



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jun 3, 2019 – 01:02 PM EDT

PDB ID : 6DRD
EMDB ID: : EMD-7997
Title : RNA Pol II(G)
Authors : Yu, X.; Jishage, M.; Shi, Y.; Ganesan, S.; Sali, A.; Chait, B.T.; Asturias, F.;
Roeder, R.G.
Deposited on : 2018-06-11
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

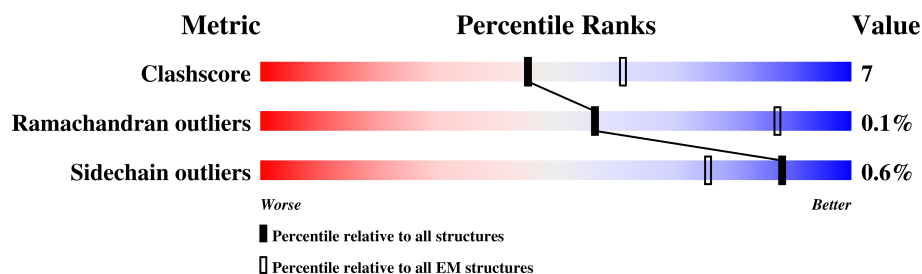
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






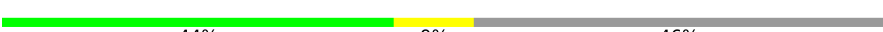



The reported resolution of this entry is 3.90 Å.

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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1970	 41% 9% 49%
2	B	1174	 70% 15% 14%
3	C	275	 76% 19% 5%
4	D	142	 78% 11% • 10%
5	E	210	 64% 23% 12%
6	F	127	 44% 9% 46%
7	G	172	 77% 20% •
8	H	150	 72% 25% •
9	I	125	 74% 14% • 12%

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Mol	Chain	Length	Quality of chain
10	J	67	<div><div></div><div>84%</div><div>9%</div><div></div><div></div></div>
11	K	117	<div><div></div><div>79%</div><div>15%</div><div>5%</div></div>
12	L	58	<div><div></div><div>48%</div><div>16%</div><div>36%</div></div>
13	M	62	<div><div></div><div>89%</div><div>11%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26708 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1000	Total	C	N	O	S	0	0
			7989	5045	1409	1493	42		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1835	THR	ALA	conflict	UNP P24928

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1009	Total	C	N	O	S	0	0
			8079	5127	1403	1499	50		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2104	1321	361	416	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1529	976	267	279	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388
E	132	GLU	GLN	conflict	UNP P19388
E	157	SER	THR	conflict	UNP P19388
E	186	ARG	LYS	conflict	UNP P19388

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	68	Total	C	N	O	S	0	0
			549	356	95	93	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	167	Total	C	N	O	S	0	0
			1307	850	211	238	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	146	Total	C	N	O	S	0	0
			1176	744	192	235	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	110	Total	C	N	O	S	0	0
			897	554	159	173	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			890	576	147	166	1		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	37	Total	C	N	O	S	0	0
			312	195	58	53	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit GRINL1A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	62	Total	C	N	O	0	0
			359	219	67	73		

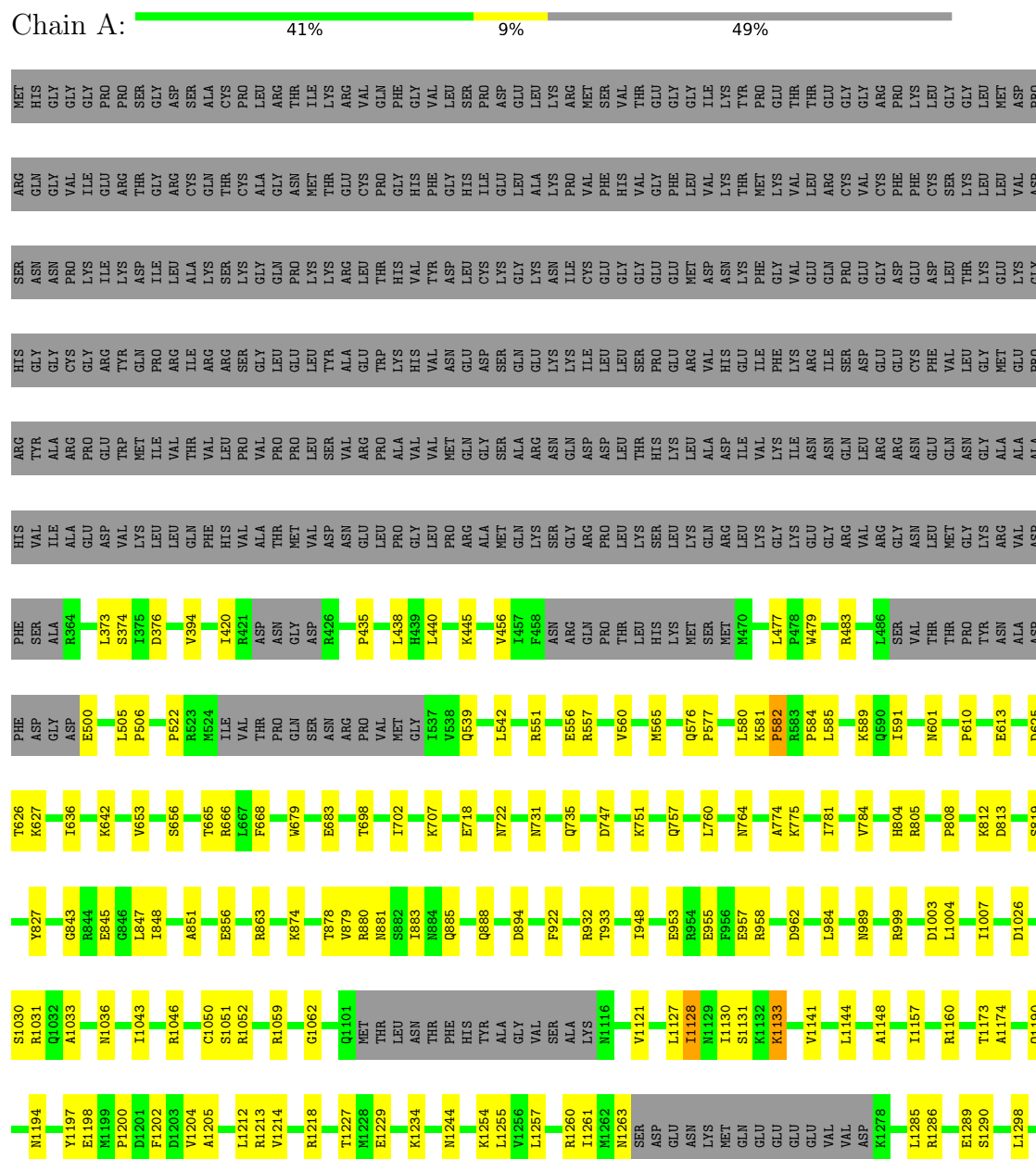
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	J	1	Total	Zn	0
			1	1	
14	I	2	Total	Zn	0
			2	2	
14	L	1	Total	Zn	0
			1	1	
14	C	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 II subunit RPB1



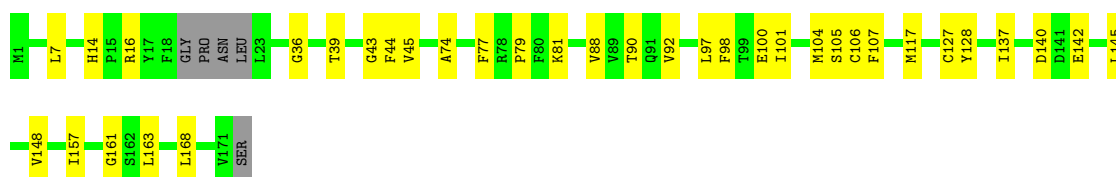
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- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:  70% 15% 14%

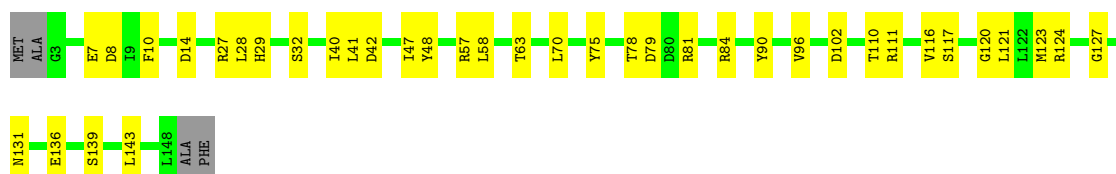
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- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 72% 25%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 74% 14% 12%



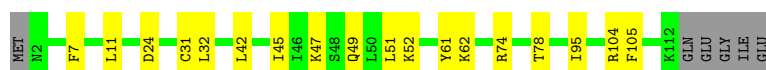
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 84% 9%



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 79% 15% 5%



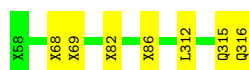
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 48% 16% 36%



- Molecule 13: DNA-directed RNA polymerase II subunit GRINL1A

Chain M: 89% 11%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: 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 >2	RMSZ	# Z >2
1	A	0.46	0/8130	0.62	0/10980
10	J	0.59	0/516	0.72	0/696
11	K	0.46	0/909	0.64	0/1232
12	L	0.48	0/315	0.67	0/416
13	M	0.30	0/134	0.81	0/179
2	B	0.55	0/8240	0.67	0/11128
3	C	0.54	0/2147	0.64	0/2917
4	D	0.26	0/1019	0.51	0/1374
5	E	0.42	0/1552	0.61	0/2091
6	F	0.40	0/558	0.62	0/752
7	G	0.32	0/1336	0.56	0/1811
8	H	0.48	0/1197	0.65	0/1614
9	I	0.41	0/917	0.60	0/1241
All	All	0.48	0/26970	0.63	0/36431

There are no bond length outliers.

There are no bond angle outliers.

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	7989	0	8058	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8079	0	8123	121	0
3	C	2104	0	2053	37	0
4	D	1005	0	964	15	0
5	E	1529	0	1565	31	0
6	F	549	0	590	8	0
7	G	1307	0	1305	20	0
8	H	1176	0	1137	28	0
9	I	897	0	831	15	0
10	J	507	0	523	9	0
11	K	890	0	913	14	0
12	L	312	0	311	5	0
13	M	359	0	195	3	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
All	All	26708	0	26568	387	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 7.

All (387) 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)
10:J:9:THR:HB	10:J:44:CYS:SG	1.82	1.20
4:D:87:LEU:HB3	4:D:97:LEU:HD11	1.15	1.09
8:H:96:VAL:HG12	8:H:116:VAL:CG2	1.87	1.05
8:H:96:VAL:CG1	8:H:116:VAL:HG22	1.90	1.01
1:A:863:ARG:HH21	1:A:1128:ILE:HG21	1.24	1.01
8:H:96:VAL:HG12	8:H:116:VAL:HG22	0.95	0.90
1:A:863:ARG:NH2	1:A:1128:ILE:HG21	1.87	0.89
1:A:863:ARG:NH2	1:A:1128:ILE:CG2	2.40	0.84
1:A:863:ARG:HH21	1:A:1128:ILE:CG2	1.90	0.83
13:M:68:UNK:O	13:M:69:UNK:CB	2.30	0.79
1:A:1133:LYS:NZ	1:A:1133:LYS:HB3	2.03	0.73
1:A:1127:LEU:HD22	1:A:1362:ILE:CD1	2.19	0.71
4:D:87:LEU:CB	4:D:97:LEU:HD11	2.08	0.71
2:B:249:LYS:HE3	2:B:255:ARG:HH21	1.55	0.71
2:B:803:ARG:NH1	10:J:8:PHE:O	2.24	0.70
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.75	0.68
7:G:36:GLY:H	7:G:45:VAL:HB	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:TRP:HB2	1:A:483:ARG:HH22	1.59	0.67
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.76	0.66
9:I:69:ILE:HG22	9:I:71:ASP:H	1.62	0.65
5:E:56:THR:HG22	5:E:58:LEU:H	1.63	0.64
2:B:941:GLN:NE2	2:B:977:THR:OG1	2.31	0.64
3:C:67:ARG:NH1	3:C:150:ILE:O	2.31	0.64
1:A:1227:THR:HG22	1:A:1229:GLU:H	1.61	0.63
1:A:610:PRO:HG2	1:A:613:GLU:HB2	1.80	0.63
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.81	0.63
1:A:1133:LYS:HZ2	1:A:1133:LYS:HB3	1.61	0.63
3:C:117:SER:HB3	3:C:148:ILE:HB	1.80	0.63
2:B:89:GLU:HB3	2:B:127:ASP:HB2	1.80	0.62
3:C:88:CYS:SG	3:C:89:THR:N	2.72	0.62
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.82	0.62
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.82	0.62
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.81	0.62
5:E:24:ARG:NH1	5:E:182:TYR:O	2.32	0.62
1:A:589:LYS:NZ	1:A:625:ASP:OD2	2.32	0.62
5:E:194:ILE:HG22	5:E:204:ILE:HG12	1.82	0.61
2:B:281:ASP:HB2	9:I:22:ASN:HA	1.82	0.61
1:A:1148:ALA:HB1	1:A:1333:GLU:HB2	1.81	0.61
12:L:26:ASN:ND2	12:L:36:CYS:SG	2.73	0.61
1:A:1213:ARG:HH22	1:A:1254:LYS:HE2	1.66	0.61
2:B:904:VAL:HG22	2:B:923:VAL:HG22	1.81	0.61
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.82	0.60
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.34	0.60
2:B:927:ARG:NH1	2:B:1054:MET:SD	2.74	0.60
7:G:44:PHE:HB2	7:G:77:PHE:HB3	1.82	0.60
2:B:111:ASN:ND2	2:B:175:ASN:O	2.33	0.60
2:B:177:CYS:HB3	2:B:180:ASP:HB2	1.84	0.60
3:C:205:LYS:NZ	3:C:212:ASP:O	2.35	0.60
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.83	0.60
1:A:1026:ASP:OD1	1:A:1031:ARG:NH2	2.35	0.60
1:A:1157:ILE:HD13	1:A:1160:ARG:HH12	1.67	0.59
2:B:625:LEU:HD12	2:B:665:ILE:HD12	1.84	0.59
7:G:100:GLU:HA	7:G:105:SER:HA	1.84	0.59
1:A:804:HIS:NE2	2:B:381:GLU:OE2	2.34	0.59
9:I:39:CYS:SG	9:I:40:ARG:N	2.76	0.59
1:A:878:THR:OG1	1:A:880:ARG:NH1	2.36	0.59
2:B:484:ARG:HH21	2:B:525:ASN:HD21	1.50	0.59
1:A:1130:ILE:HG22	1:A:1130:ILE:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:PRO:O	11:K:104:ARG:NH1	2.31	0.59
2:B:803:ARG:HD2	10:J:8:PHE:HA	1.85	0.59
8:H:111:ARG:HD2	8:H:127:GLY:HA2	1.85	0.58
2:B:192:LYS:HE2	2:B:469:VAL:HG22	1.85	0.58
2:B:861:SER:HA	2:B:901:THR:HG23	1.85	0.58
12:L:19:CYS:SG	12:L:20:GLY:N	2.75	0.58
1:A:500:GLU:OE2	2:B:1058:LYS:NZ	2.37	0.58
2:B:993:LYS:HE3	2:B:995:GLU:HB2	1.85	0.58
6:F:57:MET:HB2	6:F:123:LEU:HD21	1.86	0.58
7:G:127:CYS:HB2	7:G:137:ILE:HB	1.85	0.58
1:A:551:ARG:HH22	8:H:27:ARG:HH22	1.51	0.57
1:A:1359:SER:O	1:A:1365:ILE:HD11	2.04	0.57
4:D:117:SER:O	4:D:121:ARG:NH1	2.37	0.57
1:A:1050:CYS:SG	1:A:1051:SER:N	2.78	0.57
9:I:17:CYS:HB3	9:I:22:ASN:H	1.68	0.57
2:B:44:LEU:HD22	2:B:158:SER:HB3	1.87	0.57
8:H:42:ASP:HB2	8:H:121:LEU:HB3	1.85	0.57
3:C:7:PRO:HA	3:C:25:ASN:HB3	1.86	0.57
2:B:197:GLN:OE1	2:B:486:ASN:ND2	2.37	0.57
1:A:656:SER:O	1:A:665:THR:OG1	2.21	0.56
2:B:731:GLN:OE1	2:B:1053:HIS:NE2	2.38	0.56
1:A:863:ARG:NH2	1:A:1128:ILE:HG22	2.19	0.56
8:H:79:ASP:O	8:H:84:ARG:NH1	2.38	0.56
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	1.87	0.56
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.38	0.56
7:G:117:MET:HB3	7:G:128:TYR:HB3	1.88	0.56
2:B:83:ARG:HB2	2:B:133:ILE:HD12	1.88	0.56
8:H:116:VAL:HB	8:H:123:MET:HB3	1.88	0.56
4:D:87:LEU:HB3	4:D:97:LEU:CD1	2.10	0.56
1:A:557:ARG:HH22	11:K:51:LEU:HB3	1.71	0.56
2:B:825:GLN:NE2	2:B:872:THR:O	2.40	0.56
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.71	0.56
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.87	0.55
5:E:180:ALA:HA	5:E:185:ILE:HD12	1.87	0.55
1:A:1214:VAL:HG23	1:A:1257:LEU:HB3	1.89	0.55
4:D:90:LYS:HD3	4:D:130:ILE:HG21	1.86	0.55
2:B:674:MET:HG2	9:I:77:THR:HG22	1.89	0.55
1:A:955:GLU:HG3	1:A:1046:ARG:HH11	1.70	0.55
1:A:784:VAL:HG22	2:B:978:ILE:HD11	1.87	0.55
5:E:173:ILE:HG22	5:E:209:VAL:HA	1.88	0.55
6:F:62:ARG:NH1	6:F:126:THR:OG1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:MET:SD	2:B:599:SER:OG	2.63	0.55
3:C:52:ILE:HG21	3:C:55:ASN:HB2	1.89	0.55
2:B:347:MET:O	2:B:361:LYS:HE2	2.06	0.55
5:E:166:ARG:NH1	5:E:168:ASN:OD1	2.40	0.55
1:A:757:GLN:HE22	1:A:781:ILE:HD11	1.72	0.55
2:B:357:CYS:HA	2:B:360:LYS:HE3	1.89	0.55
13:M:315:GLN:HG2	13:M:316:GLN:HG2	1.88	0.54
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.89	0.54
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.40	0.54
2:B:998:ASP:OD2	2:B:1003:ASN:ND2	2.41	0.54
3:C:6:GLN:O	3:C:25:ASN:ND2	2.40	0.54
1:A:885:GLN:NE2	5:E:170:LEU:O	2.39	0.54
2:B:344:GLN:OE1	2:B:355:ASP:HA	2.07	0.54
1:A:879:VAL:HB	1:A:888:GLN:H	1.73	0.54
2:B:363:TYR:O	2:B:367:TYR:N	2.41	0.54
3:C:193:ARG:NH1	3:C:217:GLN:OE1	2.34	0.54
3:C:70:LEU:HB3	10:J:6:ARG:HD2	1.89	0.54
1:A:1197:TYR:HA	1:A:1200:PRO:HB3	1.90	0.54
2:B:96:PRO:HG3	2:B:154:ILE:HG13	1.90	0.54
2:B:320:PHE:O	2:B:324:ARG:NH1	2.41	0.54
2:B:49:GLU:HG3	2:B:49:GLU:O	2.07	0.54
7:G:39:THR:OG1	7:G:43:GLY:N	2.40	0.53
5:E:185:ILE:HG21	5:E:209:VAL:HG21	1.91	0.53
4:D:87:LEU:HD13	4:D:97:LEU:HD21	1.91	0.53
1:A:1234:LYS:NZ	1:A:1298:LEU:O	2.35	0.53
1:A:626:THR:OG1	1:A:627:LYS:N	2.42	0.53
2:B:51:ILE:CG2	2:B:160:TYR:CE2	2.91	0.53
2:B:794:VAL:HG22	2:B:967:ILE:HG22	1.91	0.53
1:A:1036:ASN:OD1	5:E:202:ARG:NH1	2.40	0.53
1:A:1305:SER:HB3	1:A:1339:ASP:HB3	1.90	0.52
1:A:948:ILE:HG12	1:A:1007:ILE:HD11	1.90	0.52
2:B:313:GLU:OE2	2:B:315:ASN:ND2	2.40	0.52
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.91	0.52
2:B:816:GLU:HG2	2:B:867:ILE:HG21	1.91	0.52
2:B:798:ARG:HB2	2:B:948:GLN:HB3	1.90	0.52
2:B:393:LEU:HD22	2:B:485:LEU:HD22	1.91	0.52
5:E:25:GLY:O	5:E:65:ASN:ND2	2.42	0.52
2:B:119:THR:HG21	2:B:445:LYS:HE2	1.91	0.52
6:F:107:ARG:NE	6:F:117:ASP:OD1	2.37	0.52
1:A:1144:LEU:HD12	1:A:1351:ASP:HA	1.91	0.52
2:B:425:ARG:HB3	2:B:427:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD21	1:A:477:LEU:HD11	1.92	0.51
1:A:848:ILE:O	1:A:851:ALA:N	2.43	0.51
1:A:812:LYS:NZ	9:I:77:THR:OG1	2.43	0.51
2:B:51:ILE:O	2:B:51:ILE:HG22	2.10	0.51
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.92	0.51
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	1.91	0.51
1:A:1261:ILE:HD11	1:A:1285:LEU:HD13	1.93	0.51
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	1.92	0.51
2:B:442:ASP:O	2:B:446:TYR:N	2.40	0.51
7:G:163:LEU:HA	7:G:168:LEU:HB3	1.91	0.51
8:H:7:GLU:OE1	8:H:57:ARG:NH2	2.43	0.51
1:A:585:LEU:HD22	8:H:47:ILE:HD11	1.92	0.51
2:B:866:ILE:HD11	2:B:896:LEU:HB2	1.92	0.51
2:B:51:ILE:CG2	2:B:160:TYR:HE2	2.24	0.51
7:G:90:THR:OG1	7:G:98:PHE:O	2.29	0.51
5:E:56:THR:HG23	5:E:76:PHE:HB2	1.93	0.51
11:K:24:ASP:OD2	11:K:74:ARG:NH2	2.44	0.51
11:K:42:LEU:HD12	11:K:45:ILE:HD11	1.93	0.50
2:B:872:THR:HG23	2:B:889:LYS:HE2	1.93	0.50
5:E:14:ARG:HH11	5:E:40:PHE:HE1	1.59	0.50
2:B:865:VAL:HG22	2:B:895:PHE:HE1	1.76	0.50
2:B:825:GLN:HE22	2:B:873:LEU:HA	1.77	0.50
2:B:1028:LEU:HD12	2:B:1041:ILE:HG13	1.93	0.50
1:A:1003:ASP:N	1:A:1003:ASP:OD1	2.43	0.50
2:B:51:ILE:HG21	2:B:160:TYR:CE2	2.47	0.50
1:A:698:THR:O	1:A:702:ILE:N	2.44	0.50
1:A:813:ASP:HA	9:I:98:GLN:HE21	1.77	0.50
2:B:270:ILE:HG13	2:B:305:LEU:HD23	1.94	0.49
2:B:611:GLU:OE1	2:B:613:ARG:NH2	2.46	0.49
3:C:59:LEU:HB3	3:C:63:PHE:HD2	1.76	0.49
1:A:1305:SER:OG	1:A:1306:LYS:N	2.43	0.49
2:B:799:SER:O	2:B:803:ARG:NH1	2.45	0.49
8:H:79:ASP:OD1	8:H:81:ARG:NH1	2.44	0.49
1:A:1194:ASN:O	1:A:1198:GLU:N	2.41	0.49
1:A:958:ARG:NH2	1:A:962:ASP:OD2	2.45	0.49
2:B:666:ASP:OD1	2:B:666:ASP:N	2.46	0.49
6:F:114:SER:OG	6:F:115:TYR:N	2.44	0.49
1:A:863:ARG:CZ	1:A:1128:ILE:HG21	2.41	0.49
3:C:56:SER:HG	3:C:158:GLU:H	1.61	0.49
5:E:133:GLN:HA	5:E:136:LEU:HG	1.95	0.49
4:D:61:PHE:O	4:D:65:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:106:CYS:SG	7:G:107:PHE:N	2.86	0.49
1:A:577:PRO:HG3	1:A:584:PRO:HB2	1.94	0.49
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.45	0.49
2:B:16:GLU:HG3	2:B:17:ILE:HG13	1.95	0.48
2:B:789:ASN:HA	2:B:793:SER:HB2	1.94	0.48
7:G:101:ILE:N	7:G:104:MET:O	2.44	0.48
2:B:841:ARG:HD2	2:B:895:PHE:HE2	1.78	0.48
2:B:706:VAL:HG13	2:B:767:LEU:HD22	1.94	0.48
1:A:1174:ALA:HB2	9:I:55:VAL:HG23	1.95	0.48
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.38	0.48
1:A:1173:THR:O	9:I:56:ASN:N	2.44	0.48
1:A:958:ARG:O	1:A:962:ASP:N	2.46	0.48
6:F:118:TRP:HE3	6:F:123:LEU:HD12	1.78	0.48
1:A:1365:ILE:O	1:A:1365:ILE:HG22	2.14	0.48
2:B:92:TYR:N	2:B:125:TYR:O	2.37	0.48
2:B:690:CYS:SG	2:B:691:SER:N	2.86	0.48
2:B:159:THR:H	2:B:164:ASN:HD22	1.60	0.48
2:B:776:ILE:HD12	2:B:806:PHE:H	1.79	0.48
4:D:70:ARG:NH1	7:G:140:ASP:OD2	2.46	0.48
5:E:90:TYR:O	5:E:94:MET:N	2.46	0.48
9:I:75:ASP:O	9:I:80:ARG:NH2	2.46	0.48
2:B:910:THR:HG22	12:L:43:ILE:HA	1.95	0.48
2:B:357:CYS:HA	2:B:360:LYS:HG3	1.96	0.48
2:B:709:SER:HB2	2:B:767:LEU:HD11	1.96	0.48
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	1.96	0.48
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.96	0.47
4:D:31:THR:O	4:D:84:ARG:NH2	2.47	0.47
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.94	0.47
1:A:456:VAL:HG12	1:A:505:LEU:HD13	1.96	0.47
4:D:73:ARG:NH2	7:G:142:GLU:OE2	2.48	0.47
1:A:1030:SER:HA	1:A:1033:ALA:HB3	1.96	0.47
1:A:1321:ILE:HD12	1:A:1331:LEU:HD12	1.95	0.47
1:A:565:MET:HG3	11:K:62:LYS:HD2	1.96	0.47
1:A:827:TYR:O	2:B:716:HIS:ND1	2.43	0.47
8:H:8:ASP:OD2	8:H:32:SER:OG	2.28	0.47
3:C:148:ILE:HA	10:J:16:ASN:HB3	1.95	0.47
3:C:55:ASN:ND2	3:C:61:ASP:OD1	2.42	0.47
2:B:313:GLU:HG2	2:B:315:ASN:H	1.79	0.47
2:B:721:ARG:HH21	2:B:975:ARG:HD2	1.80	0.47
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.96	0.47
2:B:420:GLN:HA	2:B:423:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:THR:HA	1:A:1059:ARG:HH12	1.80	0.47
2:B:854:ILE:HD12	2:B:866:ILE:HG23	1.97	0.47
5:E:126:ILE:HD13	5:E:186:ARG:HH21	1.80	0.47
1:A:883:ILE:O	1:A:885:GLN:N	2.48	0.46
1:A:747:ASP:O	1:A:751:LYS:N	2.41	0.46
2:B:505:LEU:HD22	2:B:509:VAL:HB	1.97	0.46
2:B:565:THR:HG21	2:B:580:PRO:HG3	1.97	0.46
5:E:81:LYS:HG2	5:E:108:GLN:HB2	1.97	0.46
1:A:874:LYS:NZ	1:A:1470:CYS:SG	2.75	0.46
1:A:374:SER:OG	1:A:666:ARG:NH1	2.48	0.46
1:A:881:ASN:OD1	1:A:881:ASN:N	2.46	0.46
2:B:845:TYR:HD1	2:B:848:LEU:HD12	1.80	0.46
3:C:205:LYS:NZ	3:C:215:GLU:O	2.39	0.46
11:K:7:PHE:HD2	11:K:11:LEU:HD12	1.80	0.46
2:B:663:GLU:OE1	2:B:695:HIS:NE2	2.36	0.46
10:J:8:PHE:CD1	10:J:8:PHE:N	2.83	0.46
2:B:483:ARG:NH2	2:B:527:ALA:O	2.33	0.46
5:E:193:ILE:N	5:E:205:THR:O	2.47	0.46
7:G:88:VAL:HG13	7:G:140:ASP:HA	1.97	0.46
1:A:376:ASP:OD1	1:A:376:ASP:N	2.48	0.46
1:A:589:LYS:HD2	8:H:120:GLY:HA2	1.98	0.46
1:A:775:LYS:HD3	2:B:974:SER:HB3	1.97	0.46
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.34	0.46
11:K:31:CYS:SG	11:K:32:LEU:N	2.89	0.46
8:H:78:THR:HG21	11:K:78:THR:HG21	1.97	0.46
1:A:922:PHE:HA	1:A:1052:ARG:HH11	1.79	0.46
2:B:124:LEU:HD23	2:B:149:ILE:HD11	1.98	0.46
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.49	0.46
8:H:14:ASP:HB2	8:H:29:HIS:HB2	1.98	0.46
1:A:1244:ASN:N	1:A:1260:ARG:O	2.47	0.45
9:I:80:ARG:HG2	9:I:95:VAL:HB	1.98	0.45
1:A:1127:LEU:HD22	1:A:1362:ILE:HD13	1.97	0.45
2:B:92:TYR:HB2	2:B:125:TYR:HB2	1.98	0.45
1:A:1366:PHE:HD1	1:A:1370:GLY:O	1.99	0.45
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.98	0.45
7:G:7:LEU:HD12	7:G:74:ALA:HB3	1.97	0.45
2:B:192:LYS:NZ	2:B:449:ALA:O	2.49	0.45
5:E:165:LEU:HD13	5:E:170:LEU:HD21	1.97	0.45
3:C:84:TYR:HE1	3:C:167:LYS:HE2	1.80	0.45
4:D:87:LEU:HD13	4:D:97:LEU:CD2	2.46	0.45
1:A:1476:ASP:HB2	6:F:105:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:22:CYS:HB3	12:L:39:CYS:HB3	1.98	0.45
7:G:101:ILE:HD11	7:G:145:LEU:HD11	1.98	0.45
1:A:843:GLY:O	1:A:847:LEU:HB2	2.16	0.45
8:H:96:VAL:HA	8:H:116:VAL:HA	1.99	0.45
2:B:51:ILE:HG22	2:B:93:LEU:HD11	1.99	0.45
7:G:107:PHE:O	7:G:161:GLY:N	2.36	0.45
2:B:47:PHE:CD2	2:B:47:PHE:O	2.70	0.45
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.99	0.45
3:C:197:TYR:HD2	3:C:217:GLN:HE21	1.65	0.45
3:C:259:LEU:O	3:C:263:LEU:N	2.32	0.45
6:F:116:GLU:OE2	6:F:118:TRP:NE1	2.47	0.45
11:K:47:LYS:HD3	11:K:61:TYR:HD1	1.81	0.45
1:A:1394:ASN:HB3	1:A:1397:HIS:CD2	2.51	0.44
9:I:86:CYS:SG	9:I:87:GLN:N	2.90	0.44
1:A:984:LEU:HD23	1:A:984:LEU:O	2.18	0.44
1:A:1366:PHE:O	1:A:1366:PHE:CD1	2.70	0.44
1:A:932:ARG:NH2	1:A:999:ARG:O	2.39	0.44
8:H:58:LEU:HD11	8:H:143:LEU:HD11	2.00	0.44
1:A:539:GLN:NE2	1:A:774:ALA:O	2.34	0.44
5:E:107:GLN:HA	5:E:132:GLU:HB2	1.99	0.44
8:H:40:ILE:HD13	8:H:124:ARG:HD3	1.98	0.44
8:H:28:LEU:HD22	8:H:41:LEU:HD23	1.98	0.44
1:A:435:PRO:HA	1:A:438:LEU:HG	1.98	0.44
2:B:912:ASN:OD1	2:B:915:GLY:N	2.39	0.44
2:B:51:ILE:CG2	2:B:93:LEU:HD11	2.48	0.44
2:B:833:THR:HB	2:B:836:THR:HG22	1.99	0.44
1:A:1286:ARG:O	1:A:1290:SER:N	2.48	0.44
1:A:760:LEU:HB3	1:A:764:ASN:HD22	1.82	0.44
1:A:805:ARG:HH12	1:A:808:PRO:HA	1.83	0.44
2:B:567:ILE:HD11	2:B:577:HIS:HB2	2.00	0.44
2:B:329:GLY:O	2:B:335:ARG:NH1	2.51	0.44
2:B:601:VAL:HG22	2:B:616:THR:HA	2.00	0.44
7:G:14:HIS:HD2	7:G:16:ARG:HG3	1.82	0.44
1:A:1205:ALA:HB3	1:A:1263:ASN:HD21	1.82	0.44
2:B:126:VAL:HG23	2:B:149:ILE:HG12	2.00	0.44
3:C:86:ARG:HG2	3:C:86:ARG:O	2.17	0.44
5:E:173:ILE:N	5:E:208:LEU:O	2.51	0.44
2:B:119:THR:HG23	2:B:187:ILE:HD13	2.00	0.43
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.53	0.43
12:L:22:CYS:SG	12:L:24:THR:OG1	2.69	0.43
3:C:45:ILE:HG22	3:C:73:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:LYS:HD3	8:H:48:TYR:HB2	2.00	0.43
1:A:653:VAL:HG22	1:A:668:PHE:HE2	1.84	0.43
2:B:929:PRO:O	2:B:948:GLN:NE2	2.51	0.43
9:I:75:ASP:HB3	9:I:78:LEU:HD13	1.99	0.43
5:E:61:LEU:HD13	5:E:73:PHE:HD1	1.84	0.43
7:G:92:VAL:HA	7:G:97:LEU:HG	2.00	0.43
1:A:1128:ILE:HA	1:A:1128:ILE:HD12	1.78	0.43
5:E:150:VAL:HA	5:E:191:VAL:HG12	2.01	0.43
3:C:259:LEU:HD11	11:K:42:LEU:HD21	1.99	0.43
1:A:505:LEU:HD12	1:A:506:PRO:HD2	2.00	0.43
3:C:30:VAL:HG22	11:K:45:ILE:HG22	2.01	0.43
1:A:580:LEU:O	1:A:580:LEU:HD23	2.19	0.43
3:C:131:THR:HG21	3:C:147:ASP:HA	2.00	0.43
9:I:54:TYR:HE2	9:I:56:ASN:HB2	1.84	0.43
2:B:42:GLN:HE22	2:B:483:ARG:HA	1.84	0.43
4:D:41:LEU:HD22	4:D:61:PHE:HE1	1.84	0.43
5:E:71:GLN:HG3	5:E:99:ILE:HG22	1.99	0.43
1:A:1341:VAL:HG12	1:A:1364:GLU:OE1	2.19	0.43
2:B:1028:LEU:HD23	2:B:1028:LEU:HA	1.84	0.42
1:A:522:PRO:HB3	1:A:666:ARG:HD3	2.01	0.42
2:B:480:SER:HB3	2:B:706:VAL:HB	2.01	0.42
3:C:253:LYS:HG3	11:K:95:ILE:HG23	2.01	0.42
1:A:1218:ARG:HH22	1:A:1255:LEU:HB2	1.85	0.42
1:A:731:ASN:HB3	1:A:735:GLN:HB2	2.01	0.42
2:B:534:VAL:N	2:B:600:GLU:OE2	2.51	0.42
1:A:542:LEU:HD21	1:A:642:LYS:HG3	2.00	0.42
1:A:856:GLU:HB3	1:A:1121:VAL:HG11	2.00	0.42
2:B:425:ARG:HD2	2:B:427:LYS:HE3	2.02	0.42
2:B:513:GLU:HG2	2:B:525:ASN:HD22	1.84	0.42
1:A:718:GLU:O	1:A:722:ASN:ND2	2.52	0.42
4:D:105:PRO:HB3	4:D:114:LEU:HD12	2.01	0.42
1:A:1144:LEU:HD11	1:A:1354:PRO:HD3	2.02	0.42
5:E:170:LEU:HA	5:E:170:LEU:HD23	1.88	0.42
5:E:171:PRO:HB2	5:E:207:ARG:HD3	2.02	0.42
1:A:1374:VAL:O	1:A:1378:LEU:N	2.46	0.42
1:A:394:VAL:HG21	1:A:440:LEU:HD11	2.02	0.42
2:B:484:ARG:HH21	2:B:525:ASN:ND2	2.17	0.42
2:B:484:ARG:HH22	2:B:730:LYS:NZ	2.18	0.42
5:E:102:ALA:HB3	5:E:127:LEU:HG	2.00	0.42
7:G:79:PRO:HG3	7:G:157:ILE:HG21	2.02	0.42
10:J:9:THR:CB	10:J:44:CYS:SG	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:PRO:HG3	8:H:47:ILE:HD13	2.02	0.42
2:B:242:ARG:HB3	2:B:254:GLN:HE21	1.85	0.41
3:C:54:ALA:HB3	3:C:160:ARG:HB3	2.02	0.41
3:C:44:ILE:HD13	3:C:44:ILE:HG21	1.85	0.41
7:G:81:LYS:NZ	7:G:148:VAL:O	2.38	0.41
1:A:1030:SER:OG	5:E:162:ARG:NE	2.34	0.41
1:A:1212:LEU:HD11	1:A:1289:GLU:HG3	2.02	0.41
2:B:951:GLN:OE1	2:B:962:THR:OG1	2.36	0.41
13:M:82:UNK:O	13:M:86:UNK:N	2.53	0.41
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	2.03	0.41
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	2.00	0.41
2:B:636:LYS:H	2:B:639:HIS:HD2	1.68	0.41
1:A:707:LYS:HB3	1:A:707:LYS:HE2	1.92	0.41
11:K:49:GLN:HE22	11:K:52:LYS:HD2	1.86	0.41
8:H:63:THR:HG21	8:H:70:LEU:HA	2.03	0.41
2:B:353:VAL:HG22	2:B:353:VAL:O	2.21	0.41
2:B:39:LEU:O	2:B:483:ARG:NH1	2.54	0.41
2:B:479:LEU:HA	2:B:479:LEU:HD23	1.88	0.41
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.48	0.41
5:E:84:ILE:HA	5:E:87:ILE:HD12	2.03	0.41
1:A:1202:PHE:HA	1:A:1204:VAL:HG23	2.02	0.41
2:B:87:LYS:O	2:B:129:THR:OG1	2.37	0.41
4:D:34:ASN:O	4:D:68:THR:OG1	2.36	0.41
8:H:10:PHE:HD1	8:H:32:SER:HA	1.86	0.41
1:A:636:ILE:HG23	8:H:117:SER:HB2	2.03	0.41
8:H:136:GLU:HB2	8:H:139:SER:HB3	2.02	0.41
2:B:505:LEU:HD23	2:B:505:LEU:HA	1.79	0.41
2:B:1038:THR:HA	3:C:195:THR:HA	2.02	0.41
4:D:41:LEU:HD12	4:D:68:THR:HG21	2.03	0.41
1:A:1319:LYS:HE2	1:A:1321:ILE:HD11	2.03	0.40
1:A:953:GLU:O	1:A:957:GLU:N	2.48	0.40
2:B:950:ARG:HG3	3:C:171:LYS:NZ	2.36	0.40
1:A:581:LYS:HB3	8:H:90:TYR:HA	2.02	0.40
1:A:819:SER:OG	1:A:819:SER:O	2.38	0.40
3:C:171:LYS:HD2	3:C:171:LYS:HA	1.81	0.40
1:A:1377:ALA:HB2	5:E:144:LEU:HD13	2.04	0.40
1:A:1386:ILE:HD13	1:A:1393:VAL:HG21	2.02	0.40
1:A:679:TRP:CH2	1:A:683:GLU:HG3	2.57	0.40
6:F:125:ILE:HA	6:F:125:ILE:HD12	1.95	0.40
9:I:86:CYS:N	9:I:91:HIS:O	2.54	0.40
2:B:268:PRO:HD2	2:B:271:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:VAL:H	5:E:74:VAL:HB	1.86	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	984/1970 (50%)	876 (89%)	106 (11%)	2 (0%)	49	83
2	B	999/1174 (85%)	870 (87%)	128 (13%)	1 (0%)	53	86
3	C	258/275 (94%)	222 (86%)	36 (14%)	0	100	100
4	D	126/142 (89%)	121 (96%)	5 (4%)	0	100	100
5	E	177/210 (84%)	166 (94%)	11 (6%)	0	100	100
6	F	64/127 (50%)	58 (91%)	6 (9%)	0	100	100
7	G	163/172 (95%)	147 (90%)	16 (10%)	0	100	100
8	H	144/150 (96%)	130 (90%)	14 (10%)	0	100	100
9	I	106/125 (85%)	90 (85%)	16 (15%)	0	100	100
10	J	62/67 (92%)	54 (87%)	7 (11%)	1 (2%)	11	49
11	K	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
12	L	33/58 (57%)	26 (79%)	7 (21%)	0	100	100
13	M	15/62 (24%)	12 (80%)	3 (20%)	0	100	100
All	All	3240/4649 (70%)	2875 (89%)	361 (11%)	4 (0%)	56	86

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	556	GLU
1	A	582	PRO

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Mol	Chain	Res	Type
2	B	159	THR
10	J	9	THR

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	890/1749 (51%)	885 (99%)	5 (1%)	87	94
2	B	889/1028 (86%)	885 (100%)	4 (0%)	92	96
3	C	239/252 (95%)	239 (100%)	0	100	100
4	D	106/126 (84%)	105 (99%)	1 (1%)	81	90
5	E	169/192 (88%)	168 (99%)	1 (1%)	87	94
6	F	59/111 (53%)	59 (100%)	0	100	100
7	G	144/153 (94%)	144 (100%)	0	100	100
8	H	129/131 (98%)	128 (99%)	1 (1%)	83	91
9	I	101/112 (90%)	100 (99%)	1 (1%)	78	89
10	J	53/56 (95%)	51 (96%)	2 (4%)	36	66
11	K	101/106 (95%)	101 (100%)	0	100	100
12	L	34/55 (62%)	33 (97%)	1 (3%)	45	72
13	M	16/16 (100%)	15 (94%)	1 (6%)	20	54
All	All	2930/4087 (72%)	2913 (99%)	17 (1%)	88	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	845	GLU
1	A	1128	ILE
1	A	1131	SER
1	A	1133	LYS
1	A	1375	ARG
2	B	185	PHE

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Mol	Chain	Res	Type
2	B	354	SER
2	B	355	ASP
2	B	356	PHE
4	D	70	ARG
5	E	162	ARG
8	H	131	ASN
9	I	40	ARG
10	J	7	CYS
10	J	8	PHE
12	L	37	ARG
13	M	312	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	HIS
1	A	620	HIS
1	A	662	HIS
1	A	704	ASN
1	A	722	ASN
1	A	792	ASN
1	A	1077	ASN
1	A	1163	HIS
1	A	1220	HIS
1	A	1310	HIS
2	B	144	HIS
2	B	164	ASN
2	B	197	GLN
2	B	486	ASN
2	B	699	HIS
2	B	825	GLN
2	B	941	GLN
4	D	93	HIS
5	E	65	ASN
7	G	14	HIS
8	H	131	ASN
11	K	49	GLN
12	L	23	HIS
12	L	26	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	102:UNK	C	300:PRO	N	51.89