEU:HG	2.56	0.45
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.51	0.45
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.81	0.45
3:D:576:ARG:HD3	3:D:593:ASN:HA	1.97	0.45
3:D:1021:ASP:HB2	3:D:1024:THR:CB	2.47	0.45
3:D:1327:GLU:HG3	3:D:1330:ARG:HB3	1.99	0.45
10:L:21:TYR:HE1	10:L:111:TYR:HD2	1.63	0.45
2:C:813:GLU:HB2	3:D:461:PHE:CD2	2.42	0.45
3:D:678:ARG:NH2	3:D:679:TYR:HB2	2.32	0.45
10:L:32:LYS:NZ	10:L:86:PRO:O	2.36	0.45
1:A:33:ARG:CZ	1:A:197:ASP:HB2	2.46	0.45
1:A:193:GLU:OE2	1:A:193:GLU:N	2.50	0.45
2:C:30:ILE:HG23	2:C:31:GLN:H	1.82	0.45
2:C:75:LEU:HD12	2:C:94:ALA:HB3	1.98	0.45
2:C:119:GLU:O	2:C:121:GLU:N	2.47	0.45
2:C:236:LYS:HA	2:C:236:LYS:HD3	1.60	0.45
2:C:489:PRO:HA	2:C:492:MET:HE2	1.99	0.45
3:D:1257:VAL:O	3:D:1260:MET:N	2.50	0.45
5:F:261:LEU:HG	5:F:262:VAL:O	2.16	0.45
6:G:18:DT:H1'	6:G:19:DC:C6	2.52	0.45
10:L:11:MET:O	10:L:11:MET:HG2	2.16	0.45
1:A:125:LYS:HE3	1:A:127:GLN:NE2	2.32	0.45
2:C:270:THR:H	2:C:273:HIS:CG	2.35	0.45
2:C:347:ILE:O	2:C:350:THR:OG1	2.33	0.45
2:C:656:SER:OG	2:C:657:THR:N	2.49	0.45
2:C:1161:LEU:HD23	2:C:1161:LEU:C	2.36	0.45
2:C:1164:PHE:O	2:C:1166:ASP:N	2.50	0.45
3:D:45:ASN:C	3:D:47:ARG:H	2.20	0.45
3:D:958:ILE:HD13	3:D:958:ILE:HA	1.78	0.45
5:F:511:ILE:HA	5:F:511:ILE:HD12	1.61	0.45
6:G:29:DT:H2''	6:G:30:DA:C8	2.52	0.45
10:K:111:TYR:CD1	10:K:164:LEU:HD12	2.52	0.45
1:B:67:GLU:N	1:B:67:GLU:OE1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.99	0.44
2:C:759:SER:OG	2:C:761:GLN:N	2.50	0.44
2:C:1014:LEU:HA	2:C:1017:GLN:HB2	1.99	0.44
2:C:1151:LEU:HD21	2:C:1198:LEU:HA	1.98	0.44
2:C:1184:THR:HG23	2:C:1189:GLY:HA2	1.99	0.44
3:D:860:ARG:HG2	3:D:861:ASN:H	1.81	0.44
3:D:1192:LYS:HE3	3:D:1192:LYS:HB2	1.84	0.44
5:F:607:LEU:HD13	5:F:610:PHE:CB	2.47	0.44
10:K:104:HIS:HD2	10:K:105:ARG:HG3	1.82	0.44
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.47	0.44
2:C:1212:LEU:HD23	2:C:1212:LEU:HA	1.76	0.44
3:D:805:GLN:HE21	3:D:805:GLN:HB3	1.52	0.44
3:D:1018:ALA:HB3	3:D:1020:TRP:HZ3	1.81	0.44
5:F:601:PRO:HA	5:F:605:GLU:OE2	2.17	0.44
10:K:126:ASP:HA	10:K:129:ARG:HB3	1.98	0.44
10:K:132:LEU:O	10:K:136:LEU:HG	2.16	0.44
1:A:235:ARG:O	1:A:235:ARG:HG3	2.17	0.44
1:B:75:GLN:HG3	1:B:76:GLU:N	2.32	0.44
2:C:881:ASP:N	2:C:881:ASP:OD1	2.50	0.44
5:F:573:LEU:H	5:F:573:LEU:HG	1.52	0.44
9:J:8:DG:C2'	9:J:9:DT:H71	2.47	0.44
2:C:358:ASP:OD1	2:C:361:SER:N	2.28	0.44
2:C:1271:GLY:HA2	3:D:344:GLY:HA2	1.98	0.44
3:D:262:THR:O	5:F:507:MET:N	2.44	0.44
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.86	0.44
3:D:963:VAL:O	3:D:964:LYS:NZ	2.29	0.44
3:D:1169:THR:C	3:D:1171:GLY:H	2.20	0.44
3:D:1356:LEU:HA	3:D:1356:LEU:HD23	1.67	0.44
7:H:36:DC:H2''	7:H:37:DC:C5	2.52	0.44
7:H:38:DG:N2	7:H:39:DC:C2	2.86	0.44
8:I:23:DG:H2''	8:I:24:DG:C8	2.52	0.44
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.98	0.44
2:C:17:LYS:N	2:C:1188:ASP:OD2	2.50	0.44
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.41	0.44
2:C:996:ARG:HA	2:C:996:ARG:HD2	1.71	0.44
2:C:1028:LYS:HB3	2:C:1028:LYS:HE2	1.74	0.44
3:D:224:LEU:HD23	3:D:224:LEU:HA	1.79	0.44
3:D:1103:GLY:O	3:D:1124:ILE:HG12	2.18	0.44
3:D:1226:VAL:O	3:D:1229:VAL:HG12	2.17	0.44
10:L:28:VAL:O	10:L:31:GLU:N	2.51	0.44
1:B:194:GLN:HG3	1:B:195:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:SER:O	2:C:33:ASP:HB2	2.18	0.44
2:C:233:ARG:H	2:C:238:GLN:CD	2.18	0.44
2:C:577:VAL:HG23	2:C:661:VAL:O	2.16	0.44
3:D:39:LYS:N	3:D:54:ASP:OD2	2.51	0.44
3:D:205:LEU:HD23	3:D:217:LEU:CB	2.48	0.44
3:D:572:THR:OG1	3:D:573:THR:N	2.49	0.44
3:D:869:CYS:SG	3:D:870:ASP:N	2.91	0.44
3:D:931:THR:O	3:D:1137:GLY:HA2	2.17	0.44
5:F:109:GLU:CD	5:F:109:GLU:H	2.21	0.44
5:F:110:LEU:HD12	5:F:110:LEU:H	1.83	0.44
10:K:15:SER:HB3	10:K:38:ILE:HD11	1.99	0.44
10:K:32:LYS:HE2	10:K:88:LEU:HD12	2.00	0.44
1:A:191:ARG:NH1	1:A:195:ARG:O	2.51	0.44
2:C:742:TYR:HB3	2:C:743:PRO:HD2	1.99	0.44
2:C:1080:ASN:HD22	2:C:1085:MET:HE2	1.83	0.44
2:C:1161:LEU:O	2:C:1161:LEU:CG	2.66	0.44
2:C:1276:TRP:CZ2	3:D:801:VAL:HG11	2.52	0.44
3:D:876:SER:HA	3:D:990:ARG:HH21	1.82	0.44
3:D:1011:VAL:HG12	3:D:1012:ALA:O	2.18	0.44
5:F:575:GLU:H	5:F:575:GLU:CD	2.19	0.44
5:F:608:ARG:O	5:F:611:LEU:HD12	2.17	0.44
10:K:23:HIS:HB2	10:K:167:ARG:HH22	1.83	0.44
1:A:58:GLU:HG2	1:A:145:LYS:HB3	1.99	0.44
1:B:50:SER:O	1:B:50:SER:OG	2.27	0.44
1:B:215:GLU:OE2	1:B:219:ARG:NH2	2.51	0.44
2:C:119:GLU:OE1	2:C:489:PRO:HD2	2.17	0.44
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.32	0.44
2:C:275:ARG:HA	2:C:278:GLU:OE2	2.16	0.44
3:D:857:LEU:HD12	3:D:871:LEU:CD2	2.48	0.44
1:B:13:LEU:O	1:B:13:LEU:HD23	2.18	0.44
2:C:246:LEU:HA	2:C:249:GLU:OE2	2.17	0.44
2:C:975:ILE:HG12	2:C:1014:LEU:HD23	1.99	0.44
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.18	0.44
3:D:1009:GLU:CD	3:D:1009:GLU:H	2.22	0.44
3:D:1064:SER:OG	3:D:1193:TRP:O	2.30	0.44
3:D:1150:PRO:O	3:D:1152:GLU:N	2.51	0.44
5:F:164:GLY:C	5:F:260:ARG:HH21	2.22	0.44
5:F:256:PHE:HD1	5:F:259:PHE:CD2	2.36	0.44
2:C:139:ASN:HD22	2:C:139:ASN:HA	1.62	0.43
2:C:466:VAL:O	2:C:469:VAL:HG22	2.18	0.43
2:C:542:ARG:HG2	8:I:15:DT:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:902:ASP:OD1	3:D:903:LEU:N	2.51	0.43
3:D:1276:GLU:CD	3:D:1277:GLY:H	2.21	0.43
7:H:48:DC:C2	7:H:49:DA:C8	3.06	0.43
10:K:16:GLY:H	10:K:22:SER:HB3	1.82	0.43
10:K:58:SER:O	10:K:61:THR:OG1	2.28	0.43
1:B:208:ASN:O	1:B:210:THR:N	2.45	0.43
2:C:19:PRO:HA	2:C:1156:ARG:HE	1.82	0.43
3:D:1162:ILE:HG13	3:D:1163:VAL:N	2.33	0.43
3:D:1332:LEU:HD23	3:D:1332:LEU:HA	1.82	0.43
5:F:231:THR:HG22	5:F:248:GLU:HB3	2.00	0.43
5:F:292:VAL:HG23	5:F:293:GLU:OE2	2.18	0.43
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.73	0.43
2:C:302:ILE:HG22	2:C:309:LEU:HA	2.00	0.43
2:C:633:LEU:HD23	2:C:633:LEU:H	1.83	0.43
3:D:704:GLU:O	3:D:706:VAL:N	2.50	0.43
3:D:1266:ILE:HD12	3:D:1274:PHE:H	1.83	0.43
5:F:429:THR:HA	6:G:40:DT:H72	2.01	0.43
3:D:478:LEU:HD23	3:D:478:LEU:HA	1.80	0.43
3:D:1098:GLN:HG2	3:D:1100:PHE:CE2	2.53	0.43
10:K:106:ILE:HD11	10:K:149:PHE:HE2	1.82	0.43
10:L:163:PRO:O	10:L:167:ARG:HD2	2.18	0.43
10:L:165:LEU:HD13	10:L:187:MET:HG2	2.00	0.43
1:B:23:HIS:CD2	1:B:206:GLU:HG2	2.53	0.43
1:B:96:ASP:HA	1:B:148:ARG:HD2	1.99	0.43
1:B:133:LEU:HD22	1:B:138:ALA:HA	1.99	0.43
1:B:162:GLU:HG3	1:B:166:ARG:NH2	2.34	0.43
2:C:27:LEU:HD13	2:C:663:VAL:HG11	2.00	0.43
2:C:557:ARG:NH2	2:C:611:GLU:OE1	2.41	0.43
2:C:1113:LEU:HG	3:D:641:ILE:HD13	2.00	0.43
3:D:332:LYS:HG2	3:D:333:GLY:N	2.30	0.43
3:D:968:ASN:HD21	3:D:972:LYS:HZ3	1.67	0.43
3:D:978:ARG:NE	3:D:999:TYR:HB3	2.30	0.43
3:D:1205:GLU:OE2	3:D:1206:ARG:N	2.52	0.43
3:D:1283:SER:HA	3:D:1286:LYS:HD2	1.99	0.43
4:E:38:LEU:HB3	4:E:58:LEU:HD23	2.00	0.43
1:A:45:ARG:NH2	1:B:34:GLY:O	2.47	0.43
1:B:103:ASN:OD1	1:B:141:SER:HB2	2.18	0.43
1:B:168:ILE:HD12	1:B:168:ILE:HA	1.89	0.43
2:C:468:LEU:HA	2:C:468:LEU:HD23	1.58	0.43
3:D:511:TYR:OH	3:D:727:ASP:OD2	2.21	0.43
3:D:536:LEU:HA	3:D:536:LEU:HD23	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:902:ASP:HB3	3:D:1251:LYS:HE3	1.99	0.43
3:D:1028:ILE:HD13	3:D:1120:THR:HG23	2.00	0.43
3:D:1191:PRO:HB3	3:D:1193:TRP:CZ3	2.54	0.43
5:F:114:GLU:OE2	5:F:115:GLY:N	2.51	0.43
10:K:46:PRO:HB2	10:K:50:LEU:HD22	2.00	0.43
10:L:168:LEU:HB2	10:L:169:PRO:HD3	2.01	0.43
1:A:33:ARG:HA	1:A:33:ARG:NE	2.33	0.43
2:C:964:LEU:HD12	2:C:964:LEU:HA	1.56	0.43
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	2.01	0.43
2:C:1164:PHE:HD2	2:C:1166:ASP:H	1.66	0.43
3:D:203:GLU:OE2	3:D:204:GLU:HG3	2.18	0.43
3:D:997:VAL:HG22	3:D:998:PRO:HD2	2.01	0.43
3:D:1025:MET:O	3:D:1124:ILE:HB	2.18	0.43
1:B:67:GLU:H	1:B:67:GLU:CD	2.19	0.43
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.00	0.43
3:D:113:HIS:HD1	3:D:115:TRP:H	1.67	0.43
3:D:368:LEU:HD12	3:D:368:LEU:HA	1.89	0.43
3:D:518:VAL:HB	3:D:716:GLN:OE1	2.19	0.43
3:D:826:ILE:HG13	3:D:831:VAL:HG12	2.00	0.43
3:D:849:LEU:HD12	3:D:856:ILE:HG12	2.01	0.43
3:D:1027:VAL:HB	3:D:1101:LEU:HD22	2.01	0.43
3:D:1049:GLN:OE1	3:D:1058:SER:HB3	2.19	0.43
5:F:141:ILE:HD12	5:F:141:ILE:HA	1.83	0.43
5:F:246:GLN:OE1	5:F:246:GLN:N	2.36	0.43
5:F:324:LYS:HG3	5:F:326:TRP:CH2	2.54	0.43
5:F:330:LEU:O	5:F:334:SER:HB3	2.18	0.43
5:F:479:THR:O	5:F:482:GLU:N	2.51	0.43
5:F:557:LYS:HE2	5:F:557:LYS:HB2	1.56	0.43
10:K:79:LEU:HD23	10:K:79:LEU:HA	1.80	0.43
1:B:192:VAL:C	1:B:194:GLN:H	2.22	0.43
2:C:235:ASN:O	2:C:238:GLN:NE2	2.51	0.43
2:C:688:GLN:HE22	2:C:1237:HIS:HE1	1.66	0.43
2:C:781:ASP:OD2	2:C:782:VAL:N	2.52	0.43
3:D:1034:PHE:CE1	3:D:1114:GLN:HB2	2.53	0.43
5:F:324:LYS:HG3	5:F:326:TRP:CZ2	2.53	0.43
5:F:385:ARG:NE	6:G:42:DT:H5'	2.34	0.43
10:K:165:LEU:HD21	10:K:187:MET:HG3	2.00	0.43
10:L:15:SER:N	10:L:39:GLU:O	2.52	0.43
2:C:74:ARG:HH22	2:C:97:ARG:HG2	1.83	0.43
2:C:372:PRO:O	5:F:94:THR:HG21	2.19	0.43
3:D:221:ILE:HD12	3:D:221:ILE:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:395:LYS:HA	3:D:395:LYS:HD2	1.81	0.43
3:D:1035:VAL:HG12	3:D:1113:VAL:H	1.83	0.43
3:D:1095:MET:SD	3:D:1096:PRO:HD2	2.59	0.43
3:D:1287:ILE:CD1	3:D:1300:ALA:CB	2.97	0.43
7:H:49:DA:C2	7:H:50:DA:C4	3.07	0.43
10:K:24:GLN:NE2	10:K:160:TYR:HA	2.34	0.43
10:K:131:GLN:HA	10:K:134:GLU:OE1	2.19	0.43
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.37	0.42
2:C:892:GLU:O	2:C:892:GLU:HG2	2.19	0.42
3:D:53:ARG:O	3:D:54:ASP:HB3	2.18	0.42
3:D:161:THR:HG22	3:D:164:GLN:OE1	2.18	0.42
3:D:393:THR:OG1	3:D:394:ILE:N	2.52	0.42
3:D:490:ILE:HD11	3:D:609:TYR:CD1	2.54	0.42
3:D:663:GLU:O	3:D:666:GLU:HG3	2.19	0.42
3:D:1065:ALA:HB2	3:D:1193:TRP:HB3	2.01	0.42
5:F:105:MET:HE1	5:F:385:ARG:HA	2.01	0.42
1:B:34:GLY:N	1:B:199:ASP:OD2	2.49	0.42
2:C:114:VAL:HG13	2:C:115:LYS:HD2	2.01	0.42
2:C:223:LEU:HA	2:C:223:LEU:HD12	1.71	0.42
2:C:243:PRO:HA	2:C:246:LEU:HD12	2.01	0.42
2:C:820:GLU:HB2	2:C:1080:ASN:O	2.20	0.42
2:C:1058:ARG:HD3	2:C:1238:LEU:HD23	2.01	0.42
3:D:57:PHE:HB3	3:D:98:ARG:NH2	2.34	0.42
3:D:88:CYS:C	3:D:90:VAL:H	2.23	0.42
3:D:744:ARG:HG3	3:D:759:ILE:HB	2.00	0.42
3:D:968:ASN:HD21	3:D:972:LYS:NZ	2.17	0.42
5:F:98:VAL:O	5:F:102:MET:HG2	2.18	0.42
5:F:216:LEU:O	5:F:220:LYS:HB2	2.19	0.42
5:F:596:ARG:O	5:F:599:ARG:N	2.52	0.42
5:F:607:LEU:HA	5:F:610:PHE:CB	2.38	0.42
10:L:18:THR:O	10:L:167:ARG:NH2	2.29	0.42
10:L:115:ASN:O	10:L:119:ASN:CB	2.68	0.42
10:L:117:ILE:HG21	10:L:171:LEU:HD22	1.99	0.42
3:D:74:LYS:HD3	3:D:75:TYR:CE2	2.54	0.42
3:D:750:PRO:HD3	3:D:777:HIS:CD2	2.55	0.42
3:D:927:GLY:C	3:D:929:GLN:H	2.22	0.42
3:D:1101:LEU:H	3:D:1101:LEU:HG	1.62	0.42
5:F:268:TYR:CD2	5:F:269:LEU:HD22	2.51	0.42
10:K:71:GLU:HG2	10:L:104:HIS:NE2	2.34	0.42
1:A:102:LEU:HD21	1:A:114:ASP:HB2	2.01	0.42
1:B:107:ILE:CD1	1:B:136:GLU:H	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.53	0.42
2:C:916:SER:O	2:C:916:SER:OG	2.35	0.42
2:C:968:GLU:OE1	2:C:971:LEU:HD23	2.19	0.42
2:C:976:ARG:HA	2:C:979:LEU:HB2	2.01	0.42
2:C:985:GLU:HB2	2:C:989:LEU:HB2	2.01	0.42
2:C:1164:PHE:CD2	2:C:1164:PHE:C	2.92	0.42
3:D:161:THR:OG1	3:D:162:GLU:N	2.52	0.42
3:D:225:GLU:O	3:D:229:GLN:HG2	2.20	0.42
3:D:318:GLY:O	3:D:320:ASN:N	2.51	0.42
3:D:534:GLU:HA	3:D:578:ILE:HD11	2.01	0.42
3:D:744:ARG:HE	3:D:744:ARG:HB2	1.43	0.42
3:D:1105:ALA:HA	3:D:1123:ARG:O	2.19	0.42
5:F:530:LEU:HD12	5:F:530:LEU:H	1.84	0.42
7:H:50:DA:C2	7:H:51:DG:C5	3.07	0.42
1:B:185:TYR:HA	1:B:202:VAL:O	2.20	0.42
2:C:124:MET:HB2	2:C:498:ILE:HD12	2.01	0.42
2:C:197:ARG:HH21	2:C:203:LYS:HB2	1.84	0.42
2:C:346:TYR:OH	2:C:436:ARG:NH1	2.53	0.42
3:D:97:VAL:C	3:D:99:ARG:H	2.21	0.42
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.02	0.42
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.45	0.42
5:F:149:ASP:OD2	5:F:225:ARG:NH1	2.53	0.42
5:F:297:MET:HG2	5:F:301:ASN:OD1	2.19	0.42
5:F:324:LYS:HB2	5:F:327:SER:HB3	2.01	0.42
5:F:344:LEU:HA	5:F:344:LEU:HD12	1.82	0.42
6:G:20:DC:H2''	6:G:21:DA:N7	2.34	0.42
10:L:12:THR:HA	10:L:37:GLU:HB3	2.02	0.42
2:C:1062:PRO:HA	2:C:1076:ILE:HG12	2.02	0.42
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.34	0.42
3:D:123:ARG:HA	3:D:123:ARG:HD3	1.67	0.42
3:D:585:LYS:O	3:D:587:LEU:N	2.53	0.42
3:D:647:PRO:HG2	3:D:650:LYS:HB2	2.00	0.42
5:F:373:ARG:HB3	5:F:373:ARG:CZ	2.50	0.42
6:G:20:DC:C2	7:H:44:DG:N2	2.87	0.42
9:J:10:DC:N3	9:J:11:DA:N6	2.68	0.42
10:L:155:SER:OG	10:L:157:VAL:HG22	2.20	0.42
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.82	0.42
2:C:185:ASP:OD1	2:C:185:ASP:N	2.52	0.42
2:C:192:ASP:HB3	2:C:346:TYR:HD1	1.84	0.42
2:C:198:ILE:HD13	2:C:388:LEU:HD21	2.01	0.42
2:C:1279:GLU:HG2	3:D:1357:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:147:ILE:HG13	3:D:177:ASP:HB3	2.02	0.42
3:D:222:LYS:HE2	3:D:1276:GLU:HG2	2.02	0.42
3:D:1196:LEU:HD12	3:D:1210:ILE:HG22	2.01	0.42
5:F:231:THR:HA	5:F:248:GLU:OE1	2.19	0.42
6:G:24:DG:N1	7:H:40:DA:C2	2.87	0.42
10:K:62:LEU:O	10:K:68:THR:HA	2.20	0.42
2:C:17:LYS:HB3	2:C:1154:ASP:OD1	2.20	0.42
2:C:38:PHE:CD2	2:C:39:ILE:HG23	2.55	0.42
2:C:347:ILE:HD13	2:C:347:ILE:HA	1.80	0.42
2:C:1326:LEU:O	2:C:1330:ILE:HG12	2.20	0.42
3:D:24:LEU:HD21	3:D:237:MET:HG2	2.02	0.42
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.34	0.42
5:F:354:THR:N	5:F:357:GLN:OE1	2.31	0.42
10:L:32:LYS:HD3	10:L:32:LYS:HA	1.84	0.42
10:L:41:VAL:HG12	10:L:47:PRO:HD3	2.01	0.42
1:A:10:LYS:HE3	1:B:226:GLU:HB3	2.02	0.42
1:B:77:ASP:O	1:B:81:ILE:HG13	2.20	0.42
1:B:83:LEU:HD12	1:B:83:LEU:HA	1.65	0.42
1:B:151:GLY:O	1:B:177:TYR:HB2	2.20	0.42
2:C:56:VAL:HG13	2:C:57:PHE:CD2	2.54	0.42
2:C:805:MET:HE2	2:C:805:MET:HB2	1.77	0.42
3:D:363:LEU:HA	3:D:363:LEU:HD12	1.83	0.42
3:D:981:GLU:HG3	3:D:983:LYS:HG3	2.02	0.42
3:D:1005:LYS:HE3	3:D:1011:VAL:HG22	2.02	0.42
3:D:1216:ALA:HB3	3:D:1219:ASP:OD1	2.20	0.42
3:D:1368:ASP:HA	3:D:1371:ARG:NH1	2.35	0.42
5:F:341:LEU:O	5:F:345:GLN:HG3	2.20	0.42
5:F:554:ARG:O	5:F:558:VAL:HG12	2.19	0.42
1:A:127:GLN:OE1	1:A:127:GLN:N	2.44	0.42
1:A:236:ASP:N	1:A:236:ASP:OD1	2.52	0.42
1:B:20:SER:OG	1:B:23:HIS:HB3	2.19	0.42
2:C:902:LEU:HA	2:C:902:LEU:HD23	1.81	0.42
2:C:1073:LYS:HB2	2:C:1073:LYS:HE3	1.72	0.42
2:C:1099:ASN:OD1	2:C:1100:PRO:HD2	2.20	0.42
3:D:235:GLU:OE1	3:D:235:GLU:N	2.42	0.42
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.77	0.42
3:D:416:ILE:HG13	3:D:441:LEU:HD21	2.01	0.42
5:F:596:ARG:HA	5:F:599:ARG:NH1	2.35	0.42
10:K:11:MET:HA	10:K:63:VAL:O	2.19	0.42
2:C:101:ARG:HD3	2:C:118:LYS:NZ	2.34	0.41
2:C:230:PHE:CZ	2:C:292:ILE:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:LYS:HE3	2:C:404:LYS:HB3	1.75	0.41
3:D:388:ARG:HH21	3:D:414:GLU:HG2	1.85	0.41
3:D:816:THR:O	3:D:860:ARG:NH2	2.53	0.41
3:D:1072:LYS:HG2	3:D:1073:ASP:N	2.35	0.41
5:F:354:THR:O	5:F:357:GLN:N	2.52	0.41
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.75	0.41
10:K:151:SER:OG	10:K:153:GLU:O	2.28	0.41
10:K:156:LEU:HD23	10:K:156:LEU:HA	1.77	0.41
10:K:186:TYR:O	10:K:190:VAL:HG12	2.20	0.41
1:B:157:THR:O	1:B:161:SER:OG	2.18	0.41
2:C:255:ILE:H	2:C:255:ILE:HG13	1.73	0.41
2:C:895:LEU:H	2:C:895:LEU:HG	1.55	0.41
3:D:929:GLN:OE1	3:D:930:LEU:HB2	2.20	0.41
5:F:355:ILE:HA	5:F:355:ILE:HD13	1.81	0.41
5:F:462:LYS:HB2	5:F:462:LYS:HE3	1.78	0.41
5:F:474:MET:HE1	5:F:476:ARG:HH11	1.84	0.41
10:K:126:ASP:OD1	10:K:126:ASP:N	2.52	0.41
2:C:207:THR:OG1	2:C:354:ASP:OD2	2.34	0.41
3:D:219:LYS:HE3	3:D:219:LYS:HB2	1.83	0.41
5:F:121:LYS:HE2	5:F:121:LYS:HB2	1.86	0.41
5:F:359:LYS:HA	5:F:362:ASN:ND2	2.35	0.41
5:F:429:THR:HA	6:G:40:DT:C7	2.51	0.41
10:L:101:LEU:HD12	10:L:101:LEU:HA	1.72	0.41
1:A:12:ARG:H	1:A:30:PRO:HD2	1.85	0.41
1:B:207:THR:HG21	1:B:211:ILE:O	2.21	0.41
2:C:102:LEU:O	2:C:116:ASP:HA	2.19	0.41
2:C:237:LEU:HD23	2:C:237:LEU:HA	1.71	0.41
2:C:288:PRO:HB2	2:C:290:GLU:OE1	2.20	0.41
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.56	0.41
3:D:596:LEU:HA	3:D:596:LEU:HD12	1.86	0.41
5:F:261:LEU:HD21	5:F:266:PHE:HB2	2.02	0.41
5:F:560:ARG:HG2	5:F:565:ILE:HB	2.03	0.41
2:C:270:THR:O	2:C:273:HIS:HB2	2.21	0.41
2:C:490:GLN:CG	5:F:472:GLN:HE22	2.33	0.41
3:D:544:LEU:HD12	3:D:544:LEU:HA	1.89	0.41
3:D:1179:PRO:CG	3:D:1184:ASP:HA	2.51	0.41
5:F:216:LEU:HA	5:F:219:GLU:HG2	2.02	0.41
5:F:604:SER:O	5:F:606:VAL:N	2.53	0.41
6:G:31:DA:H2''	6:G:32:DA:H8	1.85	0.41
6:G:38:DC:H6	6:G:38:DC:H5'	1.86	0.41
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:TYR:CD2	2:C:435:ILE:HG22	2.55	0.41
2:C:755:LYS:HA	2:C:755:LYS:HD2	1.82	0.41
2:C:813:GLU:C	2:C:815:SER:H	2.24	0.41
2:C:1292:THR:HG22	2:C:1293:VAL:N	2.34	0.41
2:C:1340:GLU:O	3:D:17:PHE:HB2	2.20	0.41
3:D:179:LYS:HB2	3:D:184:ALA:HB2	2.02	0.41
3:D:694:SER:O	3:D:697:MET:HG3	2.21	0.41
1:A:218:ARG:NH1	1:B:231:PHE:O	2.54	0.41
2:C:976:ARG:O	2:C:980:VAL:HG13	2.19	0.41
3:D:770:LEU:HD23	3:D:770:LEU:HA	1.81	0.41
3:D:868:TRP:HA	3:D:868:TRP:HE3	1.85	0.41
3:D:876:SER:HA	3:D:990:ARG:NH2	2.36	0.41
5:F:348:GLU:HG2	5:F:353:LEU:O	2.20	0.41
5:F:390:ILE:HD11	5:F:432:THR:HG23	2.02	0.41
1:A:45:ARG:NH2	1:B:37:HIS:HB2	2.36	0.41
1:A:191:ARG:HH22	1:A:197:ASP:HA	1.86	0.41
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.56	0.41
2:C:318:SER:O	2:C:321:LEU:N	2.54	0.41
2:C:849:GLU:O	2:C:886:LYS:HG3	2.20	0.41
3:D:166:LEU:O	3:D:170:GLU:HG2	2.21	0.41
3:D:346:ARG:HD3	3:D:346:ARG:HA	1.95	0.41
3:D:642:ASP:N	3:D:642:ASP:OD1	2.53	0.41
5:F:102:MET:HE2	5:F:102:MET:HB3	1.87	0.41
5:F:377:LYS:NZ	5:F:377:LYS:HB3	2.36	0.41
5:F:477:GLU:CD	5:F:478:PRO:HD2	2.41	0.41
10:K:104:HIS:ND1	10:L:71:GLU:OE1	2.53	0.41
10:K:129:ARG:HG3	10:K:173:ILE:HG12	2.02	0.41
1:A:23:HIS:NE2	1:A:204:GLU:HG3	2.36	0.41
2:C:107:ARG:O	2:C:108:GLU:HB2	2.21	0.41
2:C:207:THR:HG21	2:C:351:LEU:HG	2.03	0.41
2:C:232:ILE:HG12	2:C:237:LEU:HD23	2.02	0.41
2:C:341:LEU:HD23	2:C:342:ASP:N	2.36	0.41
2:C:414:ILE:HD13	2:C:414:ILE:HA	1.83	0.41
2:C:582:ASN:HB2	2:C:586:PHE:O	2.21	0.41
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.55	0.41
2:C:730:SER:O	2:C:730:SER:OG	2.34	0.41
2:C:1256:GLN:O	2:C:1301:ARG:NH2	2.54	0.41
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.56	0.41
3:D:371:LYS:HE2	3:D:371:LYS:HB2	1.88	0.41
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.56	0.41
3:D:566:LYS:HE2	3:D:566:LYS:HB3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:835:LEU:HD12	3:D:835:LEU:HA	1.79	0.41
3:D:1023:HIS:O	3:D:1125:PRO:HA	2.21	0.41
5:F:124:GLU:HA	5:F:127:ILE:HG22	2.03	0.41
5:F:296:LYS:HD3	5:F:296:LYS:HA	1.67	0.41
10:L:110:TRP:CD1	10:L:110:TRP:N	2.86	0.41
1:B:20:SER:O	1:B:23:HIS:N	2.53	0.41
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.68	0.41
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.77	0.41
2:C:933:VAL:HG13	2:C:1050:VAL:HG22	2.03	0.41
2:C:985:GLU:O	2:C:989:LEU:HB3	2.22	0.41
2:C:1103:VAL:HG21	2:C:1112:ILE:HD11	2.03	0.41
2:C:1113:LEU:HA	2:C:1113:LEU:HD23	1.85	0.41
2:C:1308:ILE:HD13	2:C:1308:ILE:HA	1.85	0.41
5:F:228:TYR:OH	5:F:232:ARG:NH1	2.54	0.41
5:F:272:SER:HA	5:F:275:VAL:HG12	2.03	0.41
5:F:300:LYS:O	5:F:304:THR:HG22	2.21	0.41
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.56	0.40
1:B:162:GLU:HG3	1:B:166:ARG:NH1	2.36	0.40
3:D:174:ASP:CG	3:D:175:GLU:H	2.24	0.40
3:D:543:SER:OG	3:D:544:LEU:N	2.54	0.40
3:D:865:HIS:CE1	3:D:868:TRP:CD1	3.09	0.40
3:D:901:ARG:O	3:D:903:LEU:HD12	2.21	0.40
3:D:1098:GLN:HG2	3:D:1100:PHE:HE2	1.86	0.40
3:D:1281:GLU:HG2	3:D:1282:TYR:N	2.36	0.40
6:G:15:DG:H2''	6:G:16:DC:H6	1.83	0.40
2:C:68:LEU:HD12	2:C:101:ARG:O	2.21	0.40
3:D:312:ARG:O	3:D:314:ARG:HG3	2.22	0.40
3:D:317:THR:OG1	3:D:318:GLY:N	2.54	0.40
3:D:419:HIS:HE1	3:D:471:PRO:O	2.04	0.40
3:D:980:THR:O	3:D:996:LYS:HD3	2.21	0.40
5:F:269:LEU:O	5:F:272:SER:OG	2.30	0.40
5:F:311:THR:O	5:F:341:LEU:HD21	2.21	0.40
10:K:81:GLU:CD	10:L:96:ARG:HE	2.21	0.40
10:K:170:GLN:OE1	10:K:171:LEU:HD23	2.21	0.40
1:A:14:VAL:HG13	1:A:15:ASP:OD1	2.20	0.40
1:B:214:GLU:OE2	1:B:218:ARG:NH2	2.35	0.40
2:C:179:TYR:HB2	2:C:398:SER:OG	2.21	0.40
2:C:632:ASP:OD1	2:C:632:ASP:N	2.53	0.40
2:C:971:LEU:HD12	2:C:971:LEU:HA	1.85	0.40
2:C:985:GLU:CB	2:C:989:LEU:HB2	2.51	0.40
2:C:1133:LYS:O	2:C:1135:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:139:LEU:HD23	3:D:139:LEU:HA	1.78	0.40
3:D:317:THR:HB	3:D:324:LEU:HD21	2.03	0.40
3:D:518:VAL:HA	3:D:547:ARG:HH22	1.86	0.40
3:D:985:ILE:HG22	3:D:986:ASP:N	2.37	0.40
3:D:1104:LYS:CB	3:D:1125:PRO:HD2	2.51	0.40
3:D:1116:SER:N	3:D:1119:ASP:OD1	2.53	0.40
5:F:287:ILE:HG21	5:F:306:PHE:CZ	2.56	0.40
5:F:294:GLN:OE1	5:F:333:VAL:HB	2.21	0.40
7:H:39:DC:H6	7:H:39:DC:H2'	1.72	0.40
2:C:122:VAL:HG21	2:C:493:ILE:HD13	2.03	0.40
2:C:151:ARG:HE	2:C:151:ARG:HB3	1.75	0.40
2:C:833:ILE:HA	2:C:1054:LEU:O	2.21	0.40
2:C:878:THR:OG1	2:C:879:GLY:N	2.54	0.40
2:C:1033:ARG:O	2:C:1037:THR:HG22	2.21	0.40
2:C:1259:LEU:O	2:C:1259:LEU:HG	2.15	0.40
3:D:120:LEU:HD13	3:D:120:LEU:HA	1.77	0.40
3:D:265:LEU:HD23	3:D:265:LEU:HA	1.89	0.40
3:D:442:ILE:HG22	3:D:443:GLU:O	2.21	0.40
4:E:21:LEU:HD23	4:E:21:LEU:HA	1.83	0.40
5:F:165:PHE:N	5:F:260:ARG:HH21	2.19	0.40
6:G:23:DT:H2''	6:G:24:DG:C8	2.55	0.40
10:L:9:SER:C	10:L:11:MET:H	2.24	0.40
10:L:15:SER:HG	10:L:26:ARG:HE	1.67	0.40
10:L:126:ASP:HA	10:L:129:ARG:HH11	1.86	0.40
1:A:98:VAL:HG11	1:A:121:VAL:CG2	2.51	0.40
1:A:195:ARG:HD2	1:A:195:ARG:HA	1.93	0.40
1:B:47:LEU:HD23	1:B:51:MET:CE	2.51	0.40
1:B:161:SER:O	1:B:163:GLU:N	2.51	0.40
2:C:471:VAL:HG21	2:C:498:ILE:HD11	2.04	0.40
2:C:609:ILE:H	2:C:609:ILE:HG12	1.55	0.40
3:D:298:MET:HE2	5:F:402:LEU:HB3	2.02	0.40
3:D:411:ILE:HD13	3:D:411:ILE:HA	1.88	0.40
3:D:515:ARG:HE	3:D:515:ARG:HB3	1.75	0.40
3:D:955:LYS:HE2	3:D:1010:GLN:HB3	2.04	0.40
3:D:1191:PRO:HB3	3:D:1193:TRP:CE3	2.57	0.40
3:D:1248:ILE:HG22	3:D:1249:ASN:O	2.21	0.40
3:D:1287:ILE:N	3:D:1287:ILE:HD13	2.37	0.40
4:E:50:ALA:O	4:E:54:ILE:HG12	2.21	0.40
10:L:64:ASP:C	10:L:66:GLU:H	2.21	0.40
10:L:165:LEU:HD13	10:L:187:MET:CG	2.52	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	
1	A	228/329 (69%)	208 (91%)	20 (9%)	0	100	100
1	B	226/329 (69%)	199 (88%)	25 (11%)	2 (1%)	17	54
2	C	1337/1342 (100%)	1167 (87%)	168 (13%)	2 (0%)	51	83
3	D	1359/1430 (95%)	1188 (87%)	168 (12%)	3 (0%)	47	78
4	E	85/91 (93%)	74 (87%)	11 (13%)	0	100	100
5	F	465/613 (76%)	426 (92%)	39 (8%)	0	100	100
10	K	197/232 (85%)	171 (87%)	25 (13%)	1 (0%)	29	66
10	L	202/232 (87%)	175 (87%)	23 (11%)	4 (2%)	7	35
All	All	4099/4598 (89%)	3608 (88%)	479 (12%)	12 (0%)	44	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	710	ASP
3	D	1345	ARG
1	B	21	SER
10	L	10	VAL
2	C	398	SER
10	K	65	ARG
2	C	814	ASP
10	L	48	GLN
1	B	193	GLU
3	D	338	PHE
10	L	65	ARG
10	L	72	SER

5.3.2 Protein sidechains

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/286 (69%)	184 (93%)	14 (7%)	14	45
1	B	196/286 (68%)	179 (91%)	17 (9%)	10	35
2	C	1153/1157 (100%)	1078 (94%)	75 (6%)	17	48
3	D	1116/1189 (94%)	1016 (91%)	100 (9%)	9	33
4	E	65/75 (87%)	62 (95%)	3 (5%)	27	61
5	F	419/540 (78%)	383 (91%)	36 (9%)	10	36
10	K	172/204 (84%)	162 (94%)	10 (6%)	20	53
10	L	175/204 (86%)	160 (91%)	15 (9%)	10	36
All	All	3494/3941 (89%)	3224 (92%)	270 (8%)	16	42

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	56	VAL
1	A	72	GLU
1	A	77	ASP
1	A	120	ASP
1	A	157	THR
1	A	174	ASP
1	A	191	ARG
1	A	192	VAL
1	A	205	MET
1	A	212	ASP
1	A	219	ARG
1	A	231	PHE
1	A	236	ASP
1	B	14	VAL
1	B	15	ASP
1	B	16	ILE
1	B	17	GLU
1	B	27	THR
1	B	38	THR
1	B	54	CYS
1	B	59	VAL
1	B	67	GLU

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Mol	Chain	Res	Type
1	B	127	GLN
1	B	148	ARG
1	B	150	ARG
1	B	174	ASP
1	B	186	ASN
1	B	193	GLU
1	B	207	THR
1	B	233	ASP
2	C	3	TYR
2	C	23	ASP
2	C	39	ILE
2	C	47	TYR
2	C	55	SER
2	C	70	TYR
2	C	81	ASP
2	C	97	ARG
2	C	113	THR
2	C	115	LYS
2	C	150	HIS
2	C	161	LYS
2	C	165	HIS
2	C	255	ILE
2	C	281	ASP
2	C	300	ASP
2	C	306	THR
2	C	339	ASN
2	C	340	ASP
2	C	384	LEU
2	C	393	ASP
2	C	443	ASP
2	C	484	LEU
2	C	486	THR
2	C	487	LEU
2	C	491	ASP
2	C	518	ASN
2	C	524	ILE
2	C	539	THR
2	C	553	THR
2	C	589	THR
2	C	613	ASN
2	C	632	ASP
2	C	656	SER

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Mol	Chain	Res	Type
2	C	657	THR
2	C	659	GLN
2	C	687	ARG
2	C	694	ARG
2	C	720	ARG
2	C	764	CYS
2	C	765	ILE
2	C	766	ASN
2	C	819	SER
2	C	851	THR
2	C	857	VAL
2	C	895	LEU
2	C	913	VAL
2	C	924	VAL
2	C	940	GLU
2	C	990	ASP
2	C	1004	ASP
2	C	1014	LEU
2	C	1018	TYR
2	C	1023	HIS
2	C	1041	ASP
2	C	1046	VAL
2	C	1076	ILE
2	C	1093	PRO
2	C	1127	LYS
2	C	1132	LEU
2	C	1135	GLN
2	C	1156	ARG
2	C	1172	LEU
2	C	1198	LEU
2	C	1223	ARG
2	C	1232	MET
2	C	1233	LEU
2	C	1236	ASN
2	C	1240	ASP
2	C	1246	ARG
2	C	1259	LEU
2	C	1269	ARG
2	C	1296	ASP
2	C	1302	THR
2	C	1312	ASN
3	D	18	ASP

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Mol	Chain	Res	Type
3	D	20	ILE
3	D	32	SER
3	D	46	TYR
3	D	54	ASP
3	D	60	ARG
3	D	80	HIS
3	D	91	GLU
3	D	93	THR
3	D	126	LEU
3	D	133	ARG
3	D	155	GLU
3	D	159	ILE
3	D	160	LEU
3	D	172	PHE
3	D	176	PHE
3	D	203	GLU
3	D	227	PHE
3	D	240	THR
3	D	244	VAL
3	D	314	ARG
3	D	317	THR
3	D	332	LYS
3	D	335	GLN
3	D	392	THR
3	D	393	THR
3	D	410	ASP
3	D	416	ILE
3	D	425	ARG
3	D	430	HIS
3	D	460	ASP
3	D	485	MET
3	D	505	ASP
3	D	506	VAL
3	D	518	VAL
3	D	527	LEU
3	D	543	SER
3	D	545	HIS
3	D	560	ASN
3	D	598	LYS
3	D	638	SER
3	D	674	THR
3	D	703	THR

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Mol	Chain	Res	Type
3	D	710	ASP
3	D	712	GLN
3	D	722	ILE
3	D	746	LEU
3	D	764	ARG
3	D	801	VAL
3	D	803	VAL
3	D	805	GLN
3	D	823	THR
3	D	843	VAL
3	D	847	ASP
3	D	849	LEU
3	D	858	VAL
3	D	862	THR
3	D	863	LEU
3	D	868	TRP
3	D	869	CYS
3	D	874	GLU
3	D	890	THR
3	D	901	ARG
3	D	902	ASP
3	D	918	ILE
3	D	929	GLN
3	D	959	LYS
3	D	966	VAL
3	D	980	THR
3	D	986	ASP
3	D	997	VAL
3	D	1007	ASP
3	D	1015	GLU
3	D	1034	PHE
3	D	1046	ILE
3	D	1047	THR
3	D	1072	LYS
3	D	1078	LEU
3	D	1081	VAL
3	D	1088	VAL
3	D	1093	THR
3	D	1140	ARG
3	D	1155	ILE
3	D	1170	LYS
3	D	1178	THR

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Mol	Chain	Res	Type
3	D	1181	ASP
3	D	1187	GLU
3	D	1199	PHE
3	D	1203	ARG
3	D	1204	VAL
3	D	1236	GLU
3	D	1266	ILE
3	D	1272	SER
3	D	1280	VAL
3	D	1282	TYR
3	D	1306	LEU
3	D	1307	LEU
3	D	1316	THR
3	D	1325	PHE
3	D	1357	ILE
4	E	3	ARG
4	E	46	THR
4	E	62	GLN
5	F	95	THR
5	F	109	GLU
5	F	114	GLU
5	F	147	GLN
5	F	220	LYS
5	F	225	ARG
5	F	236	LYS
5	F	250	LEU
5	F	256	PHE
5	F	296	LYS
5	F	300	LYS
5	F	346	GLN
5	F	360	ASP
5	F	395	THR
5	F	397	ARG
5	F	423	ARG
5	F	445	ASP
5	F	457	ILE
5	F	465	ARG
5	F	471	LEU
5	F	472	GLN
5	F	476	ARG
5	F	509	THR
5	F	515	GLU

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Mol	Chain	Res	Type
5	F	527	THR
5	F	533	ASP
5	F	557	LYS
5	F	569	THR
5	F	570	ASP
5	F	572	THR
5	F	573	LEU
5	F	579	GLN
5	F	580	PHE
5	F	587	ILE
5	F	588	ARG
5	F	607	LEU
10	K	19	ASP
10	K	65	ARG
10	K	70	TRP
10	K	91	VAL
10	K	121	SER
10	K	134	GLU
10	K	143	PHE
10	K	154	PHE
10	K	160	TYR
10	K	183	LEU
10	L	8	ARG
10	L	11	MET
10	L	45	ASN
10	L	56	ASN
10	L	64	ASP
10	L	112	THR
10	L	114	MET
10	L	118	ILE
10	L	146	LYS
10	L	158	ASP
10	L	164	LEU
10	L	175	PHE
10	L	194	ASP
10	L	201	THR
10	L	202	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS

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Mol	Chain	Res	Type
1	B	128	HIS
1	B	132	HIS
2	C	65	ASN
2	C	139	ASN
2	C	330	HIS
2	C	343	HIS
2	C	490	GLN
2	C	760	ASN
2	C	1008	GLN
2	C	1080	ASN
2	C	1116	HIS
2	C	1135	GLN
2	C	1237	HIS
3	D	45	ASN
3	D	294	ASN
3	D	320	ASN
3	D	365	GLN
3	D	419	HIS
3	D	477	GLN
3	D	720	ASN
3	D	739	GLN
3	D	805	GLN
3	D	951	GLN
3	D	968	ASN
3	D	1098	GLN
3	D	1108	GLN
3	D	1197	ASN
3	D	1218	HIS
3	D	1235	ASN
3	D	1238	GLN
4	E	62	GLN
4	E	70	GLN
4	E	72	GLN
5	F	271	ASN
5	F	309	ASN
5	F	323	ASN
5	F	406	GLN
5	F	446	GLN
5	F	455	HIS
5	F	464	ASN
10	K	24	GLN
10	K	40	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	K	85	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

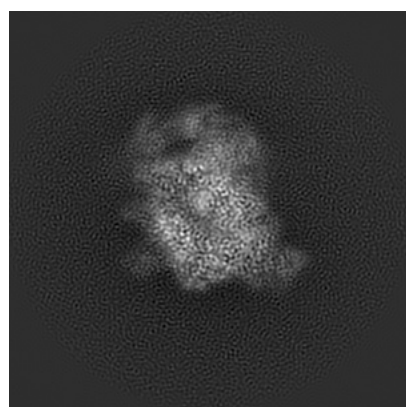
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21853. These allow visual inspection of the internal detail of the map and identification of artifacts.

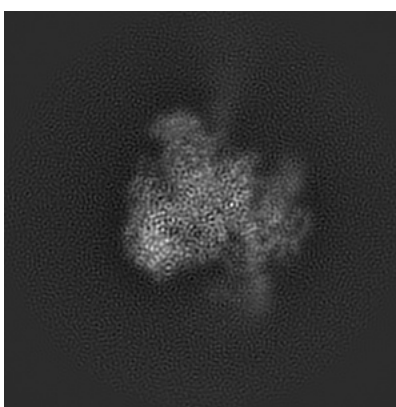
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

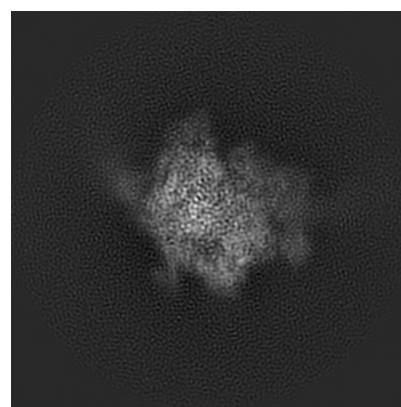
6.1.1 Primary map



X



Y

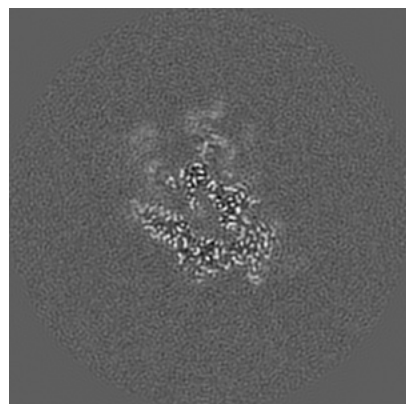


Z

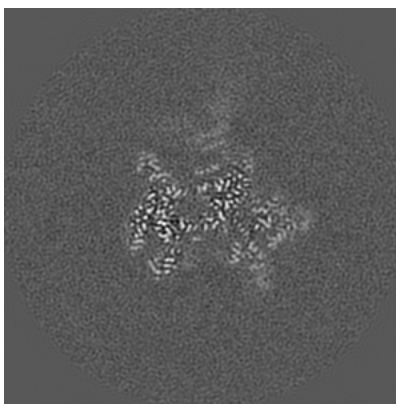
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

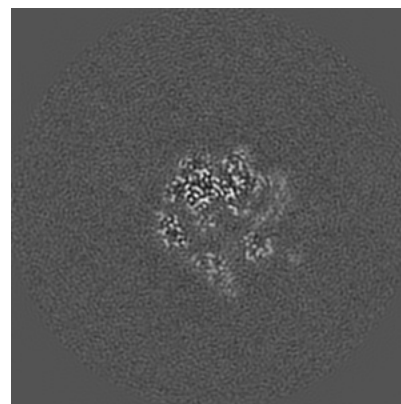
6.2.1 Primary map



X Index: 150



Y Index: 150

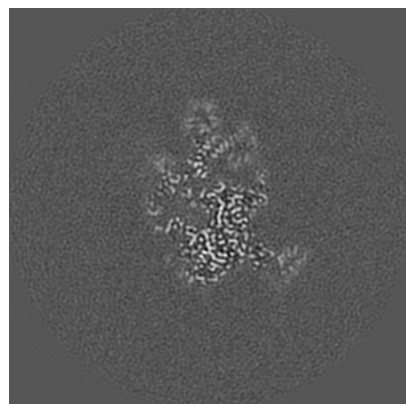


Z Index: 150

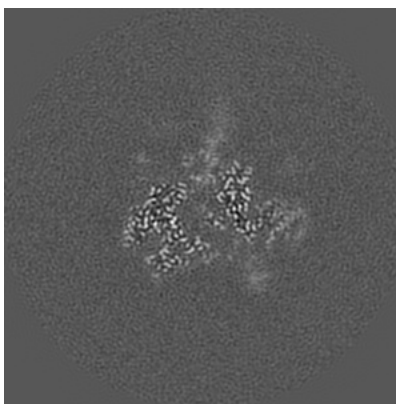
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

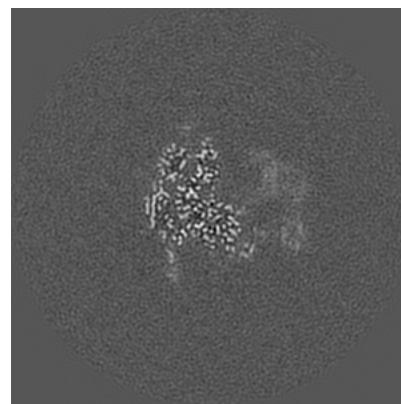
6.3.1 Primary map



X Index: 138



Y Index: 144



Z Index: 123

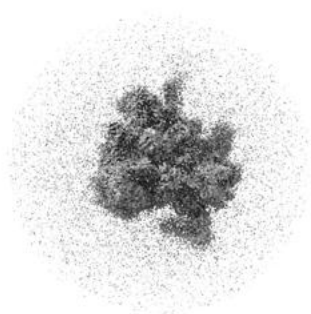
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

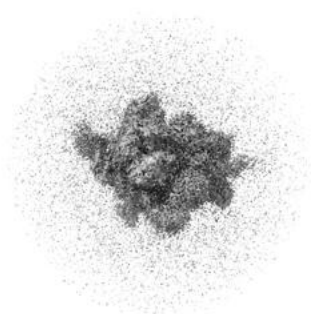
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

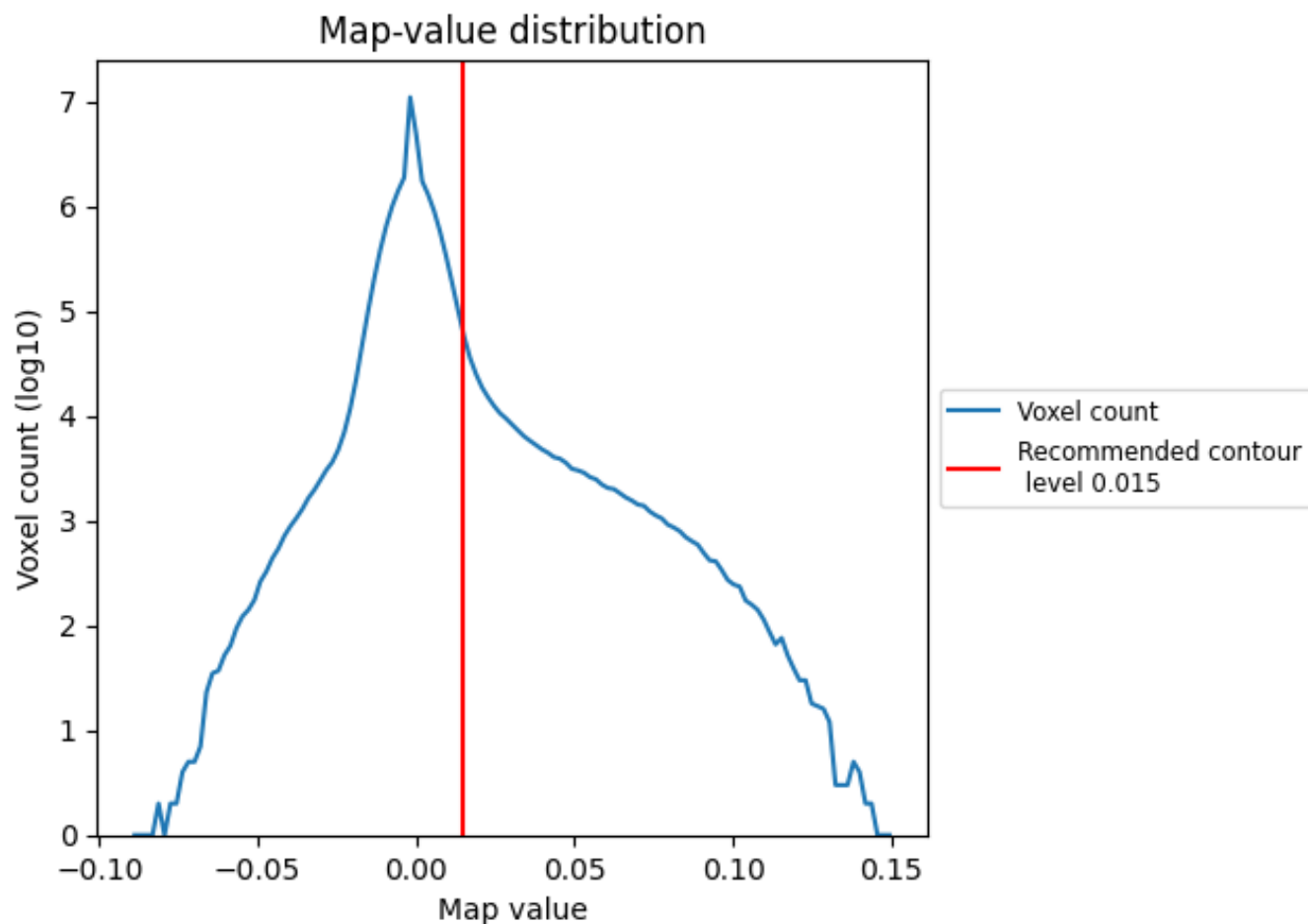
6.5 Mask visualisation

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

7 Map analysis [i](#)

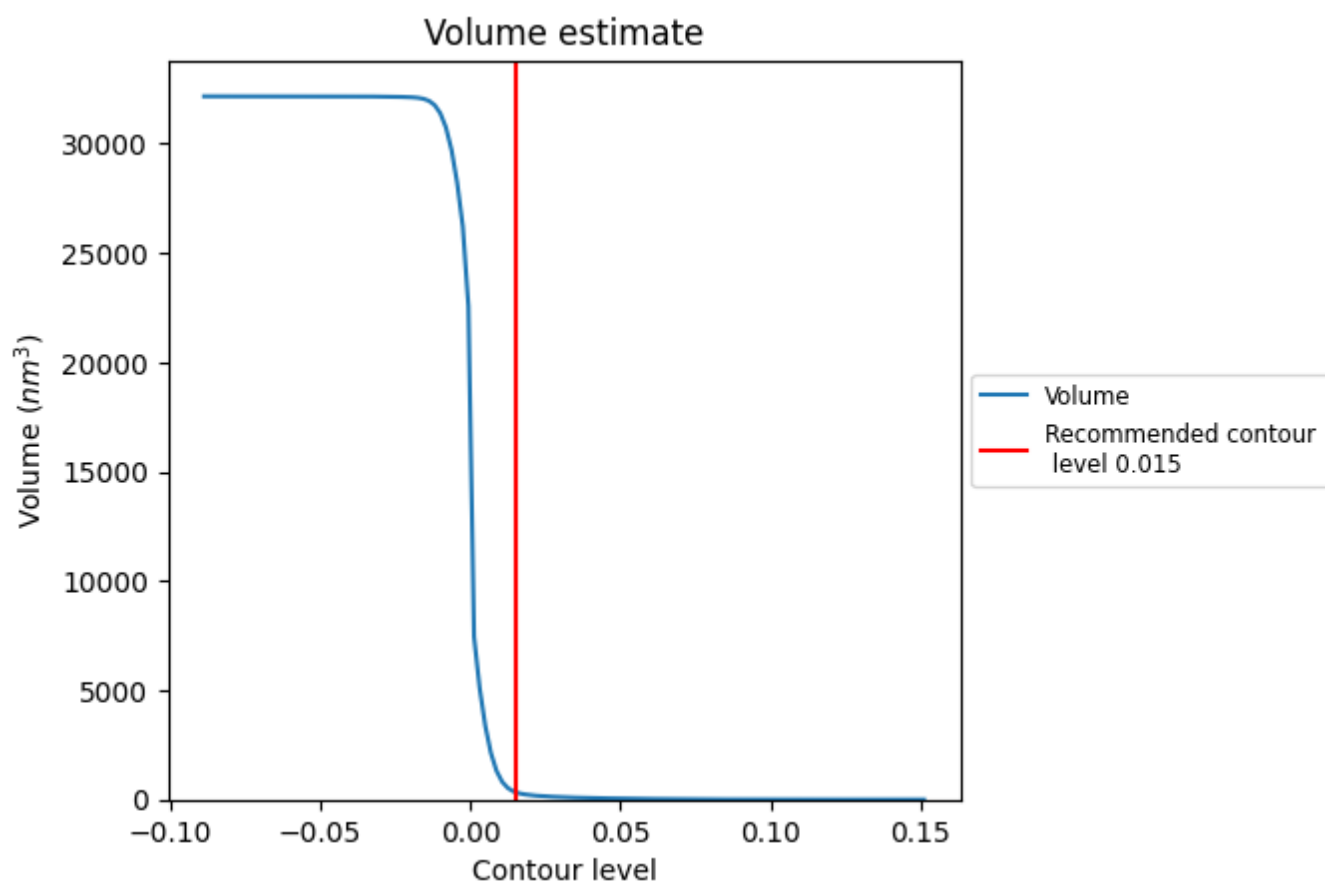
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

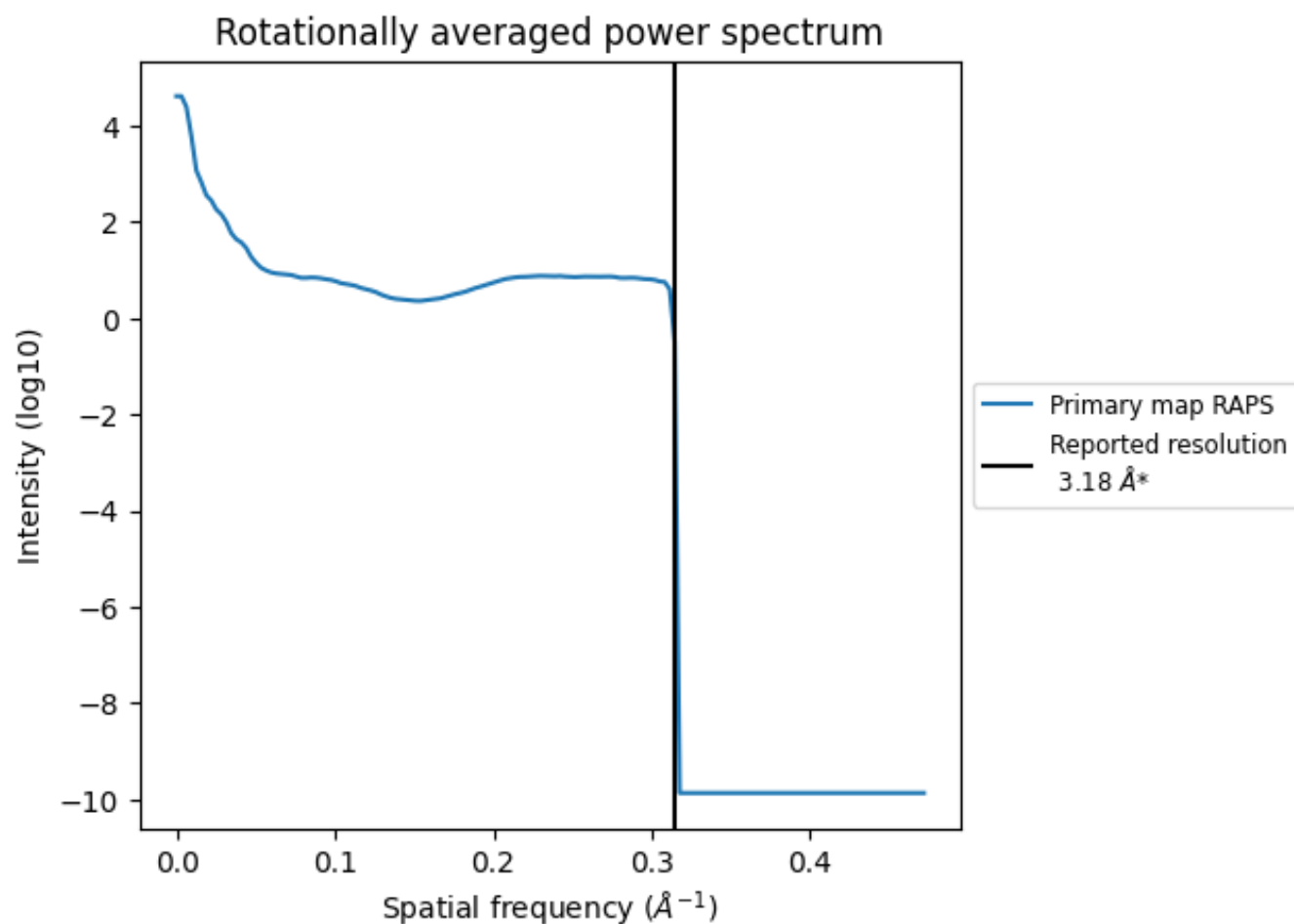
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 343 nm^3 ; this corresponds to an approximate mass of 310 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 ⓘ

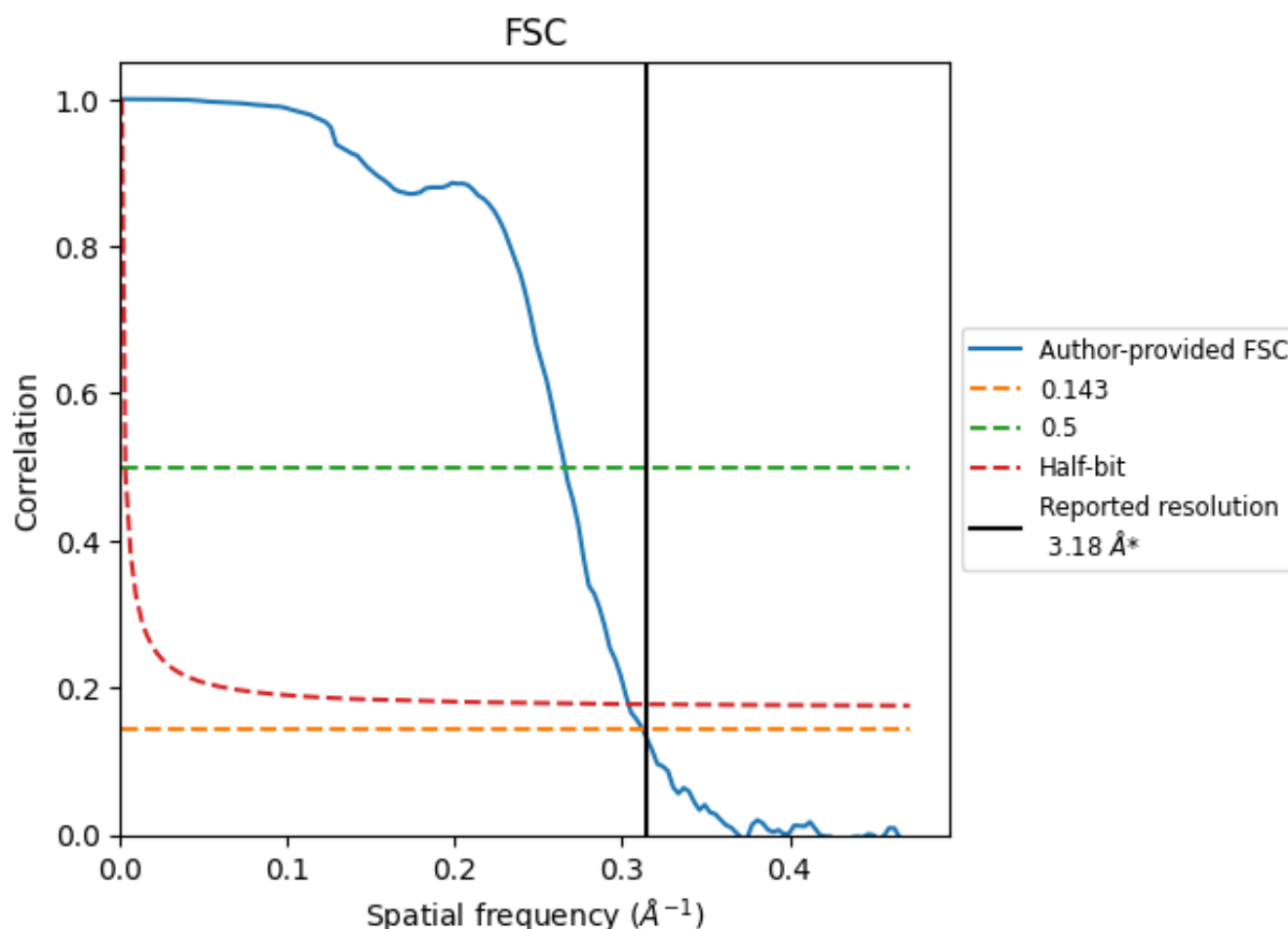


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

8.2 Resolution estimates [i](#)

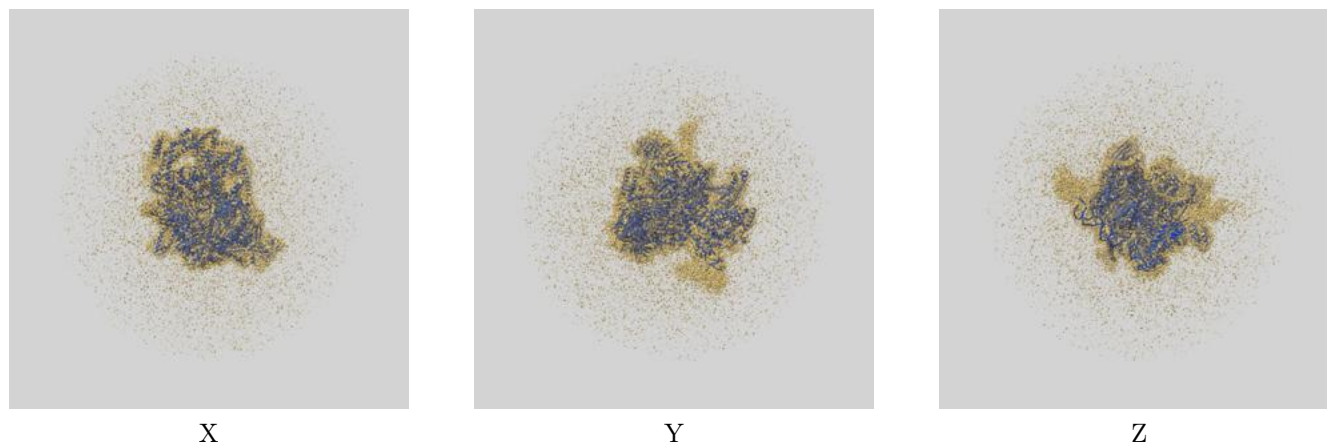
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.20	3.76	3.29
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

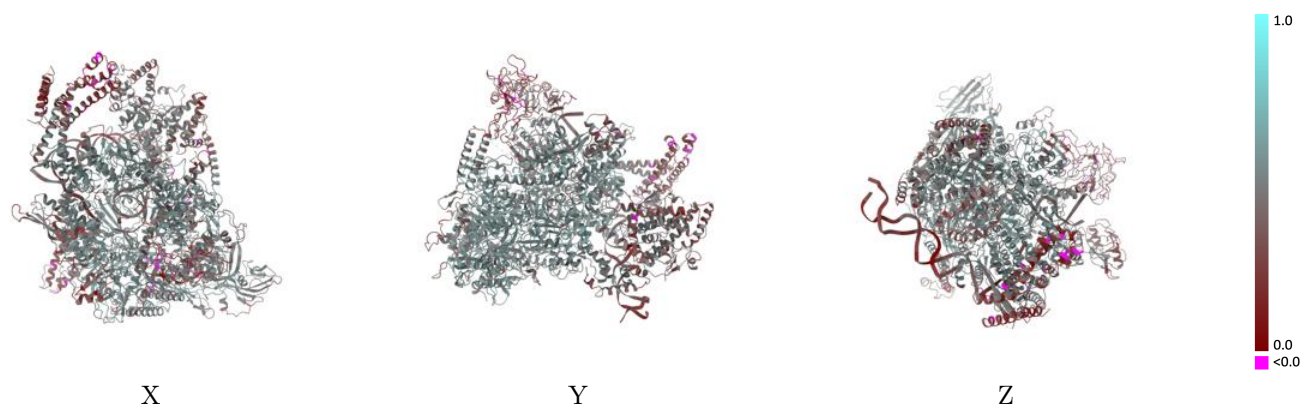
This section contains information regarding the fit between EMDB map EMD-21853 and PDB model 6WMU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



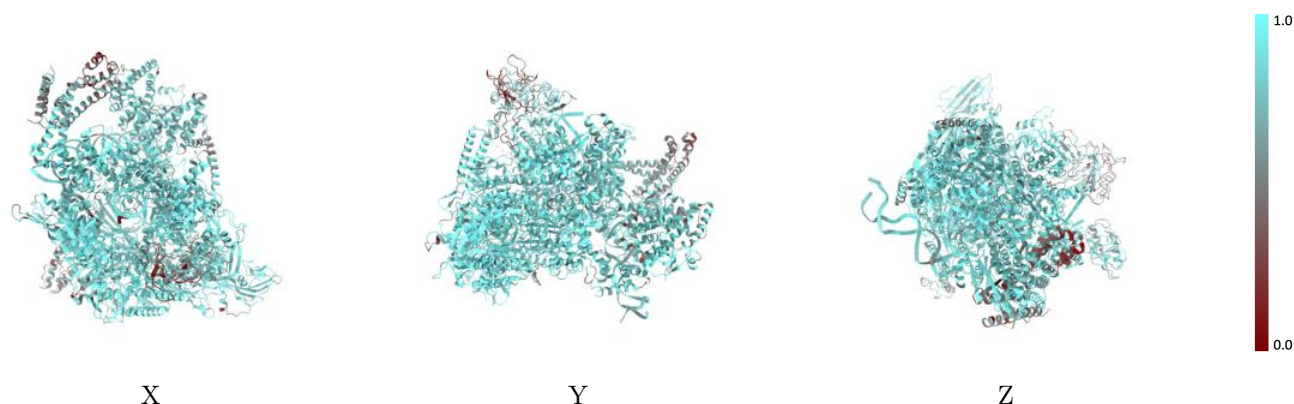
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



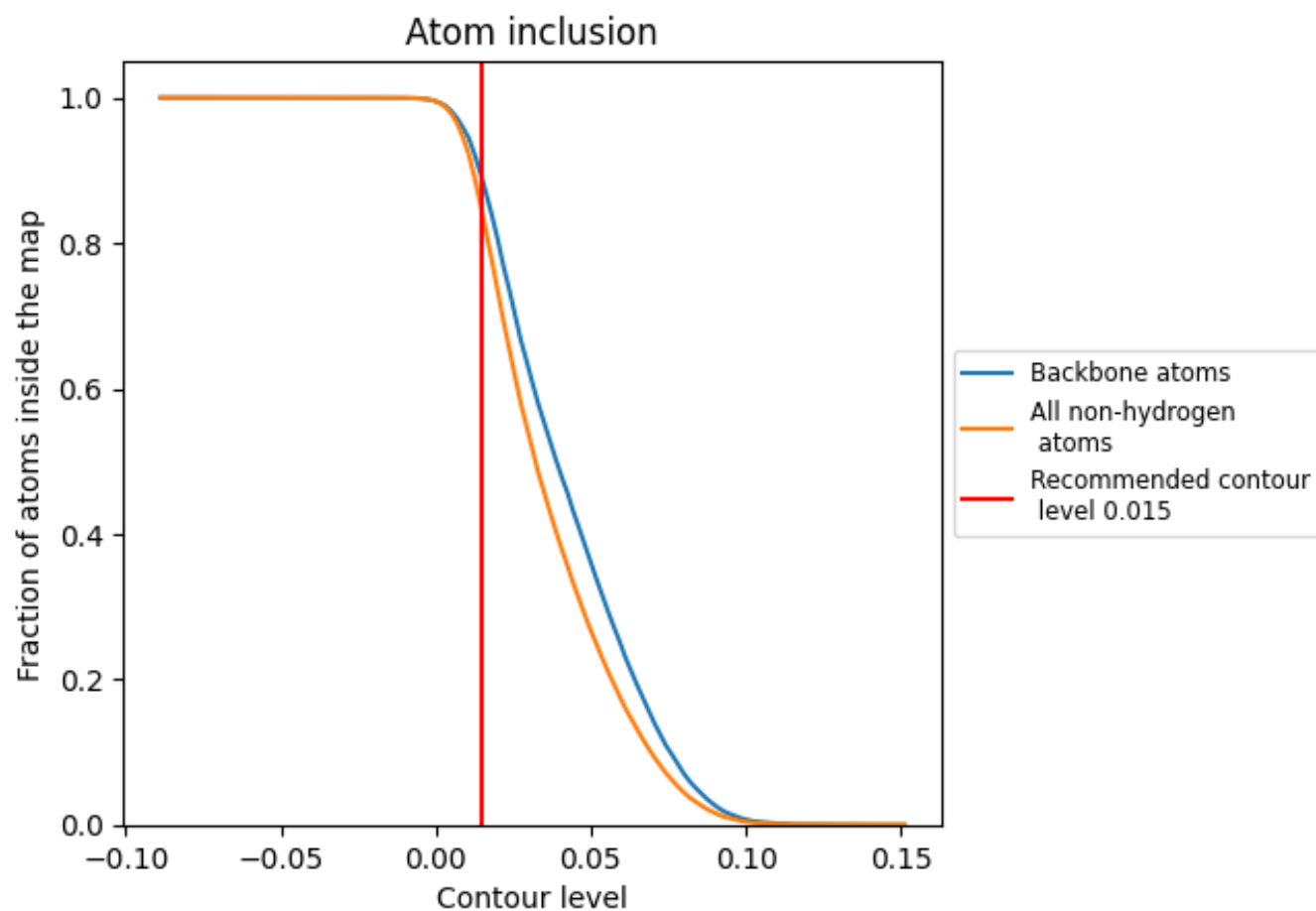
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8415</div>	<div><div></div>0.4710</div>
A	<div><div></div>0.9137</div>	<div><div></div>0.5390</div>
B	<div><div></div>0.8608</div>	<div><div></div>0.4980</div>
C	<div><div></div>0.8805</div>	<div><div></div>0.5090</div>
D	<div><div></div>0.8354</div>	<div><div></div>0.4830</div>
E	<div><div></div>0.8276</div>	<div><div></div>0.4980</div>
F	<div><div></div>0.7292</div>	<div><div></div>0.3820</div>
G	<div><div></div>0.7882</div>	<div><div></div>0.3160</div>
H	<div><div></div>0.7540</div>	<div><div></div>0.2780</div>
I	<div><div></div>0.9333</div>	<div><div></div>0.4220</div>
J	<div><div></div>0.9381</div>	<div><div></div>0.4280</div>
K	<div><div></div>0.8328</div>	<div><div></div>0.4270</div>
L	<div><div></div>0.8333</div>	<div><div></div>0.4340</div>

1.0

0.0

<0.0