



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:34 AM UTC

PDB ID : 8XX4 / pdb_00008xx4
EMDB ID : EMD-38745
Title : ASFV RNAP elongation complex
Authors : Zhu, G.L.; Zhu, Y.; Zhu, Z.X.; Sun, F.; Zheng, H.X.
Deposited on : 2024-01-17
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

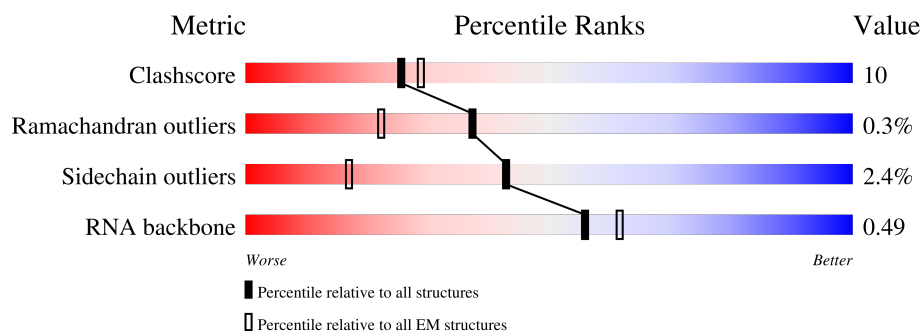
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1441	75% 21% ..
2	B	1233	68% 26% • 5%
3	C	358	73% 26%
4	D	205	77% 22%
5	F	80	61% 35% •
6	G	103	67% 31% •
7	H	80	62% 26% 11%

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Mol	Chain	Length	Quality of chain
8	P	9	56% 22% 22%
9	T	23	96%
10	E	109	72% 27%
11	N	11	27% 73%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28685 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1391	Total	C	N	O	S	0	0
			11091	7045	1925	2060	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1171	Total	C	N	O	S	0	0
			9255	5854	1624	1726	51		

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	358	Total	C	N	O	S	0	0
			2907	1885	481	529	12		

- Molecule 4 is a protein called DNA-directed RNA polymerase RPB5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1669	1088	278	295	8		

- Molecule 5 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	80	Total	C	N	O	S	0	0
			644	411	110	118	5		

- Molecule 6 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	103	Total	C	N	O	S	0	0
			800	499	136	150	15		

- Molecule 7 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	71	Total	C	N	O	S	0	0
			569	372	91	99	7		

- Molecule 8 is a RNA chain called RNA (5'-R(P*CP*UP*AP*CP*AP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	9	Total	C	N	O	P	0	0
			190	86	36	59	9		

- Molecule 9 is a DNA chain called DNA (5'-D(P*TP*TP*CP*GP*CP*CP*GP*TP*TP*GP*CP*GP*TP*AP*TP*TP*TP*GP*TP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	23	Total	C	N	O	P	0	0
			472	226	77	146	23		

- Molecule 10 is a protein called RNA polymerase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	109	Total	C	N	O	S	0	0
			854	544	146	159	5		

- Molecule 11 is a DNA chain called DNA (5'-D(P*CP*GP*CP*AP*AP*CP*GP*GP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	11	Total	C	N	O	P	0	0
			227	106	47	63	11		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	A	2	Total	Zn	0
			2	2	
12	B	1	Total	Zn	0
			1	1	
12	G	2	Total	Zn	0
			2	2	
12	H	1	Total	Zn	0
			1	1	

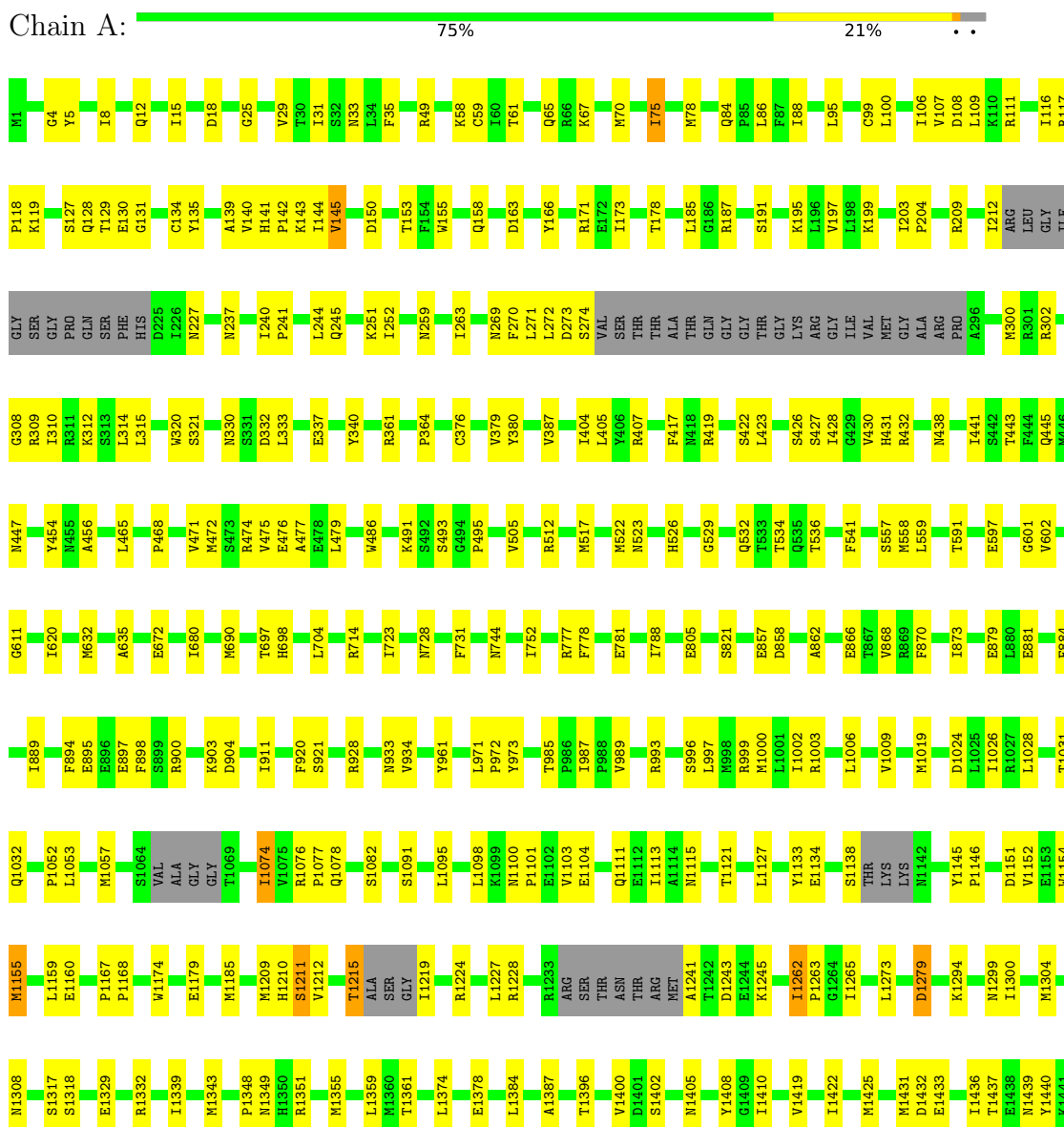
- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 1	Mg 1	0

3 Residue-property plots

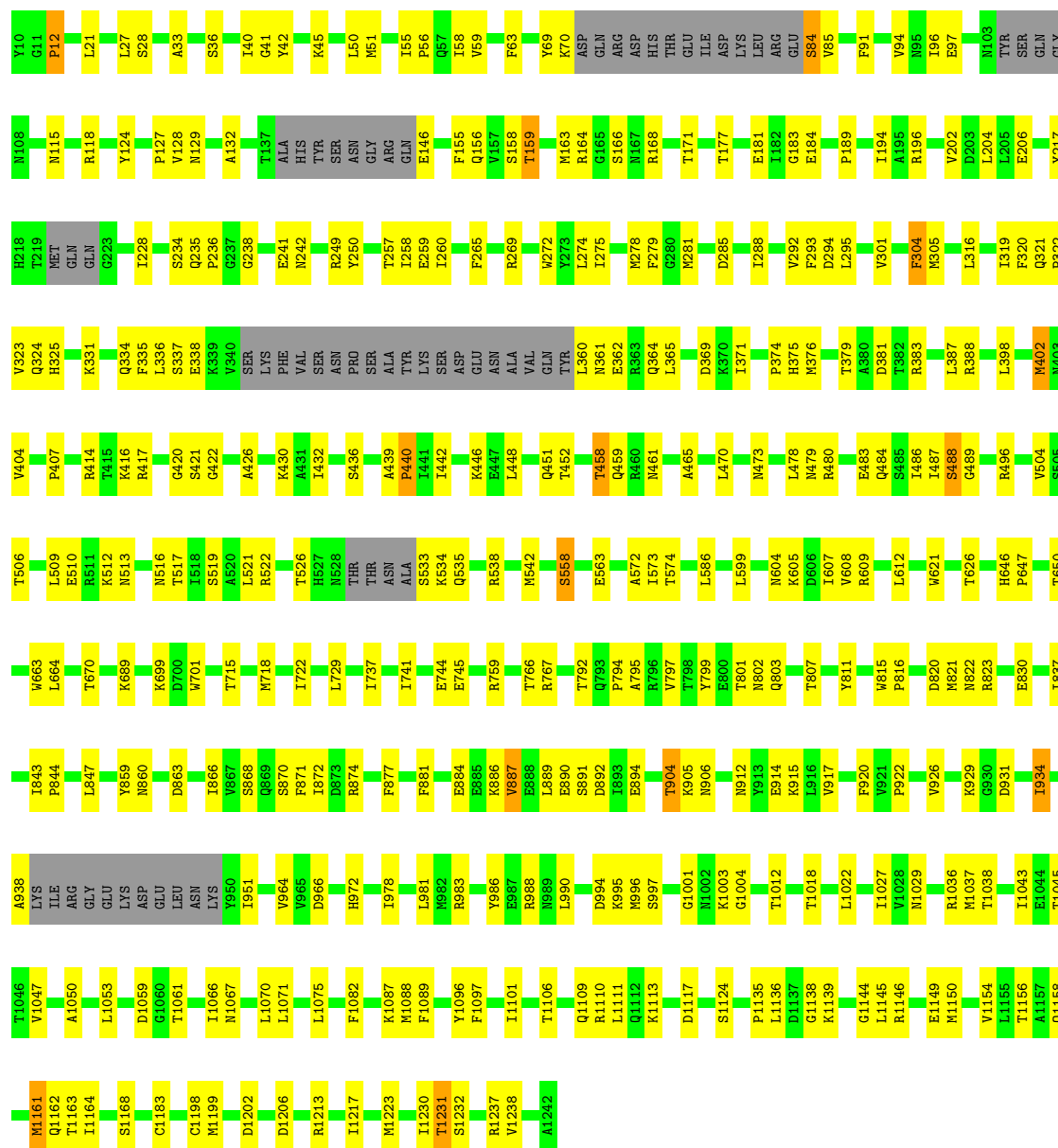
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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



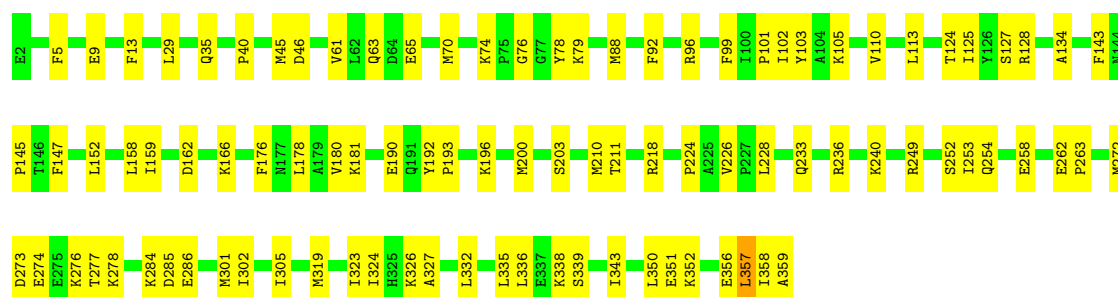
- Molecule 2: DNA-directed RNA polymerase subunit beta





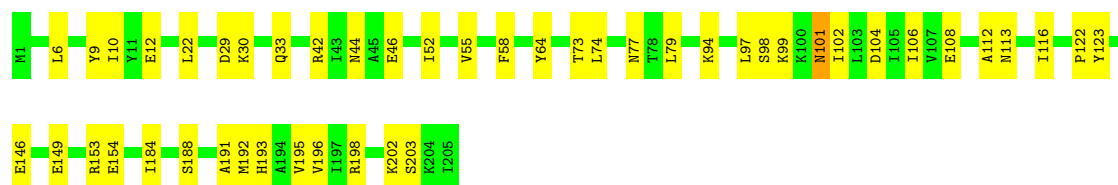
• Molecule 3: DNA-directed RNA polymerase RPB3-11 homolog

Chain C: 73% 26%



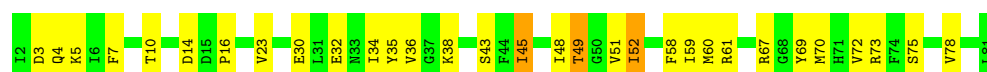
• Molecule 4: DNA-directed RNA polymerase RPB5 homolog

Chain D:  77% 22%



- Molecule 5: D339L

Chain F:  61% 35% .



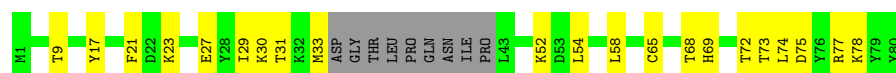
- Molecule 6: C122R

Chain G:  67% 31% .



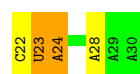
- Molecule 7: DNA-directed RNA polymerase RPB10 homolog

Chain H:  62% 26% 11%



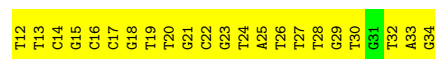
- Molecule 8: RNA (5'-R(P*CP*UP*AP*CP*AP*CP*AP*AP*A)-3')

Chain P:  56% 22% 22%



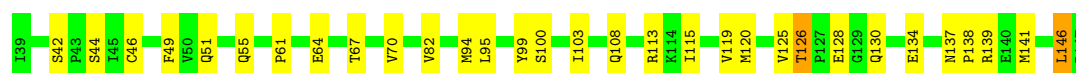
- Molecule 9: DNA (5'-D(P*TP*TP*CP*GP*CP*CP*GP*TP*TP*GP*CP*GP*TP*AP*TP*T
P*TP*GP*TP*GP*TP*AP*G)-3')

Chain T:  96%



- Molecule 10: RNA polymerase subunit 6

Chain E:  72% 27%



- Molecule 11: DNA (5'-D(P*CP*GP*CP*AP*AP*CP*GP*GP*CP*GP*A)-3')

Chain N:  27% 73%

C26	C31
G27	G32
	G33
	C34
	G35
	A36

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73192	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/11305	0.32	1/15310 (0.0%)
2	B	0.23	0/9436	0.37	3/12764 (0.0%)
3	C	0.23	0/2969	0.34	0/4012
4	D	0.21	0/1708	0.31	0/2311
5	F	0.23	0/656	0.39	0/886
6	G	0.19	0/812	0.36	0/1090
7	H	0.25	0/579	0.30	0/780
8	P	0.18	0/212	0.26	0/327
9	T	0.26	0/526	0.42	0/811
10	E	0.23	0/866	0.31	0/1172
11	N	0.19	0/255	0.38	0/391
All	All	0.22	0/29324	0.34	4/39854 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	440	PRO	CA-N-CD	-7.52	101.47	112.00
2	B	12	PRO	CA-N-CD	-5.82	103.85	112.00
1	A	1074	ILE	N-CA-C	-5.44	107.00	112.17
2	B	488	SER	CB-CA-C	-5.23	110.11	117.23

There are no chirality outliers.

There are no planarity outliers.

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	11091	0	11199	215	0
2	B	9255	0	9233	237	0
3	C	2907	0	2982	62	0
4	D	1669	0	1713	30	0
5	F	644	0	642	22	0
6	G	800	0	797	30	0
7	H	569	0	595	17	0
8	P	190	0	98	2	0
9	T	472	0	264	20	0
10	E	854	0	903	23	0
11	N	227	0	122	7	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	G	2	0	0	0	0
12	H	1	0	0	0	0
13	A	1	0	0	0	0
All	All	28685	0	28548	589	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 10.

All (589) 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)
2:B:301:VAL:HA	2:B:402:MET:HE1	1.44	0.96
2:B:1018:THR:HG22	2:B:1088:MET:HE2	1.61	0.82
9:T:33:DA:H2''	9:T:34:DG:H5'	1.59	0.82
1:A:1215:THR:HG21	1:A:1219:ILE:HG13	1.67	0.77
2:B:820:ASP:HB3	2:B:823:ARG:HG3	1.66	0.76
2:B:1238:VAL:HG12	10:E:55:GLN:HB2	1.68	0.75
8:P:24:A:H62	9:T:32:DT:H3	1.33	0.74
2:B:249:ARG:NH1	2:B:259:GLU:OE1	2.20	0.74
3:C:110:VAL:HB	3:C:134:ALA:HB3	1.68	0.74
2:B:118:ARG:NH2	2:B:184:GLU:OE2	2.20	0.73
2:B:241:GLU:OE1	2:B:241:GLU:N	2.22	0.73
3:C:61:VAL:HA	3:C:65:GLU:HB2	1.70	0.72
2:B:217:TYR:HD2	2:B:407:PRO:HG3	1.54	0.72
1:A:58:LYS:HE2	1:A:65:GLN:HG3	1.70	0.71
4:D:192:MET:O	4:D:193:HIS:ND1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:O	1:A:447:ASN:ND2	2.24	0.70
2:B:915:LYS:NZ	2:B:931:ASP:OD2	2.23	0.69
3:C:29:LEU:HD22	7:H:23:LYS:HG3	1.75	0.69
2:B:278:MET:HE1	2:B:336:LEU:HD22	1.75	0.69
2:B:115:ASN:ND2	2:B:183:GLY:O	2.26	0.69
2:B:863:ASP:OD1	2:B:1036:ARG:NH2	2.27	0.68
3:C:305:ILE:HD11	3:C:323:ILE:HG23	1.75	0.68
1:A:517:MET:HE2	1:A:517:MET:HA	1.75	0.68
1:A:777:ARG:NH1	6:G:63:ASP:OD2	2.26	0.67
9:T:20:DT:H2'	9:T:21:DG:C8	2.29	0.67
1:A:1168:PRO:HB3	1:A:1228:ARG:NH1	2.08	0.67
2:B:304:PHE:CD1	2:B:402:MET:HE3	2.29	0.67
2:B:97:GLU:OE2	2:B:129:ASN:ND2	2.26	0.67
2:B:877:PHE:O	2:B:1110:ARG:NH1	2.27	0.67
6:G:14:THR:OG1	6:G:21:ILE:O	2.11	0.67
7:H:75:ASP:HB3	7:H:78:LYS:HG3	1.77	0.67
1:A:1262:ILE:HG13	1:A:1265:ILE:HG13	1.77	0.66
1:A:1002:ILE:HG23	1:A:1006:LEU:HD12	1.77	0.66
1:A:904:ASP:OD2	1:A:1003:ARG:NH1	2.29	0.66
1:A:1052:PRO:HG2	1:A:1348:PRO:HD3	1.78	0.66
1:A:12:GLN:HB2	2:B:1231:THR:HG23	1.77	0.65
6:G:71:LYS:HD3	6:G:94:LEU:HD13	1.78	0.65
2:B:994:ASP:OD2	2:B:1110:ARG:NH2	2.28	0.65
2:B:905:LYS:HB3	2:B:951:ILE:HA	1.79	0.65
1:A:127:SER:OG	1:A:128:GLN:OE1	2.12	0.65
2:B:294:ASP:HB2	2:B:608:VAL:HG21	1.77	0.65
2:B:1161:MET:C	2:B:1163:THR:H	2.03	0.64
1:A:517:MET:HE1	3:C:192:TYR:HE2	1.62	0.64
2:B:21:LEU:O	2:B:759:ARG:NH2	2.31	0.64
4:D:58:PHE:O	4:D:123:TYR:OH	2.13	0.64
2:B:159:THR:OG1	2:B:479:ASN:ND2	2.31	0.64
1:A:523:ASN:ND2	3:C:210:MET:O	2.31	0.63
1:A:1076:ARG:NH2	1:A:1317:SER:O	2.31	0.63
5:F:14:ASP:HA	5:F:67:ARG:HG2	1.81	0.63
1:A:1152:VAL:HA	1:A:1155:MET:HE2	1.81	0.63
1:A:86:LEU:HD23	1:A:272:LEU:HD11	1.81	0.62
1:A:857:GLU:OE2	1:A:1332:ARG:NH2	2.32	0.62
1:A:431:HIS:NE2	1:A:454:TYR:OH	2.29	0.62
2:B:334:GLN:O	2:B:338:GLU:HG3	2.00	0.62
2:B:1161:MET:O	2:B:1163:THR:N	2.33	0.62
1:A:1146:PRO:HG3	6:G:34:SER:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:PRO:O	1:A:1299:ASN:ND2	2.32	0.62
1:A:134:CYS:HB3	1:A:139:ALA:H	1.65	0.61
1:A:423:LEU:HD23	2:B:1150:MET:HE1	1.82	0.61
1:A:1279:ASP:OD1	1:A:1279:ASP:N	2.30	0.61
2:B:844:PRO:HG2	7:H:74:LEU:HD11	1.83	0.61
1:A:106:ILE:HD11	1:A:141:HIS:CD2	2.36	0.61
2:B:701:TRP:H	2:B:701:TRP:CD1	2.18	0.61
7:H:69:HIS:O	7:H:73:THR:OG1	2.18	0.61
9:T:14:DC:H2''	9:T:15:DG:C8	2.35	0.61
1:A:1210:HIS:ND1	1:A:1211:SER:O	2.31	0.61
3:C:352:LYS:O	3:C:356:GLU:HG3	2.01	0.61
2:B:448:LEU:HD13	2:B:465:ALA:HB2	1.83	0.60
2:B:379:THR:HG23	2:B:381:ASP:H	1.66	0.60
2:B:236:PRO:HD3	2:B:374:PRO:HB2	1.81	0.60
2:B:322:PRO:HD2	2:B:335:PHE:HE2	1.66	0.60
2:B:650:THR:HG21	2:B:744:GLU:HG3	1.84	0.60
1:A:116:ILE:HD12	1:A:118:PRO:HG2	1.84	0.60
4:D:42:ARG:HE	4:D:44:ASN:HD21	1.50	0.59
1:A:380:TYR:HB3	1:A:404:ILE:HB	1.84	0.59
2:B:69:TYR:N	2:B:85:VAL:O	2.30	0.59
2:B:228:ILE:HG22	2:B:250:TYR:HB3	1.84	0.59
1:A:680:ILE:HD13	1:A:704:LEU:HB3	1.84	0.59
2:B:558:SER:O	2:B:802:ASN:ND2	2.34	0.59
3:C:35:GLN:HB2	3:C:228:LEU:HD11	1.84	0.59
1:A:4:GLY:HA3	5:F:10:THR:HG23	1.85	0.58
1:A:1211:SER:OG	1:A:1212:VAL:N	2.36	0.58
10:E:67:THR:OG1	10:E:134:GLU:OE1	2.14	0.58
1:A:332:ASP:OD2	2:B:859:TYR:OH	2.22	0.58
2:B:881:PHE:HB3	2:B:986:TYR:HB2	1.84	0.58
11:N:35:DG:H2'	11:N:36:DA:C8	2.38	0.58
1:A:928:ARG:HD3	1:A:997:LEU:HD21	1.85	0.58
2:B:1183:CYS:HB2	10:E:46:CYS:HB2	1.85	0.58
4:D:79:LEU:HD21	4:D:116:ILE:HG21	1.86	0.58
1:A:873:ILE:HD11	1:A:1000:MET:HE1	1.85	0.57
1:A:1410:ILE:HG12	2:B:1156:THR:HG21	1.86	0.57
1:A:1111:GLN:NE2	1:A:1115:ASN:OD1	2.36	0.57
2:B:432:ILE:HG22	2:B:478:LEU:HG	1.86	0.57
7:H:21:PHE:HB2	7:H:58:LEU:HD11	1.85	0.57
1:A:921:SER:O	1:A:921:SER:OG	2.19	0.57
1:A:900:ARG:NH2	1:A:904:ASP:OD1	2.36	0.57
1:A:973:TYR:OH	1:A:985:THR:O	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:34:SER:OG	6:G:35:GLN:N	2.33	0.57
3:C:92:PHE:O	3:C:96:ARG:HG2	2.05	0.57
11:N:26:DC:H2'	11:N:27:DG:C8	2.40	0.57
11:N:34:DC:H2''	11:N:35:DG:C8	2.39	0.57
7:H:17:TYR:HB3	7:H:58:LEU:HD22	1.87	0.57
10:E:61:PRO:HB2	10:E:64:GLU:HG3	1.87	0.57
1:A:145:VAL:HG13	1:A:155:TRP:HB2	1.87	0.56
3:C:240:LYS:HG2	3:C:351:GLU:HG2	1.86	0.56
2:B:414:ARG:HG3	2:B:744:GLU:HA	1.87	0.56
3:C:190:GLU:CD	3:C:190:GLU:H	2.14	0.56
2:B:881:PHE:HB2	2:B:988:ARG:HG3	1.87	0.56
3:C:29:LEU:CD2	7:H:23:LYS:HG3	2.35	0.56
2:B:127:PRO:HB3	2:B:156:GLN:OE1	2.05	0.56
1:A:5:TYR:HB2	5:F:60:MET:HE2	1.86	0.56
1:A:1343:MET:HA	1:A:1343:MET:HE2	1.87	0.56
2:B:40:ILE:HG21	2:B:189:PRO:HB2	1.87	0.56
1:A:315:LEU:HD11	1:A:1387:ALA:HB1	1.87	0.56
2:B:376:MET:HA	2:B:376:MET:HE2	1.88	0.56
2:B:436:SER:HB2	2:B:478:LEU:HD12	1.87	0.56
9:T:21:DG:H2'	9:T:22:DC:C6	2.41	0.56
2:B:319:ILE:HG13	2:B:320:PHE:CD1	2.42	0.55
2:B:792:THR:HG23	2:B:1038:THR:HA	1.88	0.55
9:T:12:DT:H2''	9:T:13:DT:C5	2.41	0.55
1:A:526:HIS:HB3	3:C:210:MET:HE2	1.88	0.55
1:A:70:MET:HB3	2:B:1217:ILE:HG21	1.88	0.55
1:A:468:PRO:HB2	1:A:474:ARG:HG3	1.88	0.55
1:A:889:ILE:HB	1:A:894:PHE:HE2	1.72	0.55
2:B:607:ILE:HA	2:B:612:LEU:HB2	1.89	0.55
2:B:904:THR:OG1	2:B:905:LYS:N	2.39	0.55
1:A:1433:GLU:HG2	5:F:23:VAL:HG21	1.89	0.55
2:B:295:LEU:HD11	6:G:1:MET:HE1	1.88	0.55
2:B:42:TYR:OH	2:B:521:LEU:O	2.23	0.55
2:B:56:PRO:HA	2:B:94:VAL:HG11	1.88	0.55
5:F:3:ASP:N	5:F:3:ASP:OD1	2.38	0.55
1:A:1100:ASN:HB2	1:A:1103:VAL:HG12	1.88	0.55
4:D:112:ALA:C	4:D:113:ASN:HD22	2.15	0.55
2:B:163:MET:O	2:B:166:SER:OG	2.24	0.54
2:B:335:PHE:HD1	2:B:335:PHE:O	1.89	0.54
2:B:872:ILE:HG12	2:B:990:LEU:HB3	1.89	0.54
1:A:472:MET:HE2	10:E:82:VAL:HA	1.89	0.54
1:A:1425:MET:HE3	5:F:61:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:THR:HB	2:B:663:TRP:HB2	1.87	0.54
3:C:63:GLN:OE1	3:C:181:LYS:NZ	2.35	0.54
6:G:11:MET:HG2	6:G:24:CYS:HB2	1.90	0.54
1:A:1154:TRP:HZ3	1:A:1209:MET:HG2	1.73	0.54
2:B:196:ARG:NH2	9:T:34:DG:OP1	2.41	0.54
2:B:257:THR:HB	2:B:269:ARG:HB3	1.90	0.54
1:A:1439:ASN:HB3	10:E:94:MET:SD	2.48	0.54
2:B:360:LEU:O	2:B:362:GLU:N	2.41	0.54
2:B:609:ARG:HG2	2:B:609:ARG:HH11	1.73	0.54
2:B:995:LYS:HG2	2:B:1111:LEU:HD12	1.90	0.54
1:A:1431:MET:SD	5:F:59:ILE:HD11	2.48	0.54
3:C:193:PRO:HG2	3:C:196:LYS:HD2	1.89	0.54
10:E:95:LEU:HD11	10:E:108:GLN:HB2	1.90	0.54
1:A:858:ASP:HB3	4:D:191:ALA:HB2	1.90	0.53
2:B:1237:ARG:HH11	5:F:10:THR:HG22	1.73	0.53
10:E:119:VAL:HG23	10:E:138:PRO:HG3	1.89	0.53
2:B:509:LEU:HD11	2:B:517:THR:HG23	1.89	0.53
1:A:209:ARG:NH1	1:A:227:ASN:OD1	2.39	0.53
3:C:152:LEU:HD21	3:C:158:LEU:HB2	1.90	0.53
3:C:70:MET:HG2	3:C:176:PHE:CE1	2.44	0.53
7:H:68:THR:O	7:H:72:THR:OG1	2.17	0.53
2:B:533:SER:OG	2:B:534:LYS:N	2.38	0.53
1:A:1174:TRP:HZ3	6:G:39:VAL:HG21	1.72	0.53
1:A:1057:MET:SD	1:A:1074:ILE:HG12	2.48	0.53
1:A:8:ILE:HG12	2:B:1232:SER:HB3	1.90	0.53
1:A:1422:ILE:HD11	2:B:1156:THR:HG23	1.91	0.53
2:B:292:VAL:HG12	2:B:305:MET:HG2	1.91	0.53
2:B:322:PRO:HD2	2:B:335:PHE:CE2	2.43	0.52
3:C:105:LYS:HD3	3:C:105:LYS:N	2.24	0.52
1:A:1134:GLU:OE1	1:A:1145:TYR:N	2.38	0.52
2:B:522:ARG:NH2	2:B:572:ALA:O	2.40	0.52
2:B:860:ASN:OD1	2:B:860:ASN:N	2.43	0.52
1:A:475:VAL:HG22	10:E:103:ILE:HG23	1.91	0.52
1:A:1095:LEU:HD21	1:A:1273:LEU:HD11	1.90	0.52
1:A:1174:TRP:CZ3	6:G:39:VAL:HG21	2.45	0.52
2:B:319:ILE:HG13	2:B:320:PHE:HD1	1.74	0.52
1:A:1355:MET:HA	1:A:1355:MET:HE3	1.90	0.52
1:A:1361:THR:O	4:D:198:ARG:NH2	2.38	0.52
1:A:1432:ASP:OD2	10:E:139:ARG:NH2	2.40	0.52
2:B:33:ALA:HA	2:B:729:LEU:HD22	1.90	0.52
2:B:599:LEU:HD21	2:B:621:TRP:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:HA	1:A:273:ASP:HB2	1.92	0.52
1:A:1300:ILE:O	1:A:1304:MET:HG3	2.09	0.51
2:B:510:GLU:HG2	2:B:512:LYS:HE2	1.92	0.51
1:A:18:ASP:OD2	1:A:171:ARG:NH2	2.42	0.51
1:A:117:ARG:NH2	1:A:187:ARG:O	2.42	0.51
1:A:1151:ASP:CG	1:A:1154:TRP:HE1	2.18	0.51
2:B:988:ARG:NH2	2:B:1117:ASP:OD1	2.41	0.51
1:A:142:PRO:HB3	1:A:158:GLN:HB2	1.91	0.51
1:A:191:SER:O	1:A:191:SER:OG	2.25	0.51
1:A:993:ARG:HD2	4:D:193:HIS:NE2	2.25	0.51
2:B:42:TYR:OH	2:B:522:ARG:HA	2.09	0.51
2:B:866:ILE:HB	2:B:1027:ILE:HB	1.92	0.51
4:D:9:TYR:HA	4:D:12:GLU:HG3	1.92	0.51
9:T:26:DT:H2'	9:T:27:DT:C6	2.46	0.51
10:E:126:THR:HB	10:E:130:GLN:HB2	1.92	0.51
4:D:98:SER:OG	4:D:99:LYS:NZ	2.44	0.51
1:A:512:ARG:HA	1:A:602:VAL:HG12	1.92	0.51
2:B:981:LEU:HD23	2:B:981:LEU:O	2.09	0.51
3:C:65:GLU:OE1	3:C:249:ARG:NH2	2.44	0.51
1:A:438:ASN:HB3	1:A:441:ILE:HD12	1.93	0.51
1:A:690:MET:HA	1:A:690:MET:HE3	1.92	0.51
1:A:972:PRO:HB2	1:A:987:ILE:HD13	1.92	0.51
1:A:1031:THR:HG21	10:E:70:VAL:HG21	1.92	0.51
1:A:559:LEU:HD11	1:A:635:ALA:HB1	1.91	0.51
1:A:1074:ILE:HA	1:A:1077:PRO:HG2	1.92	0.51
3:C:125:ILE:HD11	3:C:152:LEU:HG	1.93	0.51
3:C:236:ARG:NH1	3:C:359:ALA:OXT	2.44	0.51
1:A:241:PRO:HG2	1:A:244:LEU:HB2	1.93	0.51
1:A:426:SER:HB3	1:A:486:TRP:HB3	1.92	0.51
1:A:591:THR:HA	1:A:601:GLY:HA3	1.92	0.51
1:A:31:ILE:HD13	1:A:33:ASN:HB3	1.93	0.50
1:A:100:LEU:HD23	1:A:173:ILE:HD13	1.94	0.50
1:A:862:ALA:HB2	1:A:1351:ARG:HD2	1.94	0.50
2:B:926:VAL:HG22	2:B:964:VAL:HG22	1.93	0.50
2:B:442:ILE:O	2:B:446:LYS:HG2	2.10	0.50
5:F:35:TYR:HB3	5:F:45:ILE:HD13	1.91	0.50
1:A:1113:ILE:HD12	1:A:1308:ASN:HB3	1.93	0.50
2:B:483:GLU:O	2:B:487:ILE:HG12	2.10	0.50
3:C:236:ARG:HB2	3:C:358:ILE:HG21	1.94	0.50
4:D:146:GLU:O	4:D:149:GLU:HG3	2.12	0.50
6:G:73:CYS:HB2	6:G:81:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:PRO:HB3	1:A:1228:ARG:CZ	2.42	0.50
2:B:513:ASN:HA	2:B:811:TYR:HA	1.94	0.50
11:N:31:DC:H2"	11:N:32:DG:C8	2.47	0.50
1:A:315:LEU:HB3	2:B:1149:GLU:HG3	1.94	0.50
1:A:1154:TRP:CZ3	1:A:1209:MET:HG2	2.47	0.50
2:B:164:ARG:NH1	2:B:171:THR:OG1	2.45	0.50
2:B:905:LYS:HG2	2:B:951:ILE:HG23	1.94	0.50
2:B:1164:ILE:O	2:B:1168:SER:HB2	2.12	0.50
1:A:29:VAL:HG21	1:A:203:ILE:HG13	1.93	0.50
1:A:84:GLN:NE2	1:A:195:LYS:O	2.44	0.50
1:A:476:GLU:OE1	2:B:1162:GLN:HB2	2.11	0.50
2:B:821:MET:HB2	2:B:884:GLU:HG2	1.94	0.50
2:B:1053:LEU:O	7:H:52:LYS:HG3	2.11	0.50
2:B:285:ASP:HB3	6:G:3:ILE:HG13	1.94	0.49
2:B:458:THR:OG1	2:B:459:GLN:N	2.45	0.49
2:B:718:MET:HE1	2:B:737:ILE:HG21	1.94	0.49
2:B:797:VAL:O	2:B:801:THR:HG23	2.13	0.49
2:B:1045:THR:OG1	2:B:1106:THR:OG1	2.27	0.49
9:T:17:DC:H2"	9:T:18:DG:C8	2.46	0.49
9:T:22:DC:H2'	9:T:23:DG:C8	2.47	0.49
2:B:40:ILE:HD11	2:B:521:LEU:HB3	1.94	0.49
2:B:1206:ASP:OD2	2:B:1237:ARG:NH2	2.44	0.49
2:B:510:GLU:O	2:B:516:ASN:ND2	2.46	0.49
3:C:278:LYS:HG3	3:C:324:ILE:HG12	1.95	0.49
1:A:428:ILE:O	2:B:1158:GLN:NE2	2.35	0.49
2:B:234:SER:OG	2:B:375:HIS:ND1	2.38	0.49
2:B:416:LYS:O	2:B:417:ARG:NH1	2.43	0.49
2:B:586:LEU:HD23	2:B:664:LEU:HD11	1.93	0.49
10:E:126:THR:HG22	10:E:128:GLU:H	1.78	0.49
1:A:240:ILE:HD11	1:A:259:ASN:HB3	1.95	0.49
1:A:895:GLU:OE2	1:A:895:GLU:HA	2.13	0.49
1:A:971:LEU:HD23	1:A:999:ARG:HG3	1.95	0.49
2:B:886:LYS:HA	2:B:981:LEU:H	1.78	0.49
3:C:5:PHE:CE1	3:C:45:MET:HB3	2.48	0.49
1:A:302:ARG:O	1:A:309:ARG:N	2.32	0.49
1:A:523:ASN:HD22	3:C:211:THR:HA	1.76	0.49
4:D:102:ILE:O	4:D:106:ILE:HG12	2.13	0.49
10:E:113:ARG:NH1	10:E:141:MET:O	2.39	0.49
1:A:15:ILE:HD11	1:A:1400:VAL:HG12	1.94	0.48
1:A:141:HIS:ND1	1:A:142:PRO:O	2.47	0.48
1:A:166:TYR:CZ	1:A:252:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD13	10:E:146:LEU:HD13	1.95	0.48
2:B:146:GLU:N	2:B:146:GLU:OE1	2.46	0.48
3:C:76:GLY:O	3:C:79:LYS:NZ	2.43	0.48
2:B:887:VAL:HG11	2:B:934:ILE:HG21	1.94	0.48
1:A:620:ILE:HD13	1:A:632:MET:HG3	1.95	0.48
2:B:1067:ASN:ND2	2:B:1070:LEU:HD23	2.29	0.48
1:A:728:ASN:HB3	1:A:731:PHE:HB3	1.94	0.48
2:B:874:ARG:HG2	3:C:99:PHE:CE1	2.48	0.48
1:A:35:PHE:HZ	1:A:212:ILE:HD13	1.78	0.48
1:A:204:PRO:HG2	1:A:270:PHE:HZ	1.78	0.48
2:B:480:ARG:O	2:B:484:GLN:HG2	2.13	0.48
4:D:97:LEU:HD11	4:D:122:PRO:HD3	1.94	0.48
2:B:488:SER:OG	2:B:489:GLY:N	2.44	0.48
2:B:1059:ASP:OD2	2:B:1061:THR:OG1	2.28	0.48
3:C:70:MET:HE2	3:C:166:LYS:HE3	1.95	0.48
1:A:493:SER:OG	1:A:862:ALA:O	2.28	0.48
1:A:752:ILE:HB	1:A:788:ILE:HB	1.95	0.48
2:B:295:LEU:HD12	2:B:295:LEU:HA	1.61	0.48
2:B:538:ARG:O	2:B:542:MET:HG2	2.13	0.48
1:A:150:ASP:OD2	1:A:153:THR:OG1	2.31	0.48
1:A:1154:TRP:CH2	1:A:1224:ARG:HD2	2.49	0.48
1:A:320:TRP:HB3	2:B:1124:SER:HA	1.95	0.47
2:B:533:SER:HB2	11:N:26:DC:H1'	1.95	0.47
2:B:803:GLN:NE2	2:B:997:SER:OG	2.46	0.47
2:B:1043:ILE:HG21	2:B:1066:ILE:HD11	1.96	0.47
3:C:236:ARG:HH11	3:C:358:ILE:HG22	1.79	0.47
1:A:141:HIS:HE1	1:A:144:ILE:HD12	1.78	0.47
1:A:491:LYS:O	1:A:1349:ASN:N	2.41	0.47
5:F:30:GLU:O	5:F:34:ILE:HG13	2.14	0.47
1:A:897:GLU:HB2	1:A:961:TYR:CE1	2.49	0.47
1:A:900:ARG:NH1	1:A:903:LYS:HD3	2.29	0.47
4:D:22:LEU:HD11	4:D:52:ILE:HD12	1.96	0.47
6:G:51:ASP:OD1	6:G:52:LYS:N	2.47	0.47
2:B:305:MET:HE2	2:B:398:LEU:HB2	1.96	0.47
11:N:35:DG:H2'	11:N:36:DA:H8	1.80	0.47
1:A:65:GLN:O	1:A:67:LYS:N	2.42	0.47
1:A:881:GLU:HG2	1:A:898:PHE:CZ	2.49	0.47
2:B:202:VAL:HA	2:B:506:THR:HG22	1.97	0.47
2:B:1146:ARG:N	9:T:28:DT:OP1	2.47	0.47
3:C:78:TYR:OH	3:C:88:MET:O	2.27	0.47
11:N:32:DG:H1'	11:N:33:DG:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:GLU:OE1	4:D:188:SER:OG	2.25	0.47
2:B:51:MET:CE	2:B:168:ARG:HG3	2.45	0.47
2:B:321:GLN:OE1	2:B:321:GLN:HA	2.15	0.47
9:T:15:DG:H1'	9:T:16:DC:H5'	1.97	0.47
2:B:807:THR:CG2	2:B:1109:GLN:HB3	2.45	0.47
2:B:972:HIS:CE1	2:B:978:ILE:HG22	2.50	0.47
3:C:128:ARG:HB3	3:C:145:PRO:HB2	1.96	0.47
2:B:124:TYR:HB2	2:B:194:ILE:HB	1.97	0.47
2:B:420:GLY:O	2:B:422:GLY:N	2.48	0.47
2:B:830:GLU:HG3	2:B:847:LEU:HD23	1.96	0.47
1:A:134:CYS:SG	1:A:135:TYR:N	2.88	0.46
2:B:40:ILE:HD11	2:B:521:LEU:CB	2.45	0.46
2:B:274:LEU:O	2:B:278:MET:HG3	2.16	0.46
1:A:781:GLU:CD	2:B:767:ARG:HH22	2.23	0.46
1:A:911:ILE:HD13	4:D:193:HIS:HB3	1.98	0.46
1:A:934:VAL:HG13	1:A:1026:ILE:HD11	1.98	0.46
1:A:1098:LEU:HD12	1:A:1104:GLU:HA	1.97	0.46
1:A:1100:ASN:O	1:A:1103:VAL:HG12	2.15	0.46
2:B:155:PHE:CZ	2:B:470:LEU:HD23	2.50	0.46
2:B:563:GLU:OE2	2:B:563:GLU:N	2.35	0.46
2:B:1199:MET:HE3	2:B:1199:MET:HA	1.97	0.46
3:C:332:LEU:O	3:C:336:LEU:HG	2.15	0.46
9:T:25:DA:H2'	9:T:26:DT:C6	2.50	0.46
1:A:337:GLU:OE2	1:A:432:ARG:NH1	2.48	0.46
1:A:1243:ASP:OD1	1:A:1243:ASP:N	2.48	0.46
2:B:646:HIS:CD2	2:B:647:PRO:HD2	2.51	0.46
3:C:102:ILE:HG22	3:C:143:PHE:HB3	1.97	0.46
2:B:1089:PHE:HA	2:B:1096:TYR:HA	1.97	0.46
3:C:249:ARG:NH1	3:C:286:GLU:OE2	2.43	0.46
7:H:27:GLU:O	7:H:31:THR:HG23	2.16	0.46
1:A:1405:ASN:C	1:A:1405:ASN:HD22	2.24	0.46
3:C:302:ILE:HD12	3:C:305:ILE:HD12	1.97	0.46
1:A:310:ILE:HG21	1:A:1387:ALA:HA	1.98	0.46
4:D:30:LYS:HA	4:D:33:GLN:HG2	1.96	0.46
4:D:101:ASN:OD1	4:D:101:ASN:N	2.44	0.46
1:A:195:LYS:HE2	10:E:42:SER:HB2	1.98	0.46
1:A:557:SER:HB3	1:A:597:GLU:HA	1.97	0.46
1:A:1419:VAL:HG13	1:A:1425:MET:HE1	1.98	0.46
2:B:177:THR:O	2:B:181:GLU:HG3	2.15	0.46
4:D:10:ILE:HD11	4:D:55:VAL:HG11	1.98	0.46
4:D:104:ASP:O	4:D:108:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:PRO:O	1:A:611:GLY:HA2	2.15	0.46
1:A:1159:LEU:HD23	1:A:1159:LEU:HA	1.69	0.46
5:F:5:LYS:HD3	5:F:7:PHE:CZ	2.51	0.46
1:A:128:GLN:HG2	1:A:129:THR:H	1.81	0.46
1:A:361:ARG:O	1:A:364:PRO:HD2	2.16	0.46
1:A:1241:ALA:HB1	1:A:1245:LYS:HD2	1.97	0.46
2:B:891:SER:OG	2:B:892:ASP:N	2.47	0.46
9:T:28:DT:H5'	9:T:29:DG:OP2	2.16	0.46
1:A:171:ARG:HB2	1:A:197:VAL:HG11	1.98	0.45
2:B:206:GLU:HB2	2:B:526:THR:HA	1.97	0.45
2:B:715:THR:OG1	2:B:718:MET:HG3	2.16	0.45
2:B:870:SER:O	2:B:874:ARG:HG3	2.16	0.45
2:B:234:SER:HB3	2:B:374:PRO:HD2	1.97	0.45
6:G:58:LYS:HB3	6:G:58:LYS:HE3	1.56	0.45
1:A:108:ASP:HB3	1:A:111:ARG:HB3	1.99	0.45
2:B:42:TYR:CE1	2:B:204:LEU:HD11	2.52	0.45
2:B:1223:MET:HE3	2:B:1230:ILE:HG13	1.98	0.45
2:B:448:LEU:O	2:B:452:THR:HB	2.17	0.45
1:A:320:TRP:CE2	2:B:1135:PRO:HG3	2.52	0.45
1:A:330:ASN:ND2	1:A:445:GLN:OE1	2.49	0.45
1:A:1185:MET:HE3	1:A:1185:MET:HB3	1.73	0.45
1:A:1396:THR:O	1:A:1400:VAL:HG22	2.15	0.45
2:B:473:ASN:O	2:B:496:ARG:NH1	2.48	0.45
2:B:337:SER:HB3	2:B:364:GLN:HG3	1.98	0.45
2:B:1088:MET:HE3	2:B:1101:ILE:HB	1.98	0.45
7:H:21:PHE:HB2	7:H:58:LEU:CD1	2.47	0.45
2:B:58:ILE:HG23	2:B:430:LYS:HG3	1.99	0.45
2:B:281:MET:O	2:B:281:MET:HG3	2.17	0.45
2:B:324:GLN:HG2	2:B:325:HIS:CE1	2.52	0.45
5:F:4:GLN:OE1	5:F:75:SER:OG	2.29	0.45
1:A:1227:LEU:H	1:A:1227:LEU:HD12	1.81	0.45
2:B:1047:VAL:HG22	2:B:1071:LEU:HD22	1.99	0.45
1:A:672:GLU:OE1	1:A:714:ARG:NH2	2.44	0.45
1:A:1024:ASP:N	1:A:1024:ASP:OD1	2.50	0.45
3:C:284:LYS:HE3	3:C:284:LYS:HB3	1.76	0.45
1:A:522:MET:HE2	1:A:522:MET:HB3	1.89	0.45
2:B:369:ASP:OD1	2:B:369:ASP:C	2.60	0.45
2:B:379:THR:HG23	2:B:381:ASP:N	2.30	0.45
2:B:70:LYS:HA	2:B:84:SER:HA	1.99	0.44
4:D:29:ASP:OD1	4:D:29:ASP:N	2.47	0.44
5:F:52:ILE:HG12	5:F:73:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ARG:NE	10:E:100:SER:OG	2.34	0.44
1:A:1155:MET:HG3	1:A:1209:MET:SD	2.58	0.44
3:C:254:GLN:O	3:C:258:GLU:HG2	2.18	0.44
3:C:277:THR:HG23	3:C:327:ALA:O	2.17	0.44
9:T:12:DT:H2"	9:T:13:DT:C6	2.52	0.44
3:C:124:THR:OG1	7:H:77:ARG:NH1	2.50	0.44
5:F:43:SER:HB3	5:F:78:VAL:HB	1.99	0.44
1:A:49:ARG:O	1:A:61:THR:OG1	2.25	0.44
2:B:830:GLU:OE1	7:H:72:THR:OG1	2.36	0.44
5:F:58:PHE:HE1	10:E:120:MET:HE1	1.80	0.44
7:H:29:ILE:O	7:H:33:MET:HG2	2.18	0.44
1:A:100:LEU:HD13	1:A:142:PRO:HD2	1.99	0.44
1:A:422:SER:HB3	2:B:1154:VAL:HG21	2.00	0.44
1:A:1019:MET:HE2	1:A:1019:MET:HB2	1.90	0.44
1:A:1378:GLU:HG2	1:A:1408:TYR:OH	2.17	0.44
2:B:1087:LYS:HG3	3:C:203:SER:HB2	1.99	0.44
3:C:233:GLN:HG2	3:C:236:ARG:NH2	2.33	0.44
1:A:361:ARG:HE	10:E:100:SER:HG	1.61	0.44
2:B:27:LEU:HD22	2:B:837:ILE:HD12	1.98	0.44
2:B:258:ILE:HB	2:B:275:ILE:HD12	1.99	0.44
2:B:305:MET:HE2	2:B:398:LEU:CB	2.48	0.44
2:B:479:ASN:OD1	2:B:479:ASN:C	2.61	0.44
1:A:25:GLY:HA3	1:A:75:ILE:HG13	2.00	0.44
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.79	0.44
6:G:16:VAL:HA	6:G:17:ASP:HA	1.57	0.44
1:A:130:GLU:HG3	1:A:143:LYS:HB2	1.99	0.44
1:A:698:HIS:HA	6:G:90:LYS:HD2	1.99	0.44
2:B:795:ALA:O	2:B:799:TYR:HD1	1.99	0.44
2:B:843:ILE:HD11	7:H:74:LEU:HD13	2.00	0.44
2:B:966:ASP:OD2	2:B:983:ARG:NH2	2.46	0.44
3:C:127:SER:OG	3:C:147:PHE:HB2	2.18	0.44
4:D:153:ARG:NH1	4:D:154:GLU:OE2	2.48	0.44
2:B:28:SER:O	2:B:722:ILE:HG21	2.18	0.44
2:B:487:ILE:HD12	9:T:33:DA:H5"	1.99	0.44
2:B:815:TRP:CG	2:B:816:PRO:HD3	2.53	0.44
1:A:1101:PRO:HA	1:A:1104:GLU:HG2	2.00	0.43
2:B:59:VAL:HA	2:B:63:PHE:HD2	1.83	0.43
2:B:335:PHE:C	2:B:335:PHE:CD1	2.95	0.43
2:B:1139:LYS:HE3	9:T:30:DT:OP1	2.18	0.43
4:D:94:LYS:HE2	4:D:94:LYS:HB3	1.87	0.43
5:F:58:PHE:HB2	5:F:69:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:THR:HG22	1:A:536:THR:HG22	2.00	0.43
1:A:1374:LEU:HD11	1:A:1384:LEU:HD21	2.00	0.43
3:C:13:PHE:HD2	3:C:40:PRO:HB2	1.83	0.43
3:C:272:MET:SD	3:C:278:LYS:HB2	2.57	0.43
4:D:22:LEU:HD21	4:D:46:GLU:HB2	1.99	0.43
1:A:1078:GLN:O	1:A:1082:SER:OG	2.15	0.43
2:B:235:GLN:HG2	2:B:238:GLY:O	2.19	0.43
3:C:178:LEU:O	3:C:224:PRO:HD3	2.18	0.43
1:A:884:PHE:HA	1:A:1009:VAL:HG21	2.00	0.43
2:B:316:LEU:HB3	2:B:321:GLN:HE22	1.83	0.43
2:B:573:ILE:HG23	2:B:574:THR:HG23	1.99	0.43
2:B:1138:GLY:H	2:B:1144:GLY:HA3	1.84	0.43
1:A:697:THR:HB	6:G:89:GLN:HA	2.00	0.43
2:B:12:PRO:HD2	2:B:12:PRO:O	2.18	0.43
2:B:699:LYS:HB2	2:B:699:LYS:HE2	1.63	0.43
2:B:799:TYR:HD2	2:B:1003:LYS:HZ1	1.64	0.43
2:B:894:GLU:HA	2:B:938:ALA:HA	2.00	0.43
2:B:1088:MET:HE3	2:B:1088:MET:HB2	1.90	0.43
1:A:866:GLU:OE2	1:A:933:ASN:ND2	2.47	0.43
1:A:920:PHE:CE1	1:A:1294:LYS:HE3	2.54	0.43
5:F:45:ILE:HA	5:F:78:VAL:HA	2.01	0.43
10:E:49:PHE:CZ	10:E:51:GLN:HA	2.54	0.43
1:A:1127:LEU:HB2	1:A:1179:GLU:HG2	2.00	0.43
2:B:50:LEU:HD13	2:B:426:ALA:HB2	2.00	0.43
2:B:609:ARG:HG2	2:B:609:ARG:NH1	2.33	0.43
2:B:860:ASN:O	2:B:1029:ASN:HB2	2.18	0.43
3:C:46:ASP:OD1	3:C:218:ARG:HD3	2.18	0.43
10:E:100:SER:OG	10:E:100:SER:O	2.31	0.43
2:B:604:ASN:HA	2:B:607:ILE:HD12	2.00	0.43
2:B:1050:ALA:HB2	2:B:1075:LEU:HD23	2.00	0.43
3:C:350:LEU:HD23	3:C:350:LEU:HA	1.87	0.43
6:G:14:THR:HG21	6:G:23:ARG:HB3	2.00	0.43
1:A:199:LYS:HA	1:A:199:LYS:HD2	1.81	0.43
4:D:6:LEU:HD11	4:D:123:TYR:CD1	2.54	0.43
4:D:73:THR:O	4:D:77:ASN:ND2	2.47	0.43
6:G:19:ASN:OD1	6:G:19:ASN:N	2.51	0.43
5:F:32:GLU:O	5:F:36:VAL:HB	2.19	0.43
2:B:996:MET:HE3	2:B:996:MET:HB2	1.70	0.42
8:P:22:C:H2'	8:P:23:U:C6	2.54	0.42
1:A:35:PHE:HE2	1:A:212:ILE:HG21	1.84	0.42
1:A:116:ILE:HD11	1:A:119:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLY:O	1:A:312:LYS:HB3	2.19	0.42
1:A:1433:GLU:O	1:A:1437:THR:OG1	2.27	0.42
2:B:40:ILE:HD12	2:B:40:ILE:HA	1.78	0.42
2:B:316:LEU:HB3	2:B:321:GLN:NE2	2.34	0.42
2:B:917:VAL:HG22	2:B:922:PRO:HD3	2.00	0.42
1:A:379:VAL:HG22	1:A:405:LEU:HD12	2.01	0.42
1:A:541:PHE:CZ	1:A:558:MET:HE1	2.54	0.42
2:B:323:VAL:HG13	2:B:335:PHE:HD2	1.84	0.42
3:C:113:LEU:O	3:C:159:ILE:HA	2.19	0.42
1:A:889:ILE:HB	1:A:894:PHE:CE2	2.51	0.42
2:B:158:SER:CB	2:B:478:LEU:HD22	2.49	0.42
2:B:486:ILE:O	2:B:506:THR:OG1	2.28	0.42
2:B:689:LYS:HB3	2:B:689:LYS:HE3	1.74	0.42
2:B:1018:THR:HG23	2:B:1022:LEU:O	2.19	0.42
3:C:249:ARG:O	3:C:253:ILE:HD12	2.19	0.42
6:G:54:LYS:HB3	6:G:54:LYS:HE3	1.81	0.42
1:A:340:TYR:CE1	1:A:465:LEU:HD22	2.54	0.42
1:A:1145:TYR:CE1	6:G:38:LEU:HB2	2.54	0.42
2:B:1136:LEU:HD23	2:B:1136:LEU:HA	1.89	0.42
3:C:339:SER:O	3:C:343:ILE:HG13	2.20	0.42
1:A:870:PHE:HD2	1:A:1000:MET:HE2	1.85	0.42
1:A:1339:ILE:O	1:A:1343:MET:HG2	2.20	0.42
2:B:265:PHE:HE2	2:B:336:LEU:HD21	1.84	0.42
10:E:99:TYR:CZ	10:E:108:GLN:HG3	2.54	0.42
1:A:1133:TYR:CZ	6:G:15:TYR:HB3	2.54	0.42
2:B:365:LEU:HD21	2:B:383:ARG:CZ	2.49	0.42
5:F:34:ILE:O	5:F:38:LYS:HD2	2.19	0.42
5:F:45:ILE:HD11	5:F:48:ILE:HD13	2.01	0.42
6:G:100:TYR:OH	6:G:102:SER:HB2	2.20	0.42
9:T:18:DG:H1'	9:T:19:DT:H5'	2.00	0.42
10:E:137:ASN:HD21	10:E:139:ARG:NH2	2.18	0.42
1:A:59:CYS:O	1:A:61:THR:N	2.46	0.42
1:A:989:VAL:O	1:A:993:ARG:HG2	2.18	0.42
2:B:451:GLN:O	2:B:452:THR:OG1	2.34	0.42
2:B:889:LEU:HD23	2:B:889:LEU:HA	1.82	0.42
1:A:314:LEU:O	2:B:1213:ARG:NH2	2.52	0.42
1:A:529:GLY:HA2	1:A:532:GLN:HG3	2.02	0.42
2:B:55:ILE:HG21	2:B:96:ILE:HD11	2.00	0.42
2:B:535:GLN:HE22	9:T:24:DT:H2''	1.85	0.42
9:T:14:DC:H2''	9:T:15:DG:N7	2.34	0.42
2:B:293:PHE:HA	2:B:604:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:ARG:HD2	2:B:480:ARG:C	2.45	0.42
2:B:906:ASN:CG	2:B:906:ASN:O	2.62	0.42
2:B:1113:LYS:HB3	2:B:1113:LYS:HE3	1.63	0.42
1:A:1425:MET:HE2	1:A:1425:MET:HB2	1.86	0.41
1:A:1436:ILE:HG23	1:A:1440:TYR:HB2	2.02	0.41
2:B:96:ILE:HG12	2:B:128:VAL:HG22	2.01	0.41
2:B:605:LYS:HB2	2:B:605:LYS:HE3	1.76	0.41
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.87	0.41
1:A:1138:SER:HB2	1:A:1167:PRO:HG2	2.01	0.41
3:C:274:GLU:C	3:C:276:LYS:H	2.29	0.41
3:C:319:MET:HB3	3:C:319:MET:HE3	1.79	0.41
4:D:202:LYS:NZ	4:D:203:SER:O	2.38	0.41
1:A:419:ARG:HD3	1:A:456:ALA:HB2	2.01	0.41
2:B:461:ASN:HD22	2:B:461:ASN:HA	1.60	0.41
6:G:86:ILE:HD11	6:G:93:ILE:HD12	2.02	0.41
1:A:88:ILE:HD13	1:A:88:ILE:HA	1.87	0.41
1:A:131:GLY:HA2	1:A:140:VAL:HG13	2.01	0.41
1:A:380:TYR:HD1	1:A:387:VAL:HG13	1.84	0.41
1:A:1028:LEU:O	1:A:1032:GLN:HG3	2.20	0.41
2:B:331:LYS:O	2:B:331:LYS:HD3	2.20	0.41
2:B:822:ASN:HA	2:B:881:PHE:CZ	2.55	0.41
2:B:863:ASP:O	2:B:1004:GLY:HA2	2.20	0.41
6:G:1:MET:SD	6:G:3:ILE:HD11	2.61	0.41
2:B:388:ARG:NH1	2:B:599:LEU:O	2.53	0.41
2:B:1075:LEU:HD23	2:B:1075:LEU:HA	1.89	0.41
2:B:1082:PHE:HB3	3:C:200:MET:SD	2.60	0.41
3:C:357:LEU:HD23	3:C:357:LEU:HA	1.83	0.41
6:G:52:LYS:HE2	6:G:53:TYR:CE2	2.56	0.41
6:G:75:ASN:OD1	6:G:75:ASN:C	2.63	0.41
1:A:430:VAL:HG21	1:A:477:ALA:HB1	2.03	0.41
2:B:830:GLU:HG2	7:H:73:THR:HA	2.01	0.41
4:D:64:TYR:CE1	4:D:74:LEU:HB2	2.55	0.41
6:G:71:LYS:HE2	6:G:71:LYS:HB2	1.83	0.41
1:A:237:ASN:HA	1:A:263:ILE:HD11	2.03	0.41
2:B:599:LEU:HA	2:B:599:LEU:HD23	1.76	0.41
3:C:101:PRO:HD2	3:C:147:PHE:CZ	2.55	0.41
3:C:276:LYS:HG3	3:C:326:LYS:HG3	2.01	0.41
6:G:100:TYR:CZ	6:G:102:SER:HB2	2.56	0.41
2:B:439:ALA:HB3	2:B:440:PRO:HD2	2.02	0.41
2:B:929:LYS:HD3	2:B:929:LYS:HA	1.82	0.41
4:D:192:MET:O	4:D:193:HIS:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:GLU:HG2	2:B:794:PRO:HB3	2.03	0.41
1:A:1374:LEU:HD12	1:A:1374:LEU:HA	1.90	0.41
2:B:404:VAL:HA	6:G:52:LYS:HE3	2.02	0.41
2:B:741:ILE:HG23	2:B:745:GLU:HG2	2.03	0.41
2:B:803:GLN:HE22	2:B:1001:GLY:HA2	1.86	0.41
2:B:1088:MET:HB3	2:B:1097:PHE:HD2	1.86	0.41
6:G:3:ILE:HD13	6:G:3:ILE:HA	1.85	0.41
1:A:127:SER:OG	1:A:128:GLN:N	2.54	0.41
1:A:330:ASN:HB2	1:A:445:GLN:HB3	2.02	0.41
1:A:1431:MET:SD	5:F:16:PRO:HB2	2.61	0.40
2:B:260:ILE:HG21	2:B:371:ILE:HG13	2.03	0.40
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.88	0.40
2:B:912:ASN:C	2:B:914:GLU:H	2.29	0.40
1:A:31:ILE:HD12	1:A:31:ILE:C	2.47	0.40
2:B:41:GLY:O	2:B:45:LYS:HB2	2.21	0.40
2:B:91:PHE:CD2	2:B:132:ALA:HB2	2.56	0.40
2:B:96:ILE:HA	2:B:127:PRO:O	2.21	0.40
2:B:272:TRP:HH2	2:B:288:ILE:HD13	1.86	0.40
2:B:803:GLN:NE2	2:B:1001:GLY:HA2	2.36	0.40
2:B:920:PHE:CE2	2:B:934:ILE:HG12	2.56	0.40
3:C:103:TYR:CE2	3:C:105:LYS:HD2	2.57	0.40
3:C:301:MET:SD	3:C:338:LYS:HG2	2.61	0.40
1:A:78:MET:O	1:A:199:LYS:HE2	2.22	0.40
1:A:251:LYS:HD2	1:A:251:LYS:HA	1.83	0.40
1:A:517:MET:HE1	3:C:192:TYR:CE2	2.49	0.40
1:A:777:ARG:HG2	1:A:778:PHE:CD2	2.55	0.40
2:B:868:SER:HB3	2:B:871:PHE:HB3	2.02	0.40
3:C:262:GLU:HA	3:C:263:PRO:HD3	1.97	0.40
5:F:4:GLN:HE22	5:F:49:THR:HG21	1.86	0.40
1:A:271:LEU:O	1:A:300:MET:HB2	2.21	0.40
1:A:376:CYS:HA	1:A:407:ARG:HA	2.03	0.40
1:A:744:ASN:HA	2:B:1037:MET:CE	2.51	0.40
1:A:1329:GLU:HG3	4:D:184:ILE:HD13	2.03	0.40
3:C:74:LYS:HG3	3:C:162:ASP:HB3	2.04	0.40
3:C:335:LEU:HD23	3:C:335:LEU:HA	1.95	0.40
7:H:9:THR:HB	7:H:65:CYS:HB2	2.03	0.40
1:A:1074:ILE:HA	1:A:1074:ILE:HD13	1.86	0.40
1:A:1159:LEU:HD21	1:A:1167:PRO:HD3	2.04	0.40
1:A:1209:MET:HE3	1:A:1209:MET:HB2	1.87	0.40
2:B:202:VAL:HG22	2:B:506:THR:HG22	2.03	0.40
2:B:279:PHE:HB2	2:B:387:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1377/1441 (96%)	1317 (96%)	60 (4%)	0	100	100
2	B	1155/1233 (94%)	1077 (93%)	72 (6%)	6 (0%)	24	46
3	C	356/358 (99%)	340 (96%)	15 (4%)	1 (0%)	36	58
4	D	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	F	78/80 (98%)	73 (94%)	3 (4%)	2 (3%)	4	7
6	G	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	12	28
7	H	67/80 (84%)	67 (100%)	0	0	100	100
10	E	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
All	All	3444/3609 (95%)	3264 (95%)	170 (5%)	10 (0%)	37	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	361	ASN
2	B	904	THR
5	F	45	ILE
3	C	273	ASP
5	F	70	MET
6	G	49	MET
2	B	934	ILE
2	B	1145	LEU
2	B	1161	MET
2	B	890	GLU

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	1235/1270 (97%)	1203 (97%)	32 (3%)	40	68
2	B	1017/1072 (95%)	998 (98%)	19 (2%)	50	75
3	C	327/327 (100%)	321 (98%)	6 (2%)	51	76
4	D	185/185 (100%)	182 (98%)	3 (2%)	55	79
5	F	74/74 (100%)	70 (95%)	4 (5%)	20	42
6	G	95/95 (100%)	92 (97%)	3 (3%)	34	62
7	H	63/71 (89%)	61 (97%)	2 (3%)	34	62
10	E	99/99 (100%)	94 (95%)	5 (5%)	21	45
All	All	3095/3193 (97%)	3021 (98%)	74 (2%)	43	70

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	A	99	CYS
1	A	107	VAL
1	A	145	VAL
1	A	163	ASP
1	A	178	THR
1	A	185	LEU
1	A	245	GLN
1	A	274	SER
1	A	321	SER
1	A	417	PHE
1	A	427	SER
1	A	443	THR
1	A	471	VAL
1	A	505	VAL
1	A	723	ILE
1	A	821	SER
1	A	868	VAL
1	A	879	GLU

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Mol	Chain	Res	Type
1	A	996	SER
1	A	1053	LEU
1	A	1091	SER
1	A	1121	THR
1	A	1155	MET
1	A	1160	GLU
1	A	1211	SER
1	A	1215	THR
1	A	1262	ILE
1	A	1279	ASP
1	A	1318	SER
1	A	1359	LEU
1	A	1402	SER
2	B	36	SER
2	B	84	SER
2	B	159	THR
2	B	242	ASN
2	B	304	PHE
2	B	402	MET
2	B	421	SER
2	B	458	THR
2	B	504	VAL
2	B	519	SER
2	B	558	SER
2	B	626	THR
2	B	670	THR
2	B	766	THR
2	B	887	VAL
2	B	1012	THR
2	B	1198	CYS
2	B	1202	ASP
2	B	1231	THR
3	C	9	GLU
3	C	180	VAL
3	C	226	VAL
3	C	252	SER
3	C	285	ASP
3	C	357	LEU
4	D	101	ASN
4	D	195	VAL
4	D	196	VAL
5	F	49	THR

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Mol	Chain	Res	Type
5	F	51	VAL
5	F	52	ILE
5	F	72	VAL
6	G	86	ILE
6	G	89	GLN
6	G	101	MET
7	H	30	LYS
7	H	54	LEU
10	E	44	SER
10	E	115	ILE
10	E	125	VAL
10	E	126	THR
10	E	146	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	462	GLN
1	A	523	ASN
1	A	585	ASN
1	A	592	GLN
1	A	637	GLN
1	A	667	GLN
1	A	721	ASN
1	A	747	HIS
1	A	826	ASN
1	A	1055	GLN
1	A	1070	ASN
1	A	1078	GLN
1	A	1090	GLN
1	A	1106	ASN
2	B	100	GLN
2	B	115	ASN
2	B	129	ASN
2	B	172	HIS
2	B	334	GLN
2	B	361	ASN
2	B	479	ASN
2	B	525	ASN
2	B	527	HIS
2	B	597	GLN

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Mol	Chain	Res	Type
2	B	829	ASN
2	B	845	ASN
2	B	869	GLN
2	B	1039	ASN
2	B	1067	ASN
2	B	1086	GLN
2	B	1193	HIS
2	B	1204	GLN
2	B	1229	ASN
3	C	118	ASN
3	C	153	GLN
3	C	353	ASN
6	G	36	ASN
6	G	77	HIS
6	G	83	GLN
10	E	51	GLN
10	E	85	GLN
10	E	112	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	P	8/9 (88%)	3 (37%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	P	23	U
8	P	24	A
8	P	28	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38745. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.