



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 20, 2016 – 01:15 PM EST

PDB ID : 5M3M
EMDB ID: : EMD-4148
Title : Free monomeric RNA polymerase I at 4.0Å resolution
Authors : Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.;
Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on : 2016-10-15
Resolution : 4.00 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

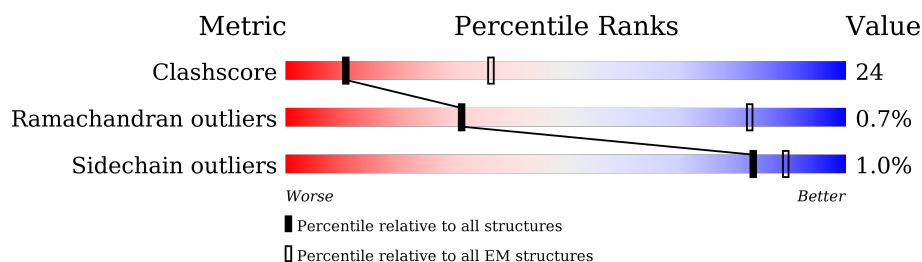
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



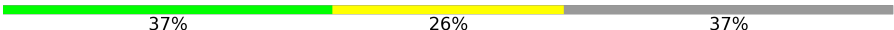

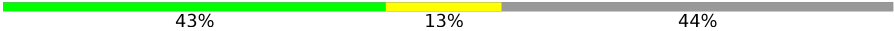

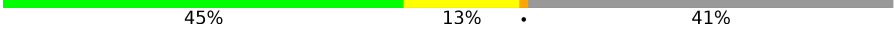
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	1664	44% 43% 12%
2	B	1203	49% 48% .
3	C	335	41% 49% 9%
4	E	215	44% 54% .
5	F	155	32% 31% 37%
6	H	146	48% 42% 10%
7	I	125	46% 46% 7%
8	J	70	44% 54% .
9	K	142	33% 38% 29%

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Mol	Chain	Length	Quality of chain
10	L	70	
11	M	415	
12	N	233	
13	D	137	
14	G	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	B	1301	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 33233 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			11558	7304	2006	2187	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1166	Total	C	N	O	S	0	0
			9266	5864	1617	1734	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	98	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	116	Total	C	N	O	S	0	0
			883	550	148	176	9		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	97	Total	C	N	O		0	0
			771	490	124	157			

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	131	Total	C	N	O	S	0	0
			1035	660	171	200	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	58	Total	C	N	O		0	0
			459	289	78	92			

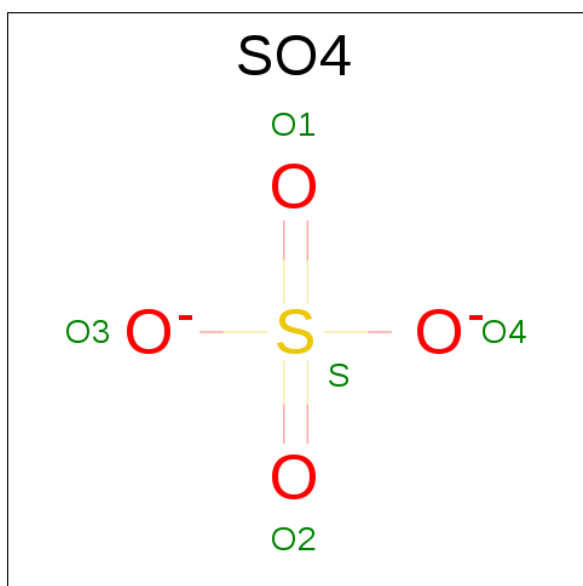
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	192	Total	C	N	O	S	0	0
			1518	979	261	273	5		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	Zn	0
			1	1	
15	A	2	Total	Zn	0
			2	2	
15	L	1	Total	Zn	0
			1	1	
15	J	1	Total	Zn	0
			1	1	
15	I	2	Total	Zn	0
			2	2	

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

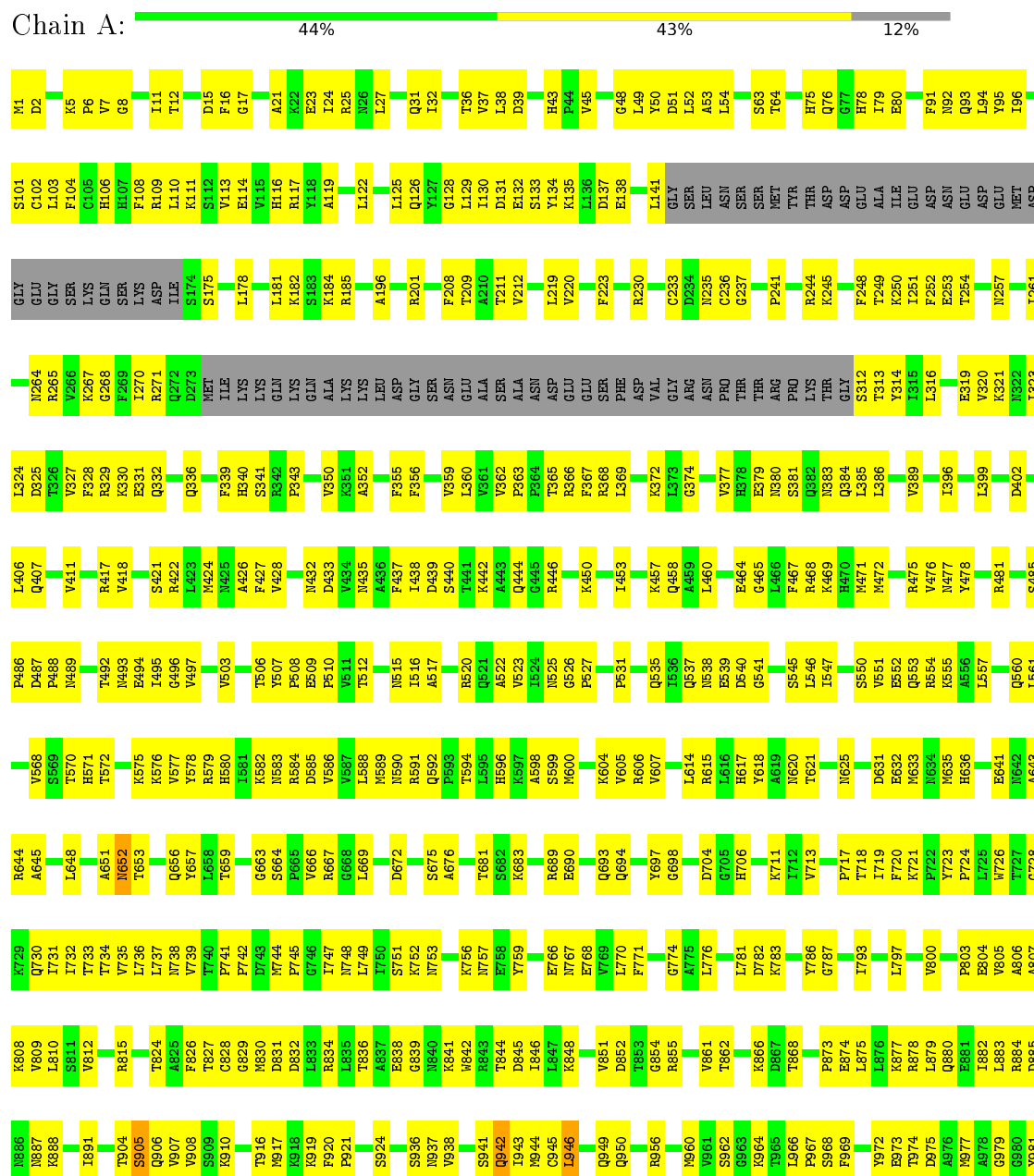


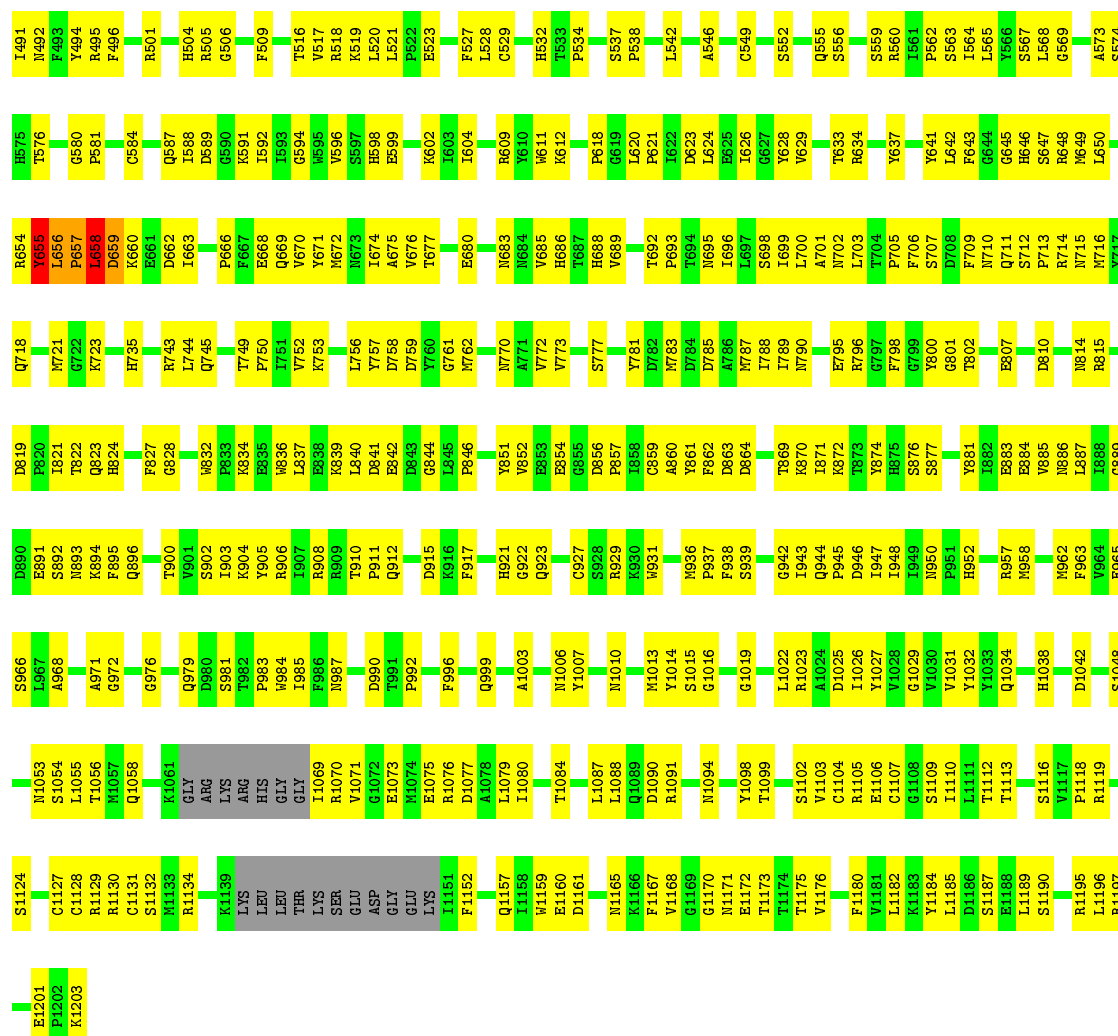
Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	O	S	0
			5	4	1	

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 errors 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.

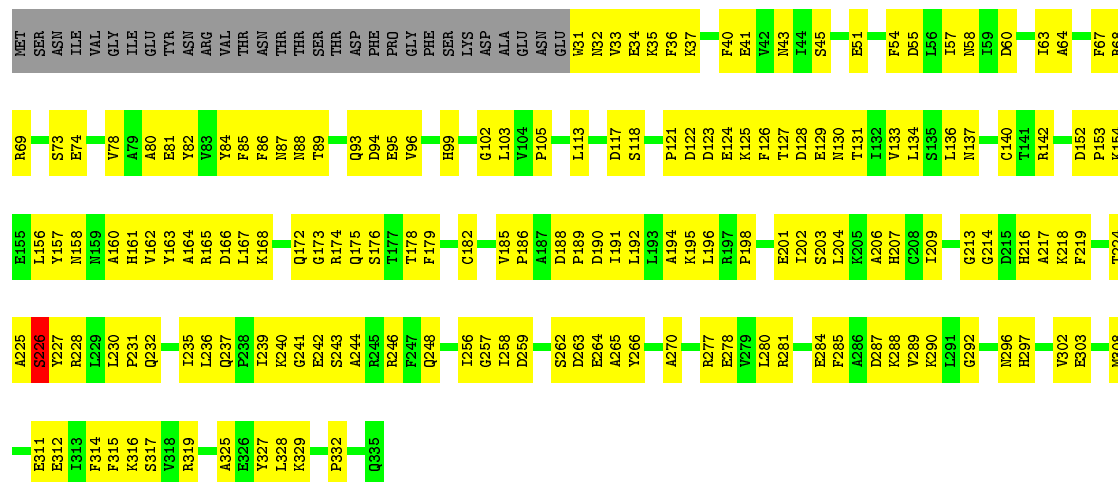
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190





- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 41% 49% 9%



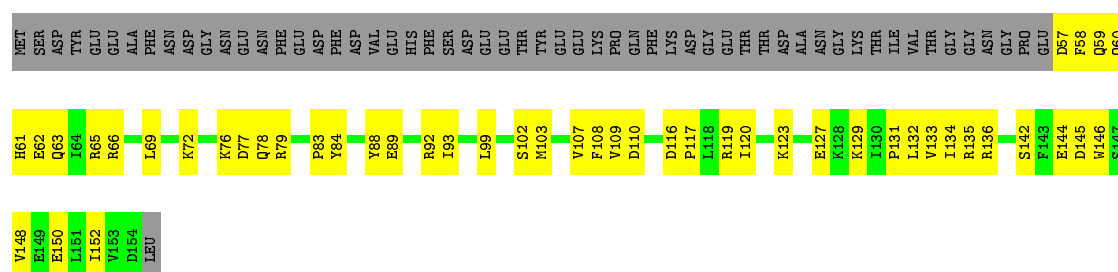
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



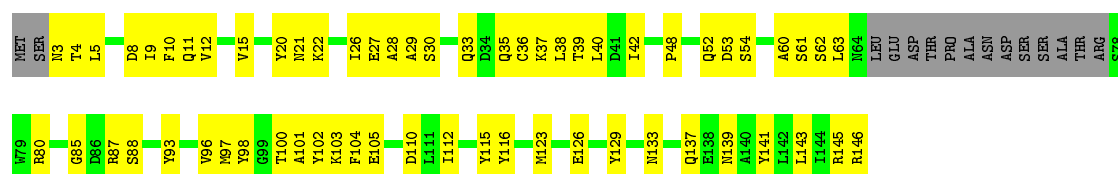
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



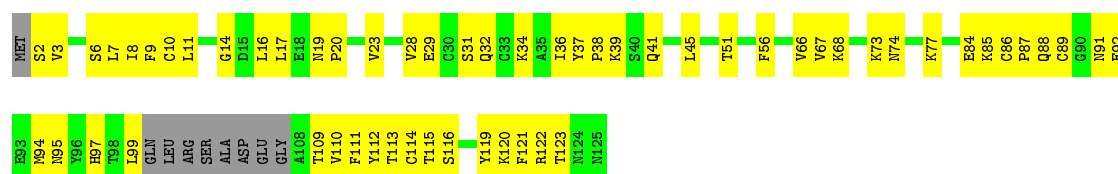
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



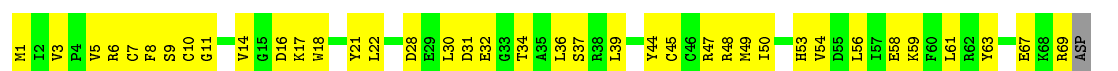
- Molecule 7: DNA-directed RNA polymerase I subunit RPA12

Chain I: 



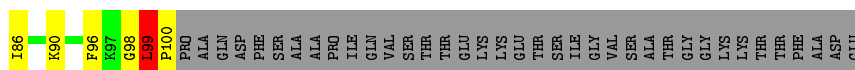
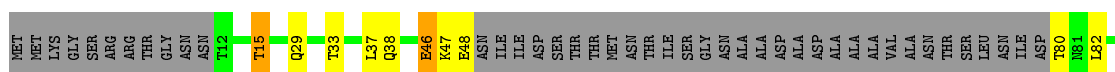
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 

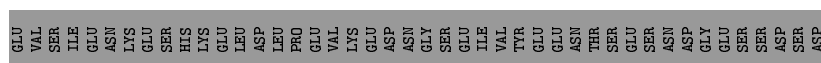
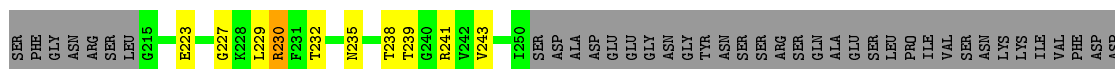
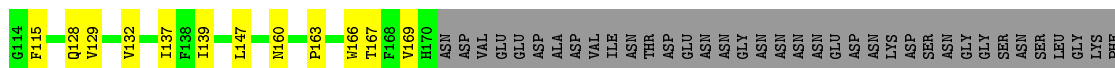
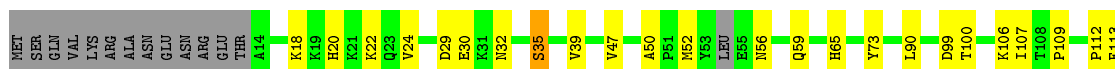


- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2



- Molecule 14: DNA-directed RNA polymerase I subunit RPA43



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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, SO4

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	0.40	0/11770	0.51	0/15895
10	L	0.40	0/354	0.53	0/468
11	M	0.40	0/786	0.55	0/1057
12	N	0.39	0/1052	0.55	0/1418
13	D	0.40	0/465	0.58	0/630
14	G	0.37	0/1555	0.66	3/2113 (0.1%)
2	B	0.45	0/9471	0.53	0/12805
3	C	0.45	0/2475	0.51	0/3354
4	E	0.40	0/1771	0.50	0/2383
5	F	0.37	0/821	0.48	0/1106
6	H	0.46	0/1070	0.54	0/1449
7	I	0.38	0/895	0.49	0/1205
8	J	0.50	0/578	0.53	0/775
9	K	0.45	0/804	0.55	0/1083
All	All	0.42	0/33867	0.53	3/45741 (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
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	241	ARG	NE-CZ-NH1	11.80	126.20	120.30
14	G	241	ARG	NE-CZ-NH2	-11.62	114.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	241	ARG	CD-NE-CZ	6.08	132.12	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1649	VAL	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	11558	0	11642	651	0
2	B	9266	0	9151	558	0
3	C	2423	0	2412	156	0
4	E	1735	0	1764	98	0
5	F	807	0	827	45	0
6	H	1052	0	1021	47	0
7	I	883	0	879	60	0
8	J	569	0	585	36	0
9	K	793	0	790	56	0
10	L	352	0	374	20	0
11	M	771	0	755	11	0
12	N	1035	0	1069	29	0
13	D	459	0	462	8	0
14	G	1518	0	1528	31	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	B	5	0	0	8	0
All	All	33233	0	33259	1613	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 24.

All (1613) 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:656:LEU:O	12:N:153:VAL:HG11	1.62	0.97
3:C:225:ALA:O	3:C:226:SER:HB2	1.63	0.95
1:A:1501:ILE:HG22	1:A:1502:PRO:HD2	1.49	0.94
2:B:894:LYS:HG2	10:L:54:ARG:HH21	1.33	0.94
5:F:66:ARG:HA	5:F:69:LEU:HD12	1.50	0.93
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.52	0.92
2:B:121:VAL:O	2:B:133:TYR:HE1	1.52	0.90
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.51	0.90
2:B:844:GLY:HA2	2:B:860:ALA:HB3	1.54	0.89
7:I:94:MET:HG2	7:I:114:CYS:HA	1.53	0.89
3:C:165:ARG:HB3	3:C:189:PRO:HB3	1.54	0.89
2:B:656:LEU:H	2:B:657:PRO:HD2	1.38	0.89
1:A:1258:ILE:O	1:A:1501:ILE:HG13	1.73	0.88
2:B:211:ARG:HH12	2:B:647:SER:HB2	1.37	0.88
2:B:894:LYS:CG	10:L:54:ARG:HH21	1.87	0.88
2:B:107:PRO:O	2:B:171:HIS:NE2	2.08	0.87
1:A:907:VAL:HG12	1:A:945:CYS:SG	2.15	0.86
1:A:675:SER:HG	2:B:952:HIS:HE2	1.18	0.86
2:B:657:PRO:O	2:B:659:ASP:N	2.09	0.86
2:B:894:LYS:HG2	10:L:54:ARG:NH2	1.89	0.86
1:A:846:ILE:HD13	1:A:906:GLN:HB3	1.54	0.86
2:B:1006:ASN:ND2	2:B:1010:ASN:O	2.08	0.85
1:A:109:ARG:NH1	1:A:230:ARG:O	2.09	0.85
1:A:908:VAL:HA	1:A:945:CYS:SG	2.16	0.84
1:A:842:TRP:CE2	1:A:910:LYS:NZ	2.45	0.84
2:B:745:GLN:HG2	2:B:800:TYR:HD2	1.43	0.84
1:A:666:VAL:HG23	1:A:667:ARG:HG3	1.59	0.83
5:F:103:MET:SD	14:G:112:PRO:CG	2.66	0.83
1:A:1655:ASP:HB2	5:F:135:ARG:HB3	1.60	0.83
1:A:526:GLY:HA3	1:A:554:ARG:HH11	1.42	0.83
2:B:655:TYR:HE1	2:B:688:HIS:HE2	1.26	0.83
2:B:70:GLU:HG2	2:B:98:SER:HB3	1.61	0.83
1:A:862:THR:O	1:A:878:ARG:NH1	2.11	0.82
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.60	0.82
1:A:1006:LEU:CD1	2:B:716:MET:SD	2.67	0.82
3:C:68:ARG:HD2	3:C:227:TYR:CD2	2.15	0.82
4:E:110:PHE:HB3	4:E:134:THR:HG22	1.61	0.82
1:A:440:SER:H	1:A:458:GLN:HE22	1.27	0.81
2:B:504:HIS:HB3	2:B:542:LEU:HD23	1.62	0.81
1:A:1263:LEU:HA	1:A:1498:ILE:HD11	1.60	0.81
1:A:943:ILE:HD11	2:B:958:MET:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.13	0.81
1:A:568:VAL:O	1:A:571:HIS:ND1	2.12	0.81
2:B:209:GLN:NE2	2:B:215:MET:SD	2.53	0.81
2:B:94:LYS:HB3	2:B:146:ASN:HA	1.63	0.81
10:L:48:CYS:HB3	10:L:52:GLY:H	1.44	0.81
2:B:501:ARG:NH2	2:B:546:ALA:O	2.13	0.81
1:A:594:THR:HG23	1:A:599:SER:HB2	1.63	0.81
5:F:62:GLU:OE2	14:G:90:LEU:CD1	2.28	0.81
1:A:1501:ILE:HB	1:A:1504:ILE:HB	1.61	0.80
1:A:943:ILE:HG23	1:A:986:PHE:HB2	1.63	0.80
1:A:1262:LEU:HD22	1:A:1496:SER:O	1.81	0.80
1:A:719:ILE:HG12	6:H:97:MET:HG2	1.61	0.80
1:A:101:SER:HA	1:A:108:PHE:HA	1.64	0.80
3:C:165:ARG:NH1	3:C:190:ASP:OD1	2.15	0.79
1:A:964:LYS:NZ	2:B:672:MET:O	2.15	0.79
1:A:936:SER:OG	1:A:938:VAL:HG23	1.81	0.79
1:A:945:CYS:O	1:A:946:LEU:CB	2.30	0.79
2:B:785:ASP:OD2	2:B:957:ARG:NH2	2.15	0.78
3:C:127:THR:H	3:C:130:ASN:HB2	1.47	0.78
2:B:201:LYS:HE2	2:B:487:VAL:HG22	1.66	0.78
1:A:1608:SER:O	1:A:1612:LYS:NZ	2.17	0.78
1:A:546:LEU:HD22	1:A:554:ARG:HG2	1.64	0.78
2:B:823:GLN:HG2	2:B:863:ASP:HA	1.65	0.77
14:G:22:LYS:HD3	14:G:128:GLN:HG2	1.65	0.77
7:I:99:LEU:HB2	7:I:109:THR:HB	1.64	0.77
9:K:88:PHE:HB3	9:K:106:GLN:HB2	1.66	0.77
5:F:103:MET:SD	14:G:112:PRO:HG2	2.25	0.77
2:B:534:PRO:HG3	2:B:542:LEU:HB2	1.66	0.77
2:B:1103:VAL:HG12	2:B:1110:ILE:HG22	1.66	0.77
1:A:1302:TYR:HA	1:A:1305:GLU:HB2	1.67	0.76
1:A:1006:LEU:HD13	2:B:716:MET:SD	2.24	0.76
2:B:807:GLU:OE1	2:B:905:TYR:OH	2.01	0.76
3:C:258:ILE:HA	3:C:265:ALA:HA	1.66	0.76
2:B:13:THR:HG21	12:N:163:VAL:HG21	1.66	0.76
2:B:1157:GLN:HB3	2:B:1168:VAL:HG13	1.66	0.76
2:B:612:LYS:NZ	2:B:624:LEU:O	2.18	0.76
8:J:9:SER:HB2	8:J:45:CYS:SG	2.26	0.76
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	1.66	0.76
2:B:211:ARG:NH1	2:B:646:HIS:O	2.19	0.76
2:B:145:VAL:HB	2:B:150:GLU:HB3	1.66	0.76
2:B:168:ASN:HA	2:B:173:ASN:HD22	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:107:VAL:HG12	5:F:109:VAL:H	1.48	0.75
2:B:144:SER:HA	2:B:151:ASN:HA	1.68	0.75
3:C:284:GLU:O	3:C:288:LYS:NZ	2.19	0.75
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.66	0.75
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.19	0.75
1:A:363:PRO:O	1:A:368:ARG:NE	2.19	0.74
1:A:824:THR:HB	2:B:1023:ARG:HB2	1.69	0.74
1:A:339:PHE:O	1:A:1629:ASN:ND2	2.20	0.74
1:A:690:GLU:HB3	9:K:77:ARG:HH22	1.50	0.74
2:B:1104:CYS:HA	2:B:1173:THR:HG22	1.69	0.74
2:B:655:TYR:HE1	2:B:688:HIS:NE2	1.85	0.74
2:B:745:GLN:NE2	8:J:1:MET:SD	2.60	0.74
3:C:68:ARG:HD2	3:C:227:TYR:HD2	1.53	0.74
1:A:1319:ASN:O	1:A:1323:HIS:ND1	2.13	0.73
1:A:636:HIS:CG	2:B:1091:ARG:HH22	2.05	0.73
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.69	0.73
2:B:122:TYR:CZ	2:B:183:HIS:CD2	2.76	0.73
2:B:655:TYR:CE1	2:B:688:HIS:NE2	2.55	0.73
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	1.69	0.73
1:A:689:ARG:NH2	9:K:87:GLU:O	2.20	0.73
2:B:58:GLY:O	2:B:62:ASN:ND2	2.21	0.73
1:A:1006:LEU:CD1	2:B:716:MET:CE	2.66	0.73
2:B:20:GLU:HG2	2:B:24:ARG:HH12	1.53	0.73
9:K:87:GLU:H	9:K:107:THR:HA	1.54	0.73
3:C:172:GLN:H	3:C:175:GLN:HB2	1.53	0.73
1:A:945:CYS:O	1:A:946:LEU:CG	2.36	0.73
2:B:75:ASP:OD1	2:B:93:ASN:N	2.20	0.72
4:E:26:ARG:NH2	4:E:186:LEU:O	2.22	0.72
6:H:29:ALA:HA	6:H:37:LYS:HA	1.71	0.72
5:F:62:GLU:OE2	14:G:90:LEU:HD11	1.90	0.72
12:N:148:ILE:O	12:N:150:TYR:CD1	2.42	0.72
3:C:153:PRO:HA	3:C:156:LEU:HB2	1.72	0.72
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.23	0.72
2:B:795:GLU:OE1	3:C:217:ALA:N	2.19	0.72
1:A:487:ASP:OD1	1:A:489:ASN:ND2	2.23	0.72
3:C:43:ASN:HB2	3:C:55:ASP:HB2	1.72	0.72
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.22	0.71
7:I:97:HIS:HB2	7:I:111:PHE:HD2	1.55	0.71
2:B:13:THR:HG21	12:N:163:VAL:CG2	2.20	0.71
2:B:239:VAL:HA	2:B:245:SER:HA	1.72	0.71
1:A:1274:GLU:OE2	1:A:1288:ARG:NH1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:815:ARG:NH2	2:B:819:ASP:O	2.22	0.71
2:B:1127:CYS:SG	2:B:1171:ASN:ND2	2.64	0.71
1:A:842:TRP:CZ2	1:A:910:LYS:NZ	2.58	0.71
7:I:23:VAL:HG21	7:I:28:VAL:HG22	1.73	0.71
6:H:63:LEU:HB3	6:H:88:SER:HB2	1.71	0.71
11:M:38:PHE:HB3	11:M:53:LEU:HD11	1.73	0.71
2:B:122:TYR:CE2	2:B:183:HIS:HD2	2.09	0.70
2:B:186:GLU:HB3	2:B:189:GLU:HB2	1.73	0.70
6:H:102:TYR:CZ	6:H:115:TYR:HB3	2.25	0.70
1:A:757:ASN:OD1	1:A:767:ASN:N	2.20	0.70
7:I:97:HIS:HB2	7:I:111:PHE:CD2	2.27	0.70
1:A:103:LEU:HD12	1:A:241:PRO:HD2	1.72	0.70
6:H:3:ASN:N	6:H:61:SER:HG	1.89	0.70
2:B:874:TYR:CZ	2:B:876:SER:HB3	2.26	0.70
2:B:122:TYR:CE2	2:B:183:HIS:CD2	2.80	0.70
2:B:657:PRO:C	2:B:659:ASP:H	1.94	0.70
1:A:908:VAL:HG22	1:A:945:CYS:HB2	1.74	0.70
2:B:915:ASP:H	2:B:927:CYS:HB3	1.57	0.70
2:B:658:LEU:O	2:B:659:ASP:C	2.31	0.69
1:A:497:VAL:HB	1:A:607:VAL:HA	1.74	0.69
1:A:782:ASP:OD1	1:A:783:LYS:N	2.24	0.69
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.24	0.69
13:D:99:LEU:HB3	13:D:100:PRO:CD	2.22	0.69
2:B:645:GLY:O	2:B:648:ARG:NE	2.22	0.69
2:B:280:LEU:O	2:B:323:ARG:NH2	2.20	0.69
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.75	0.69
2:B:161:LEU:HD12	2:B:162:PRO:HD2	1.74	0.69
1:A:945:CYS:O	1:A:946:LEU:HB3	1.91	0.69
2:B:884:GLU:H	2:B:904:LYS:HB3	1.58	0.69
1:A:1105:ARG:HH12	1:A:1138:GLU:HB3	1.56	0.69
1:A:1251:ALA:O	1:A:1255:CYS:N	2.22	0.69
1:A:130:ILE:O	1:A:133:SER:OG	2.09	0.69
2:B:122:TYR:CZ	2:B:183:HIS:HD2	2.11	0.69
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.58	0.69
2:B:504:HIS:CD2	2:B:506:GLY:H	2.11	0.69
2:B:699:ILE:N	16:B:1301:SO4:O3	2.26	0.69
2:B:1015:SER:HB2	2:B:1022:LEU:HD21	1.73	0.68
2:B:609:ARG:HH21	2:B:626:ILE:HB	1.58	0.68
2:B:714:ARG:HE	2:B:957:ARG:HB3	1.58	0.68
1:A:1573:TYR:HB3	7:I:122:ARG:HH12	1.57	0.68
2:B:700:LEU:N	16:B:1301:SO4:O4	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ILE:HG12	2:B:381:LEU:HD13	1.76	0.68
2:B:143:TRP:O	2:B:152:LEU:N	2.25	0.68
2:B:457:ILE:HG22	2:B:461:MET:HG2	1.75	0.68
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.26	0.68
7:I:97:HIS:H	7:I:111:PHE:HB2	1.58	0.68
2:B:505:ARG:HB3	2:B:509:PHE:HD2	1.58	0.68
2:B:658:LEU:N	2:B:658:LEU:HD13	2.07	0.68
3:C:160:ALA:O	3:C:196:LEU:N	2.27	0.68
9:K:86:VAL:HA	9:K:107:THR:HG22	1.75	0.68
5:F:79:ARG:NH1	5:F:145:ASP:O	2.27	0.68
1:A:1006:LEU:HD11	2:B:716:MET:SD	2.31	0.68
1:A:1263:LEU:HB3	1:A:1496:SER:HB2	1.74	0.68
2:B:1201:GLU:HG2	2:B:1203:LYS:HG2	1.76	0.68
2:B:894:LYS:CG	10:L:54:ARG:NH2	2.53	0.68
5:F:65:ARG:O	5:F:69:LEU:HG	1.94	0.68
1:A:1501:ILE:CG2	1:A:1502:PRO:HD2	2.24	0.68
1:A:1573:TYR:O	7:I:122:ARG:NH1	2.27	0.68
7:I:3:VAL:HG22	7:I:8:ILE:HG12	1.75	0.68
1:A:1275:THR:OG1	1:A:1289:SER:OG	2.12	0.68
1:A:6:PRO:O	13:D:15:THR:OG1	2.07	0.68
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.26	0.67
1:A:1504:ILE:HD13	1:A:1529:MET:HE3	1.76	0.67
6:H:8:ASP:OD1	6:H:9:ILE:N	2.26	0.67
3:C:314:PHE:O	3:C:317:SER:OG	2.09	0.67
1:A:1573:TYR:HA	7:I:122:ARG:HH22	1.60	0.67
1:A:486:PRO:O	1:A:615:ARG:NH2	2.27	0.67
2:B:752:VAL:HG22	2:B:979:GLN:HB2	1.75	0.67
4:E:37:LEU:HD11	4:E:41:ASP:HB2	1.76	0.67
1:A:475:ARG:HA	2:B:1070:ARG:HA	1.77	0.67
1:A:830:MET:SD	2:B:963:PHE:HB3	2.33	0.67
3:C:230:LEU:HD12	3:C:231:PRO:HD2	1.77	0.67
4:E:55:ARG:HB3	4:E:82:PHE:HB2	1.77	0.67
1:A:874:GLU:OE2	1:A:878:ARG:NE	2.24	0.67
1:A:1288:ARG:NE	1:A:1480:THR:O	2.27	0.67
1:A:366:ARG:HA	1:A:369:LEU:HG	1.76	0.67
1:A:509:GLU:N	1:A:577:VAL:O	2.28	0.67
3:C:240:LYS:HB3	3:C:264:GLU:HG2	1.77	0.67
3:C:88:ASN:O	10:L:60:ARG:NH1	2.28	0.67
1:A:1262:LEU:CD2	1:A:1496:SER:O	2.43	0.67
1:A:1447:GLN:HE21	1:A:1459:LYS:HA	1.60	0.67
1:A:209:THR:H	1:A:212:VAL:HB	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:N	1:A:360:LEU:O	2.29	0.66
1:A:1490:GLU:HA	7:I:56:PHE:HZ	1.59	0.66
1:A:54:LEU:HD22	1:A:76:GLN:HA	1.76	0.66
3:C:73:SER:O	3:C:214:GLY:N	2.27	0.66
7:I:20:PRO:HB3	7:I:39:LYS:HG3	1.78	0.66
1:A:537:GLN:HE21	1:A:541:GLY:HA2	1.59	0.66
1:A:584:ARG:HD2	5:F:116:ASP:HB2	1.76	0.66
2:B:862:PHE:HA	2:B:869:THR:HA	1.77	0.66
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	2.21	0.66
1:A:588:LEU:HB3	1:A:636:HIS:HB2	1.76	0.66
1:A:826:PHE:CE1	1:A:924:SER:OG	2.45	0.66
5:F:99:LEU:O	5:F:102:SER:OG	2.14	0.66
1:A:862:THR:HA	7:I:67:VAL:HG12	1.78	0.66
1:A:131:ASP:HA	1:A:134:TYR:HD2	1.60	0.66
1:A:747:ILE:HG22	1:A:774:GLY:HA2	1.78	0.66
1:A:826:PHE:CZ	1:A:924:SER:HB3	2.30	0.66
3:C:329:LYS:HE3	9:K:122:LYS:HB2	1.77	0.66
1:A:321:LYS:HB2	1:A:356:PHE:HE2	1.60	0.66
1:A:16:PHE:HB3	1:A:1626:VAL:HG22	1.77	0.65
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.30	0.65
2:B:379:ARG:HE	2:B:580:GLY:HA2	1.60	0.65
1:A:1315:ASN:OD1	1:A:1319:ASN:ND2	2.28	0.65
1:A:17:GLY:O	2:B:1195:ARG:N	2.24	0.65
1:A:1105:ARG:NH1	1:A:1138:GLU:OE1	2.29	0.65
1:A:1059:LYS:NZ	1:A:1176:ARG:O	2.26	0.65
2:B:121:VAL:O	2:B:133:TYR:CE1	2.43	0.65
1:A:1138:GLU:O	1:A:1142:ASP:N	2.25	0.65
2:B:94:LYS:N	2:B:146:ASN:OD1	2.24	0.65
2:B:335:ARG:NH2	2:B:344:GLN:O	2.28	0.65
2:B:449:VAL:HA	2:B:452:ARG:HH21	1.60	0.65
2:B:1071:VAL:HG21	2:B:1091:ARG:HD2	1.78	0.65
2:B:94:LYS:O	2:B:146:ASN:N	2.26	0.65
3:C:128:ASP:O	3:C:175:GLN:NE2	2.30	0.65
1:A:694:GLN:NE2	9:K:91:TYR:O	2.29	0.65
2:B:434:ARG:NH2	2:B:436:MET:SD	2.69	0.65
3:C:257:GLY:O	3:C:266:TYR:N	2.24	0.65
5:F:84:TYR:HA	5:F:152:ILE:HB	1.78	0.65
1:A:1242:ILE:HA	1:A:1536:ILE:HA	1.79	0.65
2:B:841:ASP:OD1	2:B:842:GLU:N	2.29	0.65
1:A:1461:ASN:OD1	1:A:1462:PHE:N	2.28	0.65
1:A:1615:TYR:CD2	1:A:1616:GLU:HG3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:PRO:O	1:A:877:LYS:N	2.26	0.65
2:B:1187:SER:O	2:B:1190:SER:OG	2.15	0.65
7:I:91:ASN:OD1	7:I:92:GLU:N	2.30	0.65
1:A:383:ASN:HA	1:A:386:LEU:HD12	1.79	0.65
1:A:492:THR:O	1:A:620:ASN:ND2	2.28	0.64
13:D:99:LEU:HB3	13:D:100:PRO:HD3	1.78	0.64
2:B:662:ASP:OD1	2:B:663:ILE:N	2.30	0.64
6:H:3:ASN:OD1	6:H:4:THR:N	2.30	0.64
9:K:88:PHE:O	9:K:106:GLN:N	2.28	0.64
2:B:13:THR:CG2	12:N:163:VAL:CG2	2.75	0.64
2:B:705:PRO:HA	2:B:981:SER:HB2	1.77	0.64
4:E:176:PRO:HB2	4:E:212:ARG:HD3	1.79	0.64
1:A:316:LEU:HD22	1:A:427:PHE:HE2	1.61	0.64
1:A:704:ASP:HB3	1:A:706:HIS:ND1	2.11	0.64
2:B:946:ASP:OD1	8:J:9:SER:OG	2.16	0.64
1:A:713:VAL:HG12	1:A:737:LEU:HD21	1.79	0.64
2:B:1016:GLY:O	3:C:69:ARG:NH2	2.31	0.64
1:A:550:SER:N	1:A:553:GLN:OE1	2.20	0.64
1:A:1654:PHE:HB2	5:F:89:GLU:HG2	1.79	0.64
3:C:225:ALA:HA	3:C:302:VAL:HA	1.79	0.64
1:A:718:THR:OG1	1:A:730:GLN:NE2	2.31	0.64
2:B:656:LEU:H	2:B:657:PRO:CD	2.11	0.64
2:B:718:GLN:HE22	2:B:1034:GLN:HE22	1.43	0.64
3:C:95:GLU:OE1	3:C:95:GLU:N	2.29	0.64
1:A:943:ILE:HD11	2:B:958:MET:CB	2.28	0.63
2:B:564:ILE:O	2:B:567:SER:OG	2.12	0.63
3:C:32:ASN:OD1	3:C:33:VAL:N	2.30	0.63
1:A:1186:GLY:O	1:A:1190:SER:N	2.31	0.63
2:B:894:LYS:O	2:B:895:PHE:CG	2.50	0.63
3:C:163:TYR:N	3:C:166:ASP:OD2	2.26	0.63
2:B:353:VAL:HG13	2:B:357:ILE:HD12	1.79	0.63
8:J:44:TYR:HA	8:J:47:ARG:HD3	1.78	0.63
1:A:1000:MET:HG2	2:B:520:LEU:HB3	1.80	0.63
2:B:938:PHE:HZ	3:C:227:TYR:CE2	2.16	0.63
7:I:28:VAL:O	7:I:37:TYR:N	2.30	0.63
1:A:1501:ILE:HG22	1:A:1502:PRO:CD	2.27	0.63
1:A:1635:ASP:OD1	1:A:1636:SER:N	2.32	0.63
1:A:1185:VAL:O	1:A:1189:ALA:N	2.28	0.63
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.79	0.63
2:B:211:ARG:NH1	2:B:401:GLU:OE1	2.32	0.63
7:I:114:CYS:N	7:I:119:TYR:O	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:THR:HG22	1:A:1120:TYR:HB3	1.80	0.62
2:B:1038:HIS:NE2	2:B:1042:ASP:OD2	2.27	0.62
2:B:676:VAL:N	2:B:680:GLU:OE1	2.31	0.62
3:C:216:HIS:ND1	3:C:218:LYS:HG2	2.14	0.62
6:H:3:ASN:N	6:H:61:SER:OG	2.33	0.62
1:A:399:LEU:HD21	1:A:422:ARG:HB3	1.80	0.62
1:A:943:ILE:HD11	2:B:958:MET:CG	2.30	0.62
2:B:629:VAL:HG22	2:B:671:TYR:HE2	1.65	0.62
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.30	0.62
2:B:286:ARG:HD3	7:I:9:PHE:CD1	2.35	0.62
2:B:576:THR:HG21	12:N:95:ILE:CG2	2.29	0.62
1:A:949:GLN:HA	1:A:981:TYR:HA	1.80	0.62
1:A:949:GLN:HB2	1:A:981:TYR:HD1	1.64	0.62
1:A:245:LYS:HA	1:A:251:ILE:HA	1.81	0.62
1:A:535:GLN:HG2	1:A:545:SER:HA	1.82	0.62
1:A:93:GLN:HA	1:A:96:ILE:HD12	1.81	0.62
2:B:480:GLN:O	2:B:484:TYR:OH	2.10	0.62
2:B:51:ALA:HA	2:B:54:GLU:HB2	1.81	0.62
2:B:757:TYR:CE2	2:B:762:MET:HB2	2.34	0.62
1:A:325:ASP:HB3	1:A:329:ARG:HH12	1.65	0.62
1:A:560:GLN:O	1:A:575:LYS:NZ	2.33	0.62
3:C:122:ASP:HA	3:C:125:LYS:HB3	1.81	0.62
4:E:26:ARG:HH21	4:E:187:TYR:C	2.03	0.62
4:E:155:ARG:HA	4:E:196:VAL:HG12	1.82	0.62
5:F:103:MET:SD	14:G:112:PRO:HG3	2.39	0.62
1:A:1497:ILE:HG23	1:A:1500:GLN:HB3	1.82	0.62
1:A:54:LEU:O	1:A:75:HIS:N	2.31	0.62
1:A:908:VAL:HG22	1:A:945:CYS:CB	2.30	0.62
4:E:41:ASP:O	4:E:45:LYS:N	2.33	0.62
6:H:21:ASN:OD1	6:H:22:LYS:N	2.33	0.62
9:K:54:THR:HA	9:K:61:ALA:HA	1.81	0.62
7:I:113:THR:OG1	7:I:120:LYS:NZ	2.28	0.61
1:A:1299:ASN:HA	1:A:1302:TYR:CE2	2.36	0.61
1:A:834:ARG:HH12	2:B:1007:TYR:HE2	1.45	0.61
2:B:96:SER:HB2	2:B:144:SER:HB3	1.80	0.61
1:A:196:ALA:HA	1:A:201:ARG:HH21	1.64	0.61
1:A:584:ARG:HG2	1:A:644:ARG:HH22	1.65	0.61
1:A:841:LYS:O	1:A:844:THR:OG1	2.18	0.61
1:A:1559:ARG:HA	1:A:1562:ILE:HD12	1.82	0.61
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.81	0.61
3:C:236:LEU:N	3:C:288:LYS:O	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:GLU:HG3	3:C:82:TYR:CD2	2.36	0.61
4:E:165:LEU:O	4:E:169:ARG:N	2.33	0.61
6:H:11:GLN:NE2	6:H:52:GLN:OE1	2.34	0.61
7:I:91:ASN:HD22	7:I:116:SER:H	1.46	0.61
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.82	0.61
1:A:1651:THR:HB	5:F:92:ARG:NH1	2.15	0.61
1:A:669:LEU:HG	1:A:810:LEU:HD11	1.83	0.61
2:B:265:ARG:O	2:B:267:ASN:ND2	2.33	0.61
1:A:1243:TRP:NE1	1:A:1533:GLU:O	2.31	0.61
1:A:264:ASN:O	1:A:268:GLY:N	2.33	0.61
4:E:183:PRO:O	4:E:187:TYR:N	2.33	0.61
2:B:1161:ASP:OD1	2:B:1165:ASN:N	2.34	0.61
1:A:1056:ASP:OD1	1:A:1057:ILE:N	2.34	0.61
1:A:1624:LYS:HA	1:A:1627:LEU:HD12	1.81	0.61
2:B:609:ARG:NH2	2:B:626:ILE:HB	2.15	0.61
2:B:714:ARG:HH21	2:B:957:ARG:HA	1.66	0.61
2:B:110:ASN:N	2:B:118:GLU:HG2	2.15	0.60
2:B:369:ASP:OD1	2:B:372:ARG:NH1	2.33	0.60
2:B:655:TYR:CD2	2:B:657:PRO:HD2	2.35	0.60
8:J:31:ASP:OD1	8:J:34:THR:N	2.33	0.60
2:B:626:ILE:N	2:B:668:GLU:OE1	2.34	0.60
7:I:6:SER:HA	7:I:45:LEU:HD22	1.83	0.60
1:A:1272:VAL:HG11	1:A:1485:MET:HG2	1.82	0.60
1:A:973:GLU:HG3	1:A:975:ASP:H	1.67	0.60
2:B:168:ASN:OD1	2:B:169:ARG:N	2.35	0.60
2:B:552:SER:OG	2:B:648:ARG:N	2.34	0.60
5:F:108:PHE:HE2	5:F:131:PRO:HG3	1.65	0.60
1:A:244:ARG:HH22	1:A:312:SER:HB3	1.65	0.60
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.83	0.60
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.83	0.60
1:A:943:ILE:HD11	2:B:958:MET:SD	2.40	0.60
1:A:945:CYS:O	1:A:946:LEU:HD23	2.01	0.60
1:A:539:GLU:HB3	1:A:570:THR:HB	1.83	0.60
6:H:105:GLU:O	6:H:112:ILE:HG23	2.00	0.60
1:A:643:ALA:HB1	2:B:1087:LEU:HD23	1.83	0.60
3:C:87:ASN:H	3:C:203:SER:HB3	1.66	0.60
4:E:155:ARG:HD3	4:E:190:LEU:HD22	1.83	0.60
1:A:36:THR:HG22	1:A:45:VAL:HG21	1.84	0.60
2:B:249:VAL:HG11	2:B:261:ARG:HH21	1.67	0.60
2:B:184:LYS:HD2	2:B:735:HIS:NE2	2.17	0.60
3:C:134:LEU:O	3:C:206:ALA:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:72:LYS:HB3	5:F:142:SER:HA	1.84	0.60
1:A:1497:ILE:CG2	1:A:1500:GLN:HB3	2.31	0.60
1:A:37:VAL:HG12	1:A:38:LEU:HG	1.83	0.60
1:A:1263:LEU:HB3	1:A:1496:SER:CB	2.32	0.60
1:A:244:ARG:O	1:A:252:PHE:N	2.32	0.60
1:A:509:GLU:HB2	1:A:577:VAL:HB	1.83	0.60
1:A:615:ARG:HH12	2:B:929:ARG:HH21	1.50	0.60
2:B:698:SER:H	2:B:701:ALA:HB3	1.66	0.60
1:A:1049:MET:HB3	4:E:208:TYR:HE1	1.67	0.59
1:A:36:THR:HB	1:A:45:VAL:HG11	1.84	0.59
2:B:444:ARG:O	2:B:448:ARG:N	2.28	0.59
2:B:588:ILE:HG12	2:B:642:LEU:HD12	1.82	0.59
2:B:796:ARG:NH2	8:J:9:SER:O	2.35	0.59
3:C:164:ALA:HB2	3:C:191:ILE:HB	1.82	0.59
3:C:277:ARG:HB3	3:C:280:LEU:HD12	1.84	0.59
4:E:114:ASN:OD1	4:E:115:ASN:N	2.35	0.59
7:I:8:ILE:HG22	7:I:17:LEU:HD12	1.84	0.59
8:J:69:ARG:NH2	10:L:33:GLU:OE2	2.35	0.59
9:K:50:LEU:O	9:K:54:THR:HG23	2.03	0.59
9:K:87:GLU:N	9:K:106:GLN:O	2.34	0.59
1:A:1603:MET:HG2	1:A:1612:LYS:HG2	1.84	0.59
1:A:497:VAL:HG21	1:A:605:VAL:HG13	1.84	0.59
2:B:341:SER:OG	2:B:343:ASP:OD1	2.12	0.59
2:B:521:LEU:HB3	2:B:523:GLU:OE1	2.02	0.59
2:B:609:ARG:HG3	2:B:655:TYR:OH	2.01	0.59
1:A:1648:ASN:HB3	1:A:1649:VAL:HG23	1.83	0.59
1:A:621:THR:O	1:A:625:ASN:N	2.35	0.59
2:B:261:ARG:NH1	2:B:268:GLU:OE2	2.35	0.59
1:A:1646:LEU:HD22	14:G:109:PRO:HB3	1.84	0.59
2:B:50:ASN:HB3	2:B:54:GLU:OE1	2.02	0.59
2:B:745:GLN:HB3	2:B:800:TYR:HB3	1.83	0.59
12:N:89:ILE:HG12	12:N:139:VAL:HG22	1.85	0.59
2:B:1128:CYS:H	2:B:1170:GLY:HA3	1.68	0.59
2:B:150:GLU:HB2	2:B:441:LYS:HE2	1.85	0.59
9:K:116:ALA:HA	9:K:119:LYS:HB3	1.85	0.59
2:B:887:LEU:HB2	10:L:56:LEU:HB2	1.84	0.59
1:A:1578:SER:HB3	1:A:1581:HIS:CD2	2.38	0.59
1:A:1640:ARG:NE	1:A:1646:LEU:O	2.34	0.59
1:A:417:ARG:O	1:A:421:SER:N	2.35	0.59
2:B:912:GLN:N	2:B:915:ASP:OD2	2.26	0.59
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HH21	1:A:137:ASP:CG	2.07	0.59
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.85	0.59
2:B:884:GLU:O	2:B:904:LYS:N	2.30	0.59
1:A:1640:ARG:O	1:A:1645:LYS:N	2.35	0.59
1:A:641:GLU:O	1:A:645:ALA:N	2.30	0.59
2:B:1128:CYS:HB3	2:B:1131:CYS:HB2	1.84	0.59
2:B:944:GLN:N	2:B:944:GLN:OE1	2.36	0.59
3:C:68:ARG:HD2	3:C:227:TYR:CE2	2.37	0.59
3:C:87:ASN:O	3:C:203:SER:N	2.33	0.59
4:E:177:ARG:HG3	4:E:215:MET:HG3	1.84	0.59
1:A:1053:ASP:OD1	1:A:1054:ALA:N	2.34	0.58
2:B:1013:MET:HB2	2:B:1022:LEU:HD12	1.84	0.58
2:B:15:ASP:OD1	2:B:16:PHE:N	2.35	0.58
2:B:996:PHE:O	2:B:999:GLN:N	2.36	0.58
9:K:122:LYS:NZ	9:K:126:ASP:OD2	2.31	0.58
1:A:267:LYS:HG2	1:A:270:ILE:HD12	1.85	0.58
2:B:1128:CYS:O	2:B:1132:SER:N	2.36	0.58
2:B:698:SER:O	2:B:702:ASN:ND2	2.36	0.58
4:E:20:LYS:NZ	4:E:34:GLU:O	2.30	0.58
11:M:10:ILE:HB	12:N:70:LEU:HB3	1.86	0.58
1:A:481:ARG:HE	1:A:632:GLU:HB2	1.68	0.58
1:A:1486:VAL:HG23	7:I:51:THR:HG22	1.86	0.58
1:A:468:ARG:HA	1:A:472:MET:HB2	1.84	0.58
2:B:523:GLU:N	2:B:523:GLU:OE1	2.34	0.58
3:C:242:GLU:HG3	3:C:246:ARG:NE	2.18	0.58
1:A:1656:VAL:HG11	14:G:107:ILE:HB	1.84	0.58
12:N:69:SER:OG	12:N:70:LEU:N	2.37	0.58
1:A:1443:GLN:O	1:A:1447:GLN:N	2.27	0.58
1:A:596:HIS:CD2	1:A:598:ALA:HB3	2.38	0.58
3:C:32:ASN:H	3:C:35:LYS:HD2	1.67	0.58
14:G:30:GLU:HA	14:G:32:ASN:N	2.18	0.58
1:A:659:THR:OG1	1:A:664:SER:N	2.33	0.58
1:A:846:ILE:HD13	1:A:906:GLN:CB	2.29	0.58
6:H:103:LYS:HD2	6:H:115:TYR:CD2	2.38	0.58
10:L:27:LEU:HA	10:L:39:SER:HB2	1.85	0.58
1:A:590:ASN:OD1	1:A:591:ARG:N	2.37	0.58
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.68	0.58
2:B:13:THR:CG2	12:N:163:VAL:HG22	2.33	0.58
2:B:576:THR:CG2	12:N:95:ILE:HG22	2.34	0.58
4:E:83:CYS:N	4:E:111:VAL:O	2.36	0.58
1:A:1101:THR:HA	1:A:1104:TYR:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:LEU:O	1:A:1158:SER:N	2.37	0.58
1:A:1497:ILE:O	1:A:1497:ILE:HG22	2.04	0.58
1:A:320:VAL:HA	1:A:323:ILE:HD12	1.85	0.58
1:A:435:ASN:ND2	1:A:442:LYS:O	2.37	0.58
2:B:832:TRP:HH2	2:B:837:LEU:HG	1.68	0.58
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.85	0.58
2:B:796:ARG:NH2	8:J:8:PHE:O	2.36	0.58
1:A:659:THR:O	1:A:663:GLY:N	2.33	0.57
1:A:1287:ALA:HA	1:A:1478:ALA:HB2	1.86	0.57
1:A:956:ARG:NH2	1:A:979:GLY:HA3	2.19	0.57
2:B:658:LEU:O	2:B:660:LYS:HG3	2.03	0.57
1:A:341:SER:N	1:A:1628:ASP:O	2.35	0.57
3:C:325:ALA:HA	3:C:328:LEU:HB3	1.86	0.57
1:A:1315:ASN:HA	1:A:1318:SER:HB2	1.85	0.57
1:A:236:CYS:HB2	1:A:271:ARG:HD2	1.86	0.57
2:B:1105:ARG:HB3	2:B:1172:GLU:HB3	1.87	0.57
2:B:894:LYS:HG3	10:L:54:ARG:HH21	1.69	0.57
1:A:522:ALA:O	1:A:526:GLY:N	2.38	0.57
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.87	0.57
2:B:757:TYR:CZ	2:B:762:MET:HB2	2.40	0.57
6:H:103:LYS:HB3	6:H:115:TYR:HB2	1.86	0.57
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.39	0.57
1:A:697:TYR:CE1	9:K:104:ARG:HG3	2.39	0.57
2:B:972:GLY:O	2:B:976:GLY:N	2.38	0.57
1:A:2:ASP:HB3	1:A:5:LYS:HD3	1.87	0.57
1:A:826:PHE:HZ	1:A:924:SER:HB3	1.68	0.57
6:H:38:LEU:HD11	6:H:123:MET:HG3	1.86	0.57
14:G:56:ASN:HB3	14:G:59:GLN:HB3	1.87	0.57
1:A:208:PHE:HA	1:A:212:VAL:HG11	1.87	0.57
1:A:975:ASP:OD2	1:A:977:MET:HB3	2.04	0.57
4:E:17:ARG:NH1	4:E:35:VAL:O	2.38	0.57
12:N:148:ILE:O	12:N:150:TYR:N	2.38	0.57
2:B:489:GLU:HG3	2:B:495:ARG:HE	1.70	0.56
4:E:110:PHE:N	4:E:133:GLU:O	2.28	0.56
2:B:656:LEU:O	12:N:153:VAL:CG1	2.46	0.56
2:B:745:GLN:HG2	2:B:800:TYR:CD2	2.33	0.56
1:A:11:ILE:HD11	2:B:1176:VAL:HG21	1.86	0.56
1:A:675:SER:OG	2:B:952:HIS:NE2	2.24	0.56
1:A:7:VAL:HG11	2:B:1176:VAL:HA	1.86	0.56
2:B:801:GLY:O	2:B:802:THR:OG1	2.23	0.56
3:C:257:GLY:HA3	3:C:266:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LEU:HD13	2:B:326:VAL:HA	1.86	0.56
1:A:836:THR:HG23	1:A:839:GLY:H	1.71	0.56
2:B:832:TRP:CH2	2:B:837:LEU:HG	2.41	0.56
6:H:85:GLY:O	6:H:87:ARG:NH1	2.38	0.56
7:I:29:GLU:HB2	7:I:36:ILE:HG13	1.87	0.56
3:C:126:PHE:HD2	3:C:131:THR:HG1	1.54	0.56
7:I:89:CYS:SG	7:I:116:SER:OG	2.59	0.56
1:A:1082:PRO:HA	1:A:1085:LEU:HD12	1.87	0.56
1:A:966:LEU:HB3	1:A:969:PHE:HD2	1.70	0.56
1:A:592:GLN:NE2	2:B:1075:GLU:OE2	2.39	0.56
2:B:852:VAL:HG13	2:B:856:ASP:HB2	1.88	0.56
2:B:893:ASN:ND2	2:B:895:PHE:CD2	2.69	0.56
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.86	0.56
1:A:1454:HIS:HB2	1:A:1457:ILE:HD12	1.88	0.56
1:A:95:TYR:CG	1:A:245:LYS:HD3	2.40	0.56
1:A:365:THR:O	1:A:369:LEU:N	2.38	0.56
1:A:846:ILE:CD1	1:A:906:GLN:HB3	2.31	0.56
1:A:683:LYS:HD2	6:H:20:TYR:CE2	2.41	0.56
1:A:828:CYS:SG	1:A:829:GLY:N	2.78	0.56
3:C:259:ASP:N	3:C:264:GLU:O	2.39	0.56
1:A:1649:VAL:HG12	1:A:1650:GLY:N	2.21	0.56
2:B:815:ARG:HE	2:B:821:ILE:HA	1.71	0.56
2:B:815:ARG:NE	2:B:821:ILE:HA	2.21	0.56
3:C:121:PRO:O	3:C:125:LYS:N	2.33	0.56
4:E:96:PHE:HE2	4:E:132:ILE:HG23	1.70	0.56
2:B:462:GLN:O	2:B:466:SER:N	2.29	0.56
2:B:750:PRO:HB3	2:B:1032:TYR:CG	2.41	0.56
2:B:787:MET:SD	2:B:917:PHE:HB2	2.46	0.56
7:I:10:CYS:HB2	7:I:17:LEU:HD21	1.88	0.56
1:A:1242:ILE:HD11	1:A:1517:ARG:NE	2.20	0.55
1:A:372:LYS:HB3	1:A:377:VAL:HA	1.88	0.55
2:B:654:ARG:NH2	2:B:659:ASP:OD2	2.37	0.55
2:B:659:ASP:O	2:B:660:LYS:HG3	2.06	0.55
2:B:987:ASN:OD1	2:B:990:ASP:N	2.35	0.55
1:A:606:ARG:NH2	9:K:98:GLU:OE2	2.39	0.55
2:B:492:ASN:OD1	2:B:495:ARG:N	2.29	0.55
8:J:32:GLU:OE1	8:J:32:GLU:N	2.38	0.55
2:B:492:ASN:HD21	2:B:723:LYS:HA	1.71	0.55
3:C:117:ASP:OD1	3:C:118:SER:N	2.39	0.55
1:A:885:ASP:OD1	1:A:887:ASN:N	2.39	0.55
2:B:218:ILE:HG23	2:B:231:HIS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:5:LEU:H	6:H:60:ALA:HA	1.70	0.55
7:I:66:VAL:HG23	7:I:67:VAL:HG13	1.89	0.55
9:K:68:GLU:H	9:K:99:ASN:HB3	1.70	0.55
1:A:316:LEU:HD22	1:A:427:PHE:CE2	2.41	0.55
2:B:700:LEU:N	16:B:1301:SO4:S	2.73	0.55
2:B:783:MET:HA	2:B:950:ASN:HD22	1.71	0.55
3:C:87:ASN:ND2	3:C:201:GLU:OE2	2.39	0.55
2:B:387:GLY:O	2:B:634:ARG:NH1	2.40	0.55
1:A:885:ASP:OD2	1:A:888:LYS:HG3	2.07	0.55
2:B:190:ILE:HD11	2:B:496:PHE:HE2	1.72	0.55
2:B:23:SER:O	2:B:27:ASN:N	2.32	0.55
2:B:362:LEU:HD12	2:B:370:LYS:HG2	1.89	0.55
3:C:179:PHE:HA	3:C:182:CYS:SG	2.47	0.55
9:K:77:ARG:HD2	9:K:91:TYR:HE1	1.71	0.55
11:M:15:VAL:HG22	11:M:90:LEU:HB2	1.88	0.55
1:A:1449:ALA:O	1:A:1452:SER:OG	2.13	0.55
1:A:1648:ASN:H	1:A:1649:VAL:HB	1.71	0.55
1:A:908:VAL:CA	1:A:945:CYS:SG	2.92	0.55
2:B:1077:ASP:HA	2:B:1080:ILE:HD12	1.89	0.55
9:K:50:LEU:HD21	9:K:64:GLN:HB2	1.88	0.55
1:A:829:GLY:N	1:A:832:ASP:OD2	2.40	0.55
9:K:63:PHE:HB2	9:K:103:ILE:HB	1.89	0.55
1:A:503:VAL:HA	1:A:580:HIS:CE1	2.42	0.55
1:A:945:CYS:C	1:A:946:LEU:HG	2.27	0.55
2:B:177:PRO:HA	2:B:180:LEU:HD12	1.89	0.55
2:B:529:CYS:SG	2:B:532:HIS:N	2.73	0.55
3:C:89:THR:OG1	3:C:201:GLU:N	2.29	0.55
2:B:675:ALA:O	2:B:689:VAL:HA	2.06	0.54
2:B:718:GLN:OE1	2:B:922:GLY:N	2.40	0.54
14:G:229:LEU:HD12	14:G:230:ARG:H	1.72	0.54
1:A:1549:VAL:O	1:A:1553:TYR:N	2.34	0.54
2:B:504:HIS:CB	2:B:542:LEU:HD23	2.36	0.54
2:B:609:ARG:HE	2:B:626:ILE:HD12	1.72	0.54
1:A:1651:THR:O	1:A:1654:PHE:N	2.39	0.54
2:B:132:SER:OG	2:B:196:VAL:HA	2.07	0.54
2:B:584:CYS:N	2:B:596:VAL:O	2.41	0.54
2:B:743:ARG:NH2	8:J:1:MET:SD	2.80	0.54
9:K:134:LYS:O	9:K:138:LYS:HG2	2.07	0.54
1:A:1105:ARG:NH2	1:A:1142:ASP:OD1	2.40	0.54
1:A:883:LEU:HD22	1:A:972:TYR:HE1	1.72	0.54
2:B:700:LEU:N	16:B:1301:SO4:O1	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HA	1:A:182:LYS:HD3	1.90	0.54
1:A:657:TYR:O	1:A:666:VAL:HG22	2.08	0.54
1:A:771:PHE:HE1	1:A:776:LEU:HD13	1.72	0.54
2:B:54:GLU:OE2	2:B:168:ASN:ND2	2.39	0.54
2:B:505:ARG:HB3	2:B:509:PHE:CD2	2.41	0.54
1:A:1204:THR:HG22	1:A:1205:PHE:H	1.73	0.54
1:A:1310:LYS:O	1:A:1314:GLN:N	2.28	0.54
4:E:143:ASN:OD1	4:E:145:THR:N	2.41	0.54
1:A:1289:SER:HA	1:A:1475:GLU:HA	1.89	0.54
1:A:535:GLN:HB2	1:A:578:TYR:HD2	1.73	0.54
2:B:656:LEU:HB3	2:B:657:PRO:HD3	1.89	0.54
5:F:117:PRO:HA	5:F:120:ILE:HD12	1.90	0.54
1:A:472:MET:HB3	2:B:1073:GLU:HG2	1.90	0.54
2:B:57:ASP:OD1	2:B:59:GLY:N	2.39	0.54
3:C:311:GLU:OE1	3:C:311:GLU:N	2.30	0.54
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.90	0.54
11:M:12:ILE:HD12	12:N:67:LEU:HB2	1.90	0.54
1:A:1111:GLU:O	1:A:1116:GLN:NE2	2.41	0.54
1:A:1533:GLU:OE2	4:E:14:ARG:NH2	2.39	0.54
1:A:916:THR:O	1:A:919:LYS:NZ	2.40	0.54
3:C:152:ASP:OD2	3:C:154:LYS:HB2	2.08	0.54
3:C:248:GLN:HG3	3:C:256:ILE:HB	1.89	0.54
4:E:83:CYS:HB2	4:E:110:PHE:CZ	2.42	0.54
1:A:368:ARG:O	1:A:383:ASN:ND2	2.38	0.54
1:A:583:ASN:OD1	1:A:606:ARG:HA	2.08	0.54
2:B:840:LEU:HA	2:B:846:PRO:HA	1.90	0.54
6:H:103:LYS:HD2	6:H:115:TYR:HD2	1.73	0.54
7:I:31:SER:O	7:I:34:LYS:NZ	2.32	0.54
2:B:21:ARG:NH2	8:J:53:HIS:O	2.41	0.54
2:B:379:ARG:HE	2:B:580:GLY:CA	2.21	0.53
6:H:112:ILE:HD12	6:H:129:TYR:HB3	1.90	0.53
1:A:467:PHE:O	1:A:471:MET:HB2	2.08	0.53
1:A:27:LEU:HA	2:B:1129:ARG:HG2	1.91	0.53
2:B:274:VAL:HA	2:B:277:LEU:HD12	1.90	0.53
6:H:36:CYS:HA	6:H:126:GLU:O	2.08	0.53
7:I:74:ASN:O	7:I:77:LYS:HG2	2.09	0.53
1:A:1298:ASP:HB2	1:A:1301:GLU:CD	2.29	0.53
1:A:1200:MET:HG2	1:A:1573:TYR:CD1	2.43	0.53
1:A:327:VAL:O	1:A:331:GLU:N	2.35	0.53
1:A:494:GLU:HG2	1:A:604:LYS:HB2	1.90	0.53
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:HA	1:A:63:SER:HB2	1.89	0.53
3:C:213:GLY:HA2	3:C:219:PHE:HB2	1.89	0.53
1:A:1559:ARG:NH2	4:E:200:ARG:HD3	2.24	0.53
1:A:32:ILE:HG21	1:A:49:LEU:HD23	1.90	0.53
2:B:1134:ARG:HD3	2:B:1167:PHE:HE1	1.72	0.53
14:G:20:HIS:O	14:G:20:HIS:ND1	2.38	0.53
1:A:1524:VAL:HG21	1:A:1545:ASP:HB2	1.91	0.53
2:B:1107:CYS:O	2:B:1197:ARG:NH1	2.42	0.53
3:C:43:ASN:O	3:C:55:ASP:N	2.39	0.53
1:A:1031:HIS:CE1	1:A:1039:ARG:HB2	2.43	0.53
1:A:39:ASP:OD1	1:A:43:HIS:N	2.41	0.53
1:A:728:GLY:HA2	1:A:731:ILE:HD12	1.91	0.53
2:B:560:ARG:O	2:B:563:SER:OG	2.19	0.53
1:A:1542:THR:HG22	4:E:149:LEU:HD11	1.90	0.53
1:A:211:THR:HG23	4:E:177:ARG:NH1	2.23	0.53
1:A:752:LYS:HG2	1:A:768:GLU:HA	1.89	0.53
2:B:560:ARG:NH1	2:B:618:PRO:HB2	2.23	0.53
7:I:91:ASN:HD21	7:I:115:THR:HB	1.74	0.53
1:A:1153:LYS:HA	1:A:1156:LYS:NZ	2.23	0.53
1:A:477:ASN:HB3	2:B:1048:SER:O	2.09	0.53
1:A:572:THR:HA	14:G:52:MET:HE1	1.91	0.53
1:A:783:LYS:HG3	1:A:787:GLY:HA3	1.89	0.53
1:A:1530:TRP:CG	4:E:142:VAL:HG21	2.44	0.53
4:E:180:ARG:N	4:E:215:MET:OXT	2.41	0.53
5:F:83:PRO:O	5:F:152:ILE:N	2.31	0.53
14:G:132:VAL:HG22	14:G:232:THR:HG22	1.90	0.53
2:B:134:ARG:HG2	2:B:162:PRO:HA	1.91	0.53
4:E:64:PRO:HG3	4:E:75:MET:HG2	1.91	0.53
1:A:1260:LYS:HE3	1:A:1500:GLN:HB2	1.90	0.53
1:A:1657:LEU:HD11	5:F:135:ARG:CB	2.39	0.53
1:A:17:GLY:N	2:B:1195:ARG:O	2.40	0.53
2:B:983:PRO:HB2	2:B:984:TRP:CE3	2.44	0.53
1:A:244:ARG:N	1:A:252:PHE:O	2.33	0.52
2:B:798:PHE:HA	8:J:8:PHE:CZ	2.44	0.52
4:E:90:VAL:HG13	4:E:123:LEU:HD11	1.89	0.52
4:E:48:ASP:OD1	4:E:52:ARG:N	2.24	0.52
4:E:6:GLU:HA	4:E:9:ILE:HD12	1.92	0.52
6:H:30:SER:HB3	6:H:33:GLN:O	2.09	0.52
1:A:648:LEU:O	1:A:652:ASN:ND2	2.42	0.52
2:B:238:SER:O	2:B:246:GLN:N	2.31	0.52
2:B:72:VAL:HG22	2:B:96:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:PRO:HB2	2:B:177:PRO:HG2	1.92	0.52
2:B:832:TRP:HZ3	2:B:836:TRP:HB2	1.74	0.52
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.43	0.52
1:A:488:PRO:HD3	1:A:618:TYR:HE2	1.75	0.52
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.92	0.52
1:A:16:PHE:CE2	1:A:1625:ALA:HB1	2.45	0.52
1:A:1301:GLU:O	1:A:1305:GLU:N	2.27	0.52
2:B:516:THR:HG22	2:B:519:LYS:HE2	1.91	0.52
2:B:757:TYR:O	2:B:761:GLY:N	2.43	0.52
2:B:832:TRP:CZ3	2:B:834:LYS:HA	2.44	0.52
3:C:121:PRO:HD2	3:C:124:GLU:OE1	2.10	0.52
2:B:1014:TYR:HE2	3:C:228:ARG:HA	1.75	0.52
3:C:84:TYR:HE2	3:C:207:HIS:HE2	1.57	0.52
1:A:1023:LEU:HD21	1:A:1226:VAL:HG11	1.92	0.52
1:A:945:CYS:O	1:A:946:LEU:HG	2.09	0.52
3:C:165:ARG:NH1	3:C:190:ASP:HA	2.25	0.52
7:I:87:PRO:HG2	7:I:119:TYR:CE2	2.43	0.52
1:A:50:TYR:OH	1:A:383:ASN:ND2	2.43	0.52
9:K:59:THR:O	9:K:106:GLN:HA	2.10	0.52
1:A:1582:LEU:O	1:A:1586:ALA:N	2.35	0.52
1:A:861:VAL:HA	7:I:68:LYS:HD3	1.92	0.52
1:A:943:ILE:O	1:A:943:ILE:HG22	2.09	0.52
2:B:1106:GLU:HB2	2:B:1172:GLU:HB2	1.90	0.52
13:D:48:GLU:OE2	13:D:90:LYS:NZ	2.43	0.52
7:I:23:VAL:HB	7:I:39:LYS:HZ1	1.75	0.52
1:A:1056:ASP:OD2	1:A:1058:THR:OG1	2.28	0.52
1:A:1254:PHE:O	1:A:1257:SER:OG	2.18	0.52
1:A:945:CYS:O	1:A:946:LEU:CD2	2.57	0.52
2:B:23:SER:HA	2:B:26:ILE:HB	1.92	0.52
3:C:232:GLN:HB3	3:C:292:GLY:C	2.30	0.52
1:A:879:LEU:O	1:A:883:LEU:N	2.30	0.51
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.92	0.51
1:A:1034:TYR:CE1	5:F:136:ARG:HD3	2.44	0.51
11:M:75:GLN:HB2	12:N:60:SER:HA	1.91	0.51
1:A:1114:TYR:HE1	1:A:1115:LYS:HE3	1.75	0.51
1:A:236:CYS:HB3	1:A:271:ARG:HH11	1.73	0.51
2:B:745:GLN:HB3	2:B:800:TYR:O	2.09	0.51
3:C:153:PRO:O	3:C:157:TYR:N	2.43	0.51
3:C:188:ASP:HB2	3:C:191:ILE:HG13	1.93	0.51
4:E:107:THR:HG23	4:E:131:THR:HG23	1.92	0.51
1:A:1238:MET:HB2	1:A:1521:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:LYS:HA	1:A:1313:LEU:HB3	1.92	0.51
2:B:404:LEU:HD12	2:B:407:PHE:CE2	2.46	0.51
2:B:576:THR:HG23	12:N:95:ILE:HG22	1.92	0.51
2:B:602:LYS:HB2	2:B:628:TYR:CZ	2.46	0.51
4:E:17:ARG:HG2	4:E:21:GLU:OE2	2.11	0.51
1:A:1264:SER:HB2	7:I:56:PHE:HD1	1.75	0.51
7:I:86:CYS:HB3	7:I:91:ASN:H	1.76	0.51
2:B:397:THR:HA	2:B:400:GLN:OE1	2.10	0.51
2:B:788:ILE:HB	2:B:948:ILE:HB	1.92	0.51
1:A:1050:TYR:CE2	1:A:1580:ARG:HD3	2.46	0.51
1:A:1100:LYS:HG2	1:A:1104:TYR:HE2	1.76	0.51
1:A:379:GLU:OE2	1:A:384:GLN:NE2	2.26	0.51
1:A:509:GLU:OE2	1:A:579:ARG:NE	2.43	0.51
2:B:335:ARG:NH2	2:B:342:PRO:O	2.44	0.51
2:B:74:PHE:HE2	2:B:343:ASP:HB3	1.74	0.51
2:B:527:PHE:O	2:B:546:ALA:N	2.29	0.51
14:G:30:GLU:HA	14:G:32:ASN:H	1.74	0.51
6:H:129:TYR:O	6:H:133:ASN:N	2.43	0.51
1:A:1193:VAL:O	1:A:1196:PRO:HD2	2.10	0.51
1:A:1647:ASN:HB3	1:A:1650:GLY:H	1.75	0.51
1:A:804:GLU:CD	1:A:804:GLU:H	2.14	0.51
2:B:167:SER:OG	2:B:170:CYS:N	2.43	0.51
2:B:589:ASP:OD1	2:B:643:PHE:HA	2.11	0.51
2:B:938:PHE:CZ	3:C:227:TYR:CE2	2.98	0.51
3:C:236:LEU:HD12	3:C:287:ASP:O	2.11	0.51
3:C:87:ASN:OD1	3:C:88:ASN:N	2.44	0.51
1:A:1303:SER:HA	1:A:1308:VAL:H	1.75	0.51
1:A:352:ALA:HA	1:A:355:PHE:HD2	1.75	0.51
1:A:949:GLN:HG3	1:A:950:GLN:O	2.11	0.51
2:B:1118:PRO:HD3	2:B:1124:SER:HB2	1.92	0.51
2:B:573:ALA:HB2	2:B:594:GLY:HA2	1.92	0.51
2:B:584:CYS:HB3	2:B:596:VAL:HG23	1.93	0.51
3:C:161:HIS:HB2	3:C:163:TYR:CE1	2.45	0.51
7:I:84:GLU:N	7:I:92:GLU:O	2.40	0.51
1:A:1609:SER:O	1:A:1612:LYS:N	2.44	0.51
1:A:675:SER:HG	2:B:952:HIS:CE1	2.28	0.51
2:B:145:VAL:N	2:B:150:GLU:O	2.41	0.51
2:B:136:LYS:HA	2:B:160:GLY:HA2	1.92	0.51
6:H:35:GLN:HE22	6:H:110:ASP:HB3	1.75	0.51
1:A:126:GLN:HB3	1:A:343:PRO:HG3	1.92	0.51
1:A:806:ALA:HA	1:A:809:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:ASP:HA	2:B:349:VAL:HB	1.93	0.51
2:B:677:THR:H	2:B:680:GLU:CD	2.14	0.51
5:F:127:GLU:HB3	5:F:129:LYS:HG2	1.93	0.51
12:N:63:ASP:OD2	12:N:66:LYS:NZ	2.35	0.51
1:A:208:PHE:CE2	1:A:1607:THR:HG23	2.47	0.50
1:A:21:ALA:HA	1:A:24:ILE:HB	1.91	0.50
1:A:321:LYS:HB2	1:A:356:PHE:CE2	2.44	0.50
3:C:174:ARG:O	3:C:178:THR:N	2.38	0.50
1:A:368:ARG:HA	1:A:380:ASN:ND2	2.27	0.50
1:A:723:TYR:CD1	1:A:724:PRO:HD2	2.47	0.50
2:B:322:ASN:HB3	2:B:325:GLN:HG3	1.93	0.50
9:K:54:THR:HG22	9:K:62:SER:H	1.77	0.50
1:A:119:ALA:HA	1:A:122:LEU:HD12	1.93	0.50
1:A:381:SER:HB2	1:A:453:ILE:HG23	1.93	0.50
1:A:826:PHE:CZ	1:A:924:SER:CB	2.95	0.50
2:B:599:GLU:CD	2:B:599:GLU:H	2.15	0.50
1:A:962:SER:HB3	2:B:670:VAL:HG12	1.92	0.50
2:B:72:VAL:HG11	2:B:94:LYS:HG3	1.94	0.50
3:C:332:PRO:HD3	9:K:42:PRO:HB2	1.94	0.50
3:C:45:SER:H	3:C:54:PHE:HA	1.76	0.50
4:E:145:THR:HG21	4:E:187:TYR:CE2	2.47	0.50
4:E:28:TYR:HE1	4:E:64:PRO:HG3	1.76	0.50
1:A:1516:LYS:HG3	1:A:1518:VAL:HG23	1.94	0.50
1:A:91:PHE:CE2	1:A:245:LYS:HD2	2.46	0.50
1:A:49:LEU:HB3	1:A:368:ARG:HH12	1.75	0.50
1:A:526:GLY:HA3	1:A:554:ARG:NH1	2.20	0.50
1:A:551:VAL:HG22	1:A:554:ARG:HH21	1.76	0.50
2:B:1131:CYS:HB2	2:B:1170:GLY:HA2	1.92	0.50
2:B:326:VAL:O	2:B:330:LEU:HG	2.11	0.50
2:B:559:SER:O	2:B:562:PRO:HD2	2.12	0.50
3:C:142:ARG:NH2	8:J:67:GLU:OE2	2.44	0.50
1:A:324:LEU:HA	1:A:327:VAL:HB	1.93	0.50
2:B:20:GLU:HG2	2:B:24:ARG:NH1	2.23	0.50
2:B:517:VAL:HG23	2:B:518:ARG:HG3	1.92	0.50
1:A:1025:LYS:HE3	1:A:1611:MET:HG3	1.93	0.50
1:A:248:PHE:CE2	1:A:444:GLN:HG2	2.46	0.50
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.94	0.50
1:A:551:VAL:HA	1:A:554:ARG:HH21	1.76	0.50
1:A:487:ASP:O	1:A:617:HIS:HA	2.12	0.50
2:B:76:GLY:H	2:B:92:GLY:HA3	1.76	0.50
3:C:87:ASN:N	3:C:203:SER:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:102:TYR:CE1	6:H:115:TYR:HB3	2.47	0.50
8:J:31:ASP:CG	8:J:34:THR:H	2.14	0.50
1:A:1138:GLU:HA	1:A:1141:GLN:HB3	1.92	0.50
1:A:1530:TRP:CD2	4:E:142:VAL:HG21	2.47	0.50
1:A:538:ASN:HB2	1:A:540:ASP:OD1	2.10	0.50
1:A:652:ASN:CG	1:A:653:THR:H	2.15	0.50
1:A:651:ALA:O	1:A:656:GLN:NE2	2.45	0.50
2:B:150:GLU:HG2	2:B:441:LYS:HG2	1.93	0.50
2:B:655:TYR:CD1	2:B:688:HIS:CD2	3.00	0.50
2:B:923:GLN:HE22	2:B:957:ARG:HD2	1.77	0.50
3:C:133:VAL:HG22	3:C:207:HIS:ND1	2.26	0.50
4:E:113:GLN:HG2	4:E:137:GLU:OE2	2.12	0.50
1:A:1288:ARG:O	1:A:1476:LEU:N	2.40	0.50
2:B:352:GLU:OE2	2:B:356:ARG:NE	2.42	0.50
1:A:488:PRO:HD2	2:B:781:TYR:CE1	2.47	0.50
1:A:618:TYR:CZ	2:B:783:MET:HB2	2.46	0.50
1:A:937:ASN:O	1:A:941:SER:HB3	2.12	0.50
2:B:368:GLN:HG3	2:B:372:ARG:NH1	2.27	0.50
2:B:393:ASN:HD22	2:B:396:ALA:HB2	1.77	0.50
4:E:46:TYR:O	4:E:53:PRO:HA	2.12	0.50
14:G:47:VAL:HB	14:G:65:HIS:CD2	2.47	0.50
1:A:721:LYS:HB3	6:H:96:VAL:HB	1.93	0.50
1:A:1074:TYR:O	1:A:1078:LYS:HG2	2.12	0.49
1:A:1224:GLU:O	1:A:1228:THR:OG1	2.27	0.49
1:A:887:ASN:O	1:A:891:ILE:HG12	2.12	0.49
2:B:211:ARG:NH1	2:B:647:SER:HB2	2.18	0.49
2:B:74:PHE:HA	2:B:93:ASN:O	2.12	0.49
6:H:28:ALA:N	6:H:38:LEU:O	2.40	0.49
2:B:966:SER:OG	2:B:1029:GLY:HA3	2.12	0.49
2:B:25:PHE:CD1	8:J:59:LYS:HD2	2.48	0.49
2:B:443:LYS:HA	2:B:446:MET:HB3	1.94	0.49
3:C:99:HIS:CE1	3:C:103:LEU:HD11	2.47	0.49
6:H:101:ALA:HB2	6:H:116:TYR:CZ	2.47	0.49
1:A:102:CYS:HB2	1:A:109:ARG:HG2	1.92	0.49
1:A:672:ASP:HA	1:A:675:SER:HB2	1.93	0.49
1:A:713:VAL:O	1:A:738:ASN:ND2	2.38	0.49
2:B:752:VAL:HA	2:B:979:GLN:O	2.12	0.49
8:J:8:PHE:HB2	8:J:48:ARG:HH22	1.77	0.49
9:K:91:TYR:CD2	9:K:101:LEU:HD11	2.46	0.49
1:A:1300:ASN:O	1:A:1304:GLU:N	2.35	0.49
1:A:1299:ASN:HA	1:A:1302:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1462:PHE:HD1	1:A:1470:CYS:HB2	1.77	0.49
1:A:1568:ASN:HA	1:A:1571:SER:HB2	1.94	0.49
1:A:717:PRO:HG2	1:A:720:PHE:CD1	2.47	0.49
4:E:54:GLN:O	4:E:58:MET:HG3	2.13	0.49
11:M:65:TYR:CE1	11:M:97:VAL:HB	2.48	0.49
1:A:1545:ASP:O	1:A:1548:ALA:N	2.44	0.49
1:A:363:PRO:HD2	1:A:368:ARG:HD3	1.94	0.49
2:B:753:LYS:O	2:B:981:SER:N	2.38	0.49
2:B:854:GLU:HG3	2:B:874:TYR:O	2.13	0.49
3:C:51:GLU:HA	3:C:303:GLU:HA	1.94	0.49
1:A:1643:VAL:HB	1:A:1645:LYS:HG2	1.95	0.49
2:B:828:GLY:HA3	2:B:862:PHE:CD1	2.48	0.49
2:B:827:PHE:CD1	2:B:869:THR:HG21	2.48	0.49
4:E:48:ASP:OD1	4:E:51:GLY:N	2.45	0.49
1:A:1066:PHE:O	1:A:1070:LEU:N	2.43	0.49
1:A:1263:LEU:HG	1:A:1267:ILE:HD11	1.95	0.49
1:A:250:LYS:HD3	1:A:428:VAL:HG22	1.94	0.49
1:A:631:ASP:N	1:A:631:ASP:OD1	2.43	0.49
3:C:41:GLU:HB3	3:C:57:ILE:HB	1.95	0.49
1:A:1129:PRO:HA	1:A:1135:SER:HB3	1.94	0.49
1:A:1504:ILE:CD1	1:A:1529:MET:HE3	2.42	0.49
1:A:942:GLN:HA	1:A:946:LEU:O	2.12	0.49
2:B:417:ILE:O	2:B:421:LEU:HG	2.11	0.49
2:B:658:LEU:O	2:B:659:ASP:O	2.30	0.49
2:B:894:LYS:C	2:B:896:GLN:H	2.16	0.49
3:C:86:PHE:HB2	3:C:203:SER:OG	2.13	0.49
6:H:62:SER:OG	6:H:63:LEU:N	2.42	0.49
1:A:219:LEU:O	1:A:223:PHE:N	2.27	0.49
1:A:636:HIS:CB	2:B:1091:ARG:HH22	2.26	0.49
2:B:371:PHE:O	2:B:375:LEU:HG	2.13	0.49
3:C:125:LYS:O	3:C:130:ASN:ND2	2.45	0.49
4:E:82:PHE:HA	4:E:111:VAL:HB	1.95	0.49
1:A:690:GLU:OE1	1:A:690:GLU:N	2.31	0.49
1:A:756:LYS:O	1:A:759:TYR:HD2	1.95	0.49
2:B:851:TYR:HB2	2:B:881:TYR:CE2	2.48	0.49
4:E:78:LEU:HD12	4:E:107:THR:O	2.12	0.49
2:B:311:ARG:HE	7:I:16:LEU:HD21	1.78	0.48
3:C:241:GLY:N	3:C:263:ASP:OD2	2.46	0.48
7:I:95:ASN:O	7:I:113:THR:N	2.45	0.48
8:J:58:GLU:O	8:J:61:LEU:N	2.44	0.48
1:A:614:LEU:O	1:A:615:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:110:PHE:O	4:E:134:THR:HA	2.12	0.48
4:E:96:PHE:CZ	4:E:110:PHE:HB2	2.48	0.48
7:I:114:CYS:HB3	7:I:119:TYR:N	2.28	0.48
2:B:576:THR:CG2	12:N:95:ILE:CG2	2.91	0.48
1:A:117:ARG:HB3	1:A:185:ARG:CZ	2.43	0.48
1:A:831:ASP:HB2	1:A:917:MET:CE	2.43	0.48
4:E:177:ARG:NE	4:E:179:GLN:HE22	2.11	0.48
4:E:46:TYR:CE1	4:E:58:MET:HA	2.48	0.48
7:I:2:SER:HB2	7:I:11:LEU:HD21	1.95	0.48
12:N:111:VAL:HG13	12:N:122:ALA:HB2	1.96	0.48
2:B:985:ILE:O	12:N:160:VAL:HG21	2.12	0.48
1:A:1127:TYR:HB3	1:A:1132:TYR:HD2	1.77	0.48
1:A:659:THR:OG1	1:A:663:GLY:N	2.46	0.48
2:B:1104:CYS:N	2:B:1109:SER:O	2.37	0.48
2:B:527:PHE:CE1	2:B:666:PRO:HG3	2.48	0.48
2:B:568:LEU:HD13	2:B:604:ILE:HG23	1.95	0.48
3:C:64:ALA:O	3:C:67:PHE:N	2.45	0.48
11:M:11:GLU:N	11:M:86:LYS:O	2.36	0.48
1:A:1603:MET:SD	1:A:1612:LYS:HA	2.54	0.48
1:A:94:LEU:HD12	1:A:355:PHE:HB3	1.95	0.48
1:A:827:THR:HG21	2:B:1026:ILE:HA	1.95	0.48
2:B:103:SER:OG	2:B:138:LEU:HB2	2.13	0.48
2:B:168:ASN:OD1	2:B:169:ARG:HG2	2.13	0.48
2:B:176:SER:O	2:B:180:LEU:HG	2.13	0.48
2:B:655:TYR:HD1	2:B:688:HIS:CD2	2.32	0.48
3:C:237:GLN:HE21	3:C:288:LYS:HG2	1.78	0.48
3:C:60:ASP:OD2	3:C:63:ILE:N	2.45	0.48
4:E:98:ILE:O	4:E:102:GLU:N	2.42	0.48
1:A:1189:ALA:HA	1:A:1581:HIS:ND1	2.29	0.48
1:A:950:GLN:HE21	1:A:982:VAL:HG21	1.78	0.48
2:B:212:ASN:OD1	2:B:238:SER:HA	2.14	0.48
2:B:341:SER:N	2:B:344:GLN:OE1	2.47	0.48
3:C:315:PHE:HB3	3:C:319:ARG:HH12	1.79	0.48
1:A:1654:PHE:CD2	5:F:92:ARG:HD3	2.49	0.48
1:A:1636:SER:O	1:A:1640:ARG:HG2	2.13	0.48
1:A:464:GLU:O	1:A:468:ARG:HD3	2.14	0.48
2:B:21:ARG:HA	2:B:24:ARG:HH11	1.78	0.48
2:B:388:GLU:O	2:B:634:ARG:HA	2.13	0.48
2:B:587:GLN:HG2	2:B:592:ILE:HG12	1.94	0.48
1:A:884:ARG:NH2	2:B:633:THR:O	2.43	0.48
3:C:248:GLN:NE2	3:C:256:ILE:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.96	0.48
9:K:50:LEU:HB2	9:K:62:SER:HB2	1.95	0.48
1:A:1648:ASN:N	1:A:1649:VAL:HB	2.28	0.48
1:A:855:ARG:NH1	1:A:868:THR:O	2.45	0.48
1:A:968:SER:HA	2:B:674:ILE:O	2.13	0.48
2:B:156:ARG:NE	2:B:455:GLU:OE2	2.36	0.48
3:C:185:VAL:HG12	3:C:186:PRO:O	2.14	0.48
8:J:5:VAL:O	8:J:14:VAL:N	2.44	0.48
1:A:1172:LEU:O	1:A:1176:ARG:N	2.34	0.48
1:A:257:ASN:O	1:A:261:ILE:HD12	2.14	0.48
1:A:368:ARG:HA	1:A:380:ASN:HD22	1.78	0.48
1:A:830:MET:HG2	2:B:1027:TYR:CE1	2.49	0.48
2:B:449:VAL:HG22	2:B:452:ARG:HH21	1.79	0.48
1:A:1336:GLN:NE2	1:A:1483:LEU:HD21	2.29	0.48
2:B:173:ASN:OD1	2:B:174:LYS:HG3	2.14	0.48
2:B:18:THR:O	2:B:22:GLU:HG2	2.12	0.48
2:B:641:TYR:HB3	2:B:643:PHE:CE2	2.49	0.48
3:C:235:ILE:HA	3:C:289:VAL:HG22	1.95	0.48
1:A:1052:GLY:HA2	4:E:208:TYR:CE1	2.49	0.48
1:A:1258:ILE:O	1:A:1501:ILE:CG1	2.53	0.47
1:A:1256:LYS:O	1:A:1259:SER:HB2	2.13	0.47
1:A:1638:SER:O	1:A:1642:VAL:HG23	2.14	0.47
1:A:591:ARG:HB2	1:A:633:MET:HE3	1.96	0.47
1:A:717:PRO:HG2	1:A:720:PHE:CE1	2.49	0.47
2:B:827:PHE:HE2	2:B:842:GLU:HA	1.79	0.47
2:B:939:SER:OG	2:B:942:GLY:N	2.47	0.47
3:C:154:LYS:HZ3	3:C:161:HIS:H	1.62	0.47
3:C:34:GLU:OE1	3:C:37:LYS:HD3	2.14	0.47
1:A:1501:ILE:HB	1:A:1504:ILE:CB	2.38	0.47
1:A:457:LYS:HG3	1:A:1619:CYS:SG	2.54	0.47
1:A:220:VAL:HA	1:A:223:PHE:HB3	1.95	0.47
2:B:937:PRO:HB2	2:B:1013:MET:HE2	1.97	0.47
2:B:1019:GLY:O	3:C:227:TYR:OH	2.32	0.47
2:B:135:GLY:O	2:B:161:LEU:N	2.36	0.47
2:B:832:TRP:CZ3	2:B:836:TRP:HB2	2.49	0.47
1:A:1183:GLU:HA	5:F:88:TYR:OH	2.14	0.47
8:J:36:LEU:HD21	8:J:50:ILE:HG21	1.95	0.47
2:B:13:THR:HG23	12:N:163:VAL:HG22	1.96	0.47
1:A:1451:ILE:HG12	1:A:1457:ILE:HG22	1.96	0.47
1:A:1656:VAL:C	1:A:1657:LEU:HD12	2.35	0.47
1:A:253:GLU:N	1:A:313:THR:O	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ILE:O	1:A:520:ARG:HG3	2.14	0.47
1:A:848:LYS:O	1:A:851:VAL:HG23	2.14	0.47
2:B:758:ASP:C	2:B:761:GLY:H	2.17	0.47
3:C:40:PHE:CE2	9:K:131:VAL:HG22	2.50	0.47
3:C:86:PHE:HB3	10:L:62:LYS:HE3	1.95	0.47
5:F:110:ASP:O	5:F:123:LYS:NZ	2.33	0.47
9:K:54:THR:HG22	9:K:61:ALA:HA	1.96	0.47
1:A:1034:TYR:CZ	5:F:136:ARG:HB3	2.49	0.47
1:A:1317:ILE:O	1:A:1322:ILE:HG12	2.14	0.47
1:A:1326:GLU:OE2	1:A:1457:ILE:HG13	2.14	0.47
1:A:977:MET:HB2	1:A:983:LYS:NZ	2.29	0.47
2:B:641:TYR:HB3	2:B:643:PHE:HE2	1.80	0.47
2:B:800:TYR:HE2	3:C:96:VAL:HG22	1.79	0.47
2:B:824:HIS:NE2	2:B:864:ASP:OD2	2.46	0.47
3:C:113:LEU:HD11	3:C:131:THR:N	2.29	0.47
2:B:284:SER:HB2	7:I:14:GLY:HA3	1.95	0.47
2:B:421:LEU:HA	2:B:424:ILE:HD12	1.97	0.47
4:E:13:TRP:CD1	4:E:39:LEU:HA	2.49	0.47
6:H:100:THR:OG1	6:H:139:ASN:OD1	2.22	0.47
6:H:93:TYR:CD2	6:H:143:LEU:HD23	2.49	0.47
10:L:41:SER:N	10:L:44:ASP:OD2	2.25	0.47
10:L:29:TYR:HD1	10:L:58:LYS:HA	1.79	0.47
1:A:1256:LYS:HD3	1:A:1305:GLU:O	2.14	0.47
1:A:523:VAL:HG21	1:A:561:LEU:HD11	1.97	0.47
2:B:335:ARG:HG3	2:B:340:ALA:HB3	1.96	0.47
2:B:449:VAL:HG22	2:B:452:ARG:NH2	2.30	0.47
3:C:154:LYS:HZ3	3:C:161:HIS:N	2.12	0.47
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.97	0.47
1:A:1049:MET:HB3	4:E:208:TYR:CE1	2.47	0.47
1:A:114:GLU:OE1	1:A:117:ARG:HD3	2.14	0.47
1:A:1482:LYS:HB3	2:B:308:LEU:HD21	1.96	0.47
1:A:380:ASN:HB3	1:A:383:ASN:ND2	2.29	0.47
1:A:437:PHE:HD2	1:A:438:ILE:HG13	1.79	0.47
1:A:49:LEU:HD22	1:A:386:LEU:HD13	1.94	0.47
2:B:861:TYR:CE2	2:B:870:LYS:HB2	2.50	0.47
2:B:810:ASP:HB2	2:B:900:THR:HG23	1.95	0.47
2:B:943:ILE:O	2:B:945:PRO:HD3	2.15	0.47
3:C:162:VAL:N	3:C:194:ALA:O	2.47	0.47
3:C:232:GLN:O	3:C:292:GLY:N	2.47	0.47
3:C:284:GLU:HG3	3:C:285:PHE:N	2.29	0.47
2:B:1152:PHE:HZ	14:G:235:ASN:OD1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:72:LEU:O	9:K:76:LEU:N	2.34	0.47
1:A:1545:ASP:O	1:A:1547:ALA:N	2.48	0.47
1:A:517:ALA:HA	1:A:520:ARG:HD3	1.96	0.47
2:B:1105:ARG:N	2:B:1172:GLU:O	2.47	0.47
2:B:382:TYR:O	2:B:386:ALA:N	2.29	0.47
2:B:745:GLN:CB	2:B:800:TYR:HB3	2.45	0.47
1:A:852:ASP:OD2	1:A:855:ARG:NH2	2.47	0.47
2:B:1053:ASN:OD1	2:B:1055:LEU:N	2.47	0.47
1:A:476:VAL:N	2:B:1069:ILE:O	2.41	0.47
2:B:172:LEU:HA	2:B:175:MET:SD	2.55	0.47
2:B:472:SER:OG	2:B:474:SER:O	2.33	0.47
3:C:60:ASP:HB2	9:K:78:TYR:CZ	2.50	0.47
14:G:137:ILE:HG13	14:G:227:GLY:O	2.13	0.47
7:I:38:PRO:HD2	7:I:41:GLN:OE1	2.15	0.47
2:B:286:ARG:HD3	7:I:9:PHE:CG	2.49	0.47
1:A:51:ASP:OD1	1:A:52:LEU:N	2.48	0.47
1:A:838:GLU:HA	1:A:841:LYS:HB3	1.97	0.47
2:B:146:ASN:HB2	2:B:149:GLU:HB3	1.96	0.47
2:B:648:ARG:O	2:B:650:LEU:HG	2.15	0.47
2:B:894:LYS:O	2:B:895:PHE:CD2	2.68	0.47
1:A:1243:TRP:HD1	1:A:1535:PHE:C	2.19	0.47
1:A:24:ILE:HG21	1:A:359:VAL:HG21	1.97	0.47
1:A:512:THR:OG1	1:A:515:ASN:OD1	2.20	0.47
2:B:103:SER:O	2:B:137:LEU:HD12	2.15	0.47
2:B:228:SER:O	2:B:254:ASN:N	2.33	0.47
2:B:399:HIS:O	2:B:400:GLN:HG3	2.15	0.47
2:B:859:CYS:SG	2:B:860:ALA:N	2.88	0.47
2:B:921:HIS:NE2	2:B:962:MET:HA	2.29	0.47
3:C:231:PRO:HG2	3:C:270:ALA:HB1	1.96	0.47
13:D:46:GLU:OE1	13:D:47:LYS:HE2	2.15	0.47
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.96	0.47
7:I:2:SER:O	7:I:8:ILE:HA	2.15	0.47
1:A:1094:ALA:O	1:A:1098:SER:N	2.36	0.46
1:A:175:SER:HA	1:A:178:LEU:HD12	1.97	0.46
1:A:781:LEU:HB3	1:A:786:TYR:HE2	1.79	0.46
2:B:1152:PHE:CE2	14:G:129:VAL:HG21	2.51	0.46
2:B:1119:ARG:NH2	2:B:1160:GLU:OE2	2.48	0.46
3:C:161:HIS:CD2	3:C:195:LYS:HG2	2.50	0.46
3:C:262:SER:O	3:C:264:GLU:HG3	2.15	0.46
3:C:78:VAL:HA	3:C:209:ILE:O	2.16	0.46
4:E:118:PRO:O	4:E:121:MET:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:91:TYR:HD2	9:K:101:LEU:HD11	1.80	0.46
1:A:1034:TYR:CE2	5:F:136:ARG:HB3	2.51	0.46
1:A:1539:ASP:HA	4:E:147:HIS:CD2	2.50	0.46
1:A:332:GLN:HE22	1:A:350:VAL:N	2.13	0.46
1:A:440:SER:H	1:A:458:GLN:NE2	2.03	0.46
1:A:672:ASP:O	1:A:676:ALA:N	2.46	0.46
1:A:681:THR:HG21	1:A:781:LEU:HG	1.97	0.46
2:B:822:THR:HG22	2:B:823:GLN:HG3	1.97	0.46
2:B:929:ARG:HG2	2:B:931:TRP:HE3	1.80	0.46
3:C:136:LEU:HB3	3:C:204:LEU:HD11	1.98	0.46
3:C:137:ASN:HA	3:C:202:ILE:O	2.14	0.46
9:K:66:VAL:HG12	9:K:67:GLU:N	2.31	0.46
1:A:641:GLU:OE1	1:A:644:ARG:HD3	2.15	0.46
1:A:781:LEU:HB3	1:A:786:TYR:CE2	2.50	0.46
5:F:57:ASP:O	5:F:61:HIS:N	2.34	0.46
8:J:18:TRP:CH2	8:J:22:LEU:HD21	2.51	0.46
1:A:1113:HIS:HA	1:A:1116:GLN:HG2	1.97	0.46
1:A:91:PHE:HE2	1:A:245:LYS:HD2	1.80	0.46
1:A:261:ILE:O	1:A:265:ARG:HG2	2.15	0.46
1:A:267:LYS:HA	1:A:270:ILE:HD12	1.97	0.46
1:A:487:ASP:HA	2:B:781:TYR:HE1	1.80	0.46
1:A:943:ILE:HG12	1:A:986:PHE:CD2	2.51	0.46
2:B:677:THR:OG1	2:B:680:GLU:HG3	2.15	0.46
2:B:693:PRO:O	2:B:696:ILE:HG12	2.15	0.46
3:C:308:MET:SD	3:C:316:LYS:NZ	2.86	0.46
4:E:163:GLU:O	4:E:167:ARG:N	2.44	0.46
4:E:197:LYS:HA	4:E:211:TYR:CE1	2.50	0.46
4:E:90:VAL:O	4:E:94:LYS:N	2.35	0.46
8:J:34:THR:HA	8:J:37:SER:HB2	1.96	0.46
1:A:108:PHE:CE2	1:A:331:GLU:HG3	2.50	0.46
1:A:1272:VAL:HG22	1:A:1292:ILE:HG23	1.98	0.46
1:A:129:LEU:HB3	1:A:132:GLU:CD	2.36	0.46
1:A:842:TRP:CD2	1:A:910:LYS:NZ	2.74	0.46
1:A:842:TRP:CE3	1:A:910:LYS:HG2	2.50	0.46
2:B:202:LEU:O	2:B:486:VAL:HG12	2.15	0.46
2:B:377:MET:O	2:B:381:LEU:N	2.35	0.46
2:B:190:ILE:HD11	2:B:496:PHE:CE2	2.51	0.46
2:B:65:VAL:HA	2:B:68:ILE:HD12	1.97	0.46
3:C:131:THR:O	3:C:175:GLN:NE2	2.47	0.46
7:I:91:ASN:HD22	7:I:116:SER:N	2.13	0.46
1:A:1311:GLU:O	1:A:1315:ASN:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:GLU:OE1	1:A:1311:GLU:N	2.38	0.46
1:A:1322:ILE:O	1:A:1325:LEU:N	2.46	0.46
1:A:64:THR:HB	1:A:75:HIS:CD2	2.51	0.46
2:B:246:GLN:NE2	2:B:247:THR:H	2.14	0.46
2:B:489:GLU:HB3	2:B:491:ILE:HG12	1.98	0.46
3:C:167:LEU:C	3:C:168:LYS:HD2	2.36	0.46
3:C:162:VAL:O	3:C:192:LEU:HD12	2.15	0.46
13:D:33:THR:HG23	13:D:96:PHE:HD1	1.80	0.46
1:A:1100:LYS:HG2	1:A:1104:TYR:CE2	2.51	0.46
1:A:135:LYS:HA	1:A:138:GLU:CD	2.36	0.46
1:A:551:VAL:HG22	1:A:554:ARG:NH2	2.31	0.46
1:A:694:GLN:O	1:A:698:GLY:N	2.39	0.46
2:B:102:VAL:HA	2:B:139:LEU:HD23	1.97	0.46
2:B:322:ASN:OD1	2:B:323:ARG:N	2.49	0.46
2:B:749:THR:O	2:B:770:ASN:ND2	2.48	0.46
3:C:57:ILE:HG22	3:C:58:ASN:ND2	2.30	0.46
4:E:93:MET:HG2	4:E:120:ALA:HB1	1.98	0.46
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.46	0.46
1:A:1312:GLU:O	1:A:1316:VAL:N	2.26	0.46
1:A:141:LEU:HD21	1:A:184:LYS:HZ2	1.80	0.46
1:A:1570:PHE:O	1:A:1574:ALA:N	2.49	0.46
1:A:719:ILE:HG12	6:H:97:MET:CG	2.40	0.46
1:A:756:LYS:HB2	1:A:759:TYR:CE2	2.50	0.46
1:A:831:ASP:N	1:A:831:ASP:OD1	2.49	0.46
2:B:321:GLN:HB3	7:I:32:GLN:NE2	2.31	0.46
2:B:889:GLY:HA3	10:L:54:ARG:HB3	1.96	0.46
4:E:113:GLN:HA	4:E:137:GLU:CD	2.36	0.46
8:J:16:ASP:OD1	8:J:17:LYS:N	2.48	0.46
1:A:478:TYR:CE1	2:B:1048:SER:HB2	2.51	0.46
2:B:445:TYR:HA	2:B:448:ARG:NH1	2.31	0.46
1:A:880:GLN:HE22	2:B:633:THR:H	1.63	0.46
2:B:712:SER:N	2:B:713:PRO:HD2	2.30	0.46
4:E:136:ASN:HB3	4:E:139:ALA:HB3	1.98	0.46
1:A:1657:LEU:HD11	5:F:135:ARG:HB2	1.98	0.46
1:A:131:ASP:HA	1:A:134:TYR:CD2	2.47	0.46
1:A:1504:ILE:HD13	1:A:1529:MET:CE	2.45	0.46
1:A:907:VAL:HG12	1:A:945:CYS:HG	1.80	0.46
2:B:1110:ILE:O	2:B:1113:THR:OG1	2.19	0.46
2:B:28:PRO:HG2	2:B:178:TYR:HD1	1.80	0.46
2:B:668:GLU:HG3	2:B:672:MET:HE3	1.98	0.46
2:B:699:ILE:N	16:B:1301:SO4:S	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:ARG:HD2	1:A:1043:GLY:O	2.17	0.45
1:A:314:TYR:CE2	1:A:316:LEU:HA	2.50	0.45
1:A:435:ASN:O	1:A:439:ASP:N	2.48	0.45
1:A:985:ARG:HG3	1:A:988:SER:H	1.81	0.45
2:B:322:ASN:HB3	2:B:325:GLN:CG	2.46	0.45
2:B:501:ARG:HH22	2:B:549:CYS:HB3	1.82	0.45
2:B:576:THR:HG21	12:N:95:ILE:HG22	1.98	0.45
5:F:109:VAL:HG22	5:F:110:ASP:H	1.82	0.45
11:M:65:TYR:HE1	11:M:97:VAL:HB	1.81	0.45
1:A:741:PRO:HA	1:A:742:PRO:HD3	1.86	0.45
2:B:658:LEU:HD13	2:B:658:LEU:H	1.79	0.45
2:B:814:ASN:OD1	2:B:815:ARG:N	2.50	0.45
1:A:943:ILE:CD1	2:B:958:MET:HB3	2.42	0.45
3:C:31:TRP:CH2	3:C:33:VAL:HA	2.52	0.45
3:C:325:ALA:O	3:C:329:LYS:N	2.25	0.45
8:J:17:LYS:HD3	8:J:39:LEU:HB3	1.97	0.45
11:M:26:PHE:CE1	11:M:98:SER:HB2	2.51	0.45
1:A:1550:LEU:HA	1:A:1554:GLY:O	2.16	0.45
1:A:324:LEU:O	1:A:328:PHE:N	2.27	0.45
1:A:367:PHE:CD1	2:B:1184:TYR:HD1	2.34	0.45
2:B:301:PHE:O	2:B:305:ARG:HG2	2.16	0.45
2:B:756:LEU:HD23	2:B:759:ASP:OD2	2.15	0.45
2:B:857:PRO:HB3	2:B:871:ILE:HD11	1.99	0.45
5:F:77:ASP:OD1	5:F:78:GLN:N	2.50	0.45
1:A:1302:TYR:O	1:A:1306:TYR:N	2.48	0.45
1:A:588:LEU:HD11	1:A:600:MET:HG2	1.99	0.45
1:A:826:PHE:HA	2:B:1023:ARG:HH22	1.82	0.45
2:B:1105:ARG:NH1	2:B:1172:GLU:OE1	2.49	0.45
2:B:1099:THR:OG1	2:B:1180:PHE:HB2	2.16	0.45
2:B:307:GLU:OE1	7:I:7:LEU:HD11	2.17	0.45
2:B:556:SER:OG	2:B:623:ASP:OD2	2.32	0.45
9:K:77:ARG:HD2	9:K:91:TYR:CE1	2.52	0.45
9:K:92:SER:O	9:K:101:LEU:HD12	2.17	0.45
1:A:460:LEU:HB3	1:A:1618:THR:HG21	1.97	0.45
2:B:1053:ASN:OD1	2:B:1054:SER:N	2.49	0.45
2:B:286:ARG:O	2:B:290:ASP:N	2.26	0.45
2:B:657:PRO:C	2:B:659:ASP:N	2.59	0.45
2:B:649:MET:O	2:B:666:PRO:HD3	2.17	0.45
2:B:921:HIS:CD2	2:B:962:MET:HA	2.51	0.45
3:C:93:GLN:H	3:C:93:GLN:CD	2.20	0.45
4:E:29:PHE:HB2	4:E:65:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:57:ASP:HA	5:F:60:GLN:HB3	1.98	0.45
1:A:1061:SER:OG	1:A:1062:HIS:N	2.49	0.45
1:A:706:HIS:CD2	1:A:808:LYS:HD3	2.51	0.45
2:B:468:GLY:HA2	2:B:485:THR:HG23	1.98	0.45
3:C:152:ASP:O	3:C:156:LEU:HG	2.16	0.45
3:C:154:LYS:HE2	3:C:161:HIS:CE1	2.51	0.45
6:H:80:ARG:HG3	9:K:108:TYR:CZ	2.52	0.45
1:A:23:GLU:O	1:A:27:LEU:HG	2.17	0.45
2:B:263:SER:HA	2:B:268:GLU:HA	1.98	0.45
2:B:31:ASP:OD1	2:B:32:LYS:N	2.43	0.45
2:B:527:PHE:CZ	2:B:666:PRO:HG3	2.51	0.45
2:B:968:ALA:HA	2:B:971:ALA:HB3	1.99	0.45
3:C:315:PHE:HE1	9:K:136:THR:HG1	1.64	0.45
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.51	0.45
8:J:7:CYS:HA	8:J:49:MET:HG3	1.98	0.45
1:A:1124:LEU:HD23	1:A:1135:SER:OG	2.17	0.45
1:A:1024:THR:HG22	1:A:1190:SER:HB3	1.99	0.45
1:A:418:VAL:O	1:A:422:ARG:HG2	2.17	0.45
1:A:855:ARG:NH1	1:A:866:LYS:O	2.50	0.45
2:B:1182:LEU:HA	2:B:1185:LEU:HB3	1.98	0.45
2:B:96:SER:N	2:B:144:SER:O	2.44	0.45
2:B:427:GLN:HG2	2:B:449:VAL:HG13	1.99	0.45
2:B:443:LYS:O	2:B:446:MET:HB3	2.17	0.45
2:B:772:VAL:O	2:B:946:ASP:HB2	2.17	0.45
3:C:239:ILE:HD11	3:C:288:LYS:HB2	1.99	0.45
5:F:108:PHE:CE2	5:F:131:PRO:HG3	2.49	0.45
6:H:40:LEU:HD23	6:H:42:ILE:HD11	1.98	0.45
1:A:316:LEU:HB2	1:A:319:GLU:HG3	1.98	0.45
1:A:475:ARG:NH2	2:B:1070:ARG:HH22	2.15	0.45
2:B:1112:THR:OG1	2:B:1128:CYS:SG	2.55	0.45
1:A:15:ASP:N	2:B:1197:ARG:O	2.30	0.45
2:B:537:SER:N	2:B:538:PRO:HD2	2.32	0.45
2:B:128:GLN:NE2	2:B:735:HIS:O	2.50	0.45
3:C:240:LYS:HB3	3:C:264:GLU:CG	2.46	0.45
1:A:1654:PHE:HE1	5:F:134:ILE:HG12	1.81	0.45
1:A:424:MET:O	1:A:428:VAL:HG23	2.17	0.45
1:A:92:ASN:O	1:A:96:ILE:HG13	2.17	0.45
2:B:46:ILE:HD12	2:B:46:ILE:H	1.82	0.45
2:B:750:PRO:HB3	2:B:1032:TYR:CD1	2.52	0.45
1:A:1580:ARG:NH2	4:E:204:THR:HG21	2.31	0.45
7:I:2:SER:HA	7:I:9:PHE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:ILE:HG13	2:B:1080:ILE:HG22	1.99	0.44
1:A:208:PHE:HE2	1:A:1607:THR:HG23	1.80	0.44
2:B:30:LYS:HG2	2:B:178:TYR:CG	2.52	0.44
2:B:555:GLN:HB2	2:B:646:HIS:CE1	2.51	0.44
2:B:827:PHE:HD1	2:B:869:THR:HG21	1.82	0.44
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.99	0.44
8:J:18:TRP:CE2	8:J:22:LEU:HD11	2.52	0.44
9:K:66:VAL:O	9:K:68:GLU:HG2	2.17	0.44
1:A:1040:ASP:HB3	1:A:1042:ASP:OD1	2.17	0.44
1:A:106:HIS:HB2	1:A:330:LYS:HE3	1.99	0.44
1:A:753:ASN:ND2	1:A:766:GLU:O	2.50	0.44
5:F:144:GLU:OE1	5:F:146:TRP:NE1	2.40	0.44
5:F:66:ARG:HA	5:F:69:LEU:CD1	2.34	0.44
6:H:98:TYR:HD1	6:H:141:TYR:CD1	2.35	0.44
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.52	0.44
2:B:106:LYS:HE2	2:B:168:ASN:O	2.17	0.44
2:B:371:PHE:CE2	2:B:375:LEU:HD11	2.53	0.44
2:B:372:ARG:HH21	2:B:574:SER:HA	1.83	0.44
2:B:692:THR:H	2:B:695:ASN:ND2	2.16	0.44
2:B:938:PHE:CZ	2:B:1014:TYR:HB2	2.51	0.44
2:B:709:PHE:CE2	2:B:992:PRO:HG2	2.52	0.44
3:C:319:ARG:NH2	9:K:132:GLU:OE2	2.51	0.44
3:C:36:PHE:CE1	3:C:40:PHE:HB2	2.52	0.44
4:E:88:VAL:HB	4:E:116:ILE:HA	1.99	0.44
9:K:116:ALA:O	9:K:120:GLY:N	2.36	0.44
1:A:659:THR:HG23	1:A:664:SER:O	2.17	0.44
1:A:945:CYS:C	1:A:946:LEU:CG	2.85	0.44
2:B:218:ILE:HA	2:B:231:HIS:O	2.17	0.44
2:B:286:ARG:HD2	2:B:286:ARG:HA	1.75	0.44
2:B:854:GLU:OE1	2:B:877:SER:HA	2.17	0.44
2:B:999:GLN:O	2:B:1003:ALA:N	2.46	0.44
1:A:1000:MET:HG3	2:B:520:LEU:HD23	1.98	0.44
1:A:1158:SER:OG	1:A:1159:ASP:N	2.50	0.44
1:A:39:ASP:OD2	1:A:43:HIS:HB2	2.17	0.44
1:A:771:PHE:CD1	1:A:776:LEU:HA	2.52	0.44
1:A:79:ILE:HB	1:A:360:LEU:HB2	1.99	0.44
2:B:968:ALA:HB2	2:B:996:PHE:CE1	2.52	0.44
4:E:112:TYR:CD2	4:E:116:ILE:HD11	2.52	0.44
4:E:17:ARG:HH12	4:E:36:GLU:HA	1.82	0.44
6:H:48:PRO:O	6:H:146:ARG:NH2	2.50	0.44
1:A:1233:ILE:HD11	1:A:1236:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:HA	1:A:24:ILE:HD12	2.00	0.44
2:B:228:SER:O	2:B:254:ASN:ND2	2.50	0.44
2:B:442:ASP:HB3	2:B:445:TYR:HB3	1.99	0.44
2:B:705:PRO:HB2	2:B:706:PHE:HD2	1.82	0.44
3:C:332:PRO:HG2	9:K:44:ARG:HA	1.99	0.44
8:J:28:ASP:HB3	8:J:30:LEU:HG	2.00	0.44
1:A:1316:VAL:HG13	1:A:1320:GLN:HE21	1.82	0.44
1:A:237:GLY:HA3	1:A:267:LYS:HE2	1.99	0.44
1:A:507:TYR:O	1:A:578:TYR:HA	2.18	0.44
2:B:1159:TRP:CE2	2:B:1167:PHE:HB2	2.53	0.44
2:B:683:ASN:O	2:B:685:VAL:HG23	2.17	0.44
2:B:1152:PHE:CZ	14:G:235:ASN:OD1	2.71	0.44
9:K:133:SER:O	9:K:137:GLU:HG3	2.17	0.44
9:K:50:LEU:HB2	9:K:62:SER:CB	2.47	0.44
10:L:33:GLU:HB3	10:L:53:HIS:CD2	2.52	0.44
1:A:552:GLU:HA	1:A:555:LYS:HB2	1.98	0.44
1:A:842:TRP:CE3	1:A:910:LYS:CG	3.00	0.44
1:A:842:TRP:O	1:A:845:ASP:N	2.51	0.44
2:B:104:ILE:O	2:B:169:ARG:NE	2.51	0.44
2:B:275:MET:SD	2:B:330:LEU:HD21	2.58	0.44
2:B:428:VAL:O	2:B:431:ASP:HB2	2.17	0.44
3:C:123:ASP:N	3:C:123:ASP:OD1	2.49	0.44
3:C:68:ARG:CD	3:C:227:TYR:CE2	3.00	0.44
9:K:83:ASN:OD1	9:K:85:ASP:N	2.51	0.44
1:A:336:GLN:O	1:A:340:HIS:ND1	2.50	0.44
2:B:35:PHE:CE1	2:B:761:GLY:HA3	2.53	0.44
2:B:861:TYR:CE1	2:B:872:LYS:HE2	2.53	0.44
3:C:57:ILE:HG13	3:C:297:HIS:CD2	2.53	0.44
2:B:908:ARG:HD2	3:C:95:GLU:HG3	1.99	0.44
8:J:18:TRP:CZ2	8:J:22:LEU:HD21	2.53	0.44
9:K:69:ASP:OD1	9:K:69:ASP:N	2.51	0.44
1:A:95:TYR:CD2	1:A:245:LYS:HD3	2.53	0.43
1:A:960:MET:HG2	2:B:523:GLU:OE2	2.18	0.43
3:C:140:CYS:HA	3:C:158:ASN:O	2.18	0.43
3:C:73:SER:OG	3:C:74:GLU:HG3	2.18	0.43
3:C:95:GLU:O	3:C:99:HIS:N	2.36	0.43
4:E:177:ARG:CZ	4:E:179:GLN:HE22	2.31	0.43
1:A:117:ARG:NH2	1:A:137:ASP:OD2	2.49	0.43
1:A:1537:ASP:OD1	1:A:1538:VAL:N	2.51	0.43
1:A:525:ASN:ND2	1:A:531:PRO:O	2.45	0.43
1:A:996:TYR:CZ	2:B:520:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1056:THR:O	2:B:1058:GLN:HG3	2.18	0.43
2:B:1102:SER:OG	2:B:1175:THR:HG22	2.17	0.43
2:B:676:VAL:HB	2:B:680:GLU:OE2	2.18	0.43
3:C:243:SER:N	3:C:246:ARG:HH21	2.15	0.43
4:E:20:LYS:NZ	4:E:34:GLU:HG2	2.33	0.43
14:G:163:PRO:HG2	14:G:166:TRP:CD1	2.52	0.43
6:H:12:VAL:HG11	6:H:15:VAL:HG23	1.99	0.43
8:J:17:LYS:O	8:J:21:TYR:N	2.40	0.43
1:A:31:GLN:HB2	1:A:78:HIS:CE1	2.53	0.43
1:A:352:ALA:HA	1:A:355:PHE:CD2	2.52	0.43
1:A:440:SER:N	1:A:458:GLN:HE22	2.06	0.43
1:A:32:ILE:HD12	1:A:48:GLY:O	2.18	0.43
3:C:311:GLU:HG2	3:C:312:GLU:N	2.33	0.43
4:E:67:GLU:HA	4:E:70:SER:OG	2.18	0.43
7:I:19:ASN:O	7:I:23:VAL:HG23	2.18	0.43
11:M:8:SER:O	12:N:71:PRO:HA	2.19	0.43
1:A:389:VAL:HG22	1:A:433:ASP:HB3	2.00	0.43
1:A:711:LYS:NZ	9:K:60:SER:HB2	2.33	0.43
2:B:840:LEU:HD13	2:B:860:ALA:HB2	2.01	0.43
3:C:216:HIS:CD2	10:L:70:ARG:HE	2.36	0.43
1:A:506:THR:HA	1:A:579:ARG:O	2.19	0.43
1:A:27:LEU:O	2:B:1129:ARG:HD2	2.18	0.43
2:B:208:VAL:O	2:B:401:GLU:N	2.41	0.43
3:C:173:GLY:O	3:C:176:SER:OG	2.19	0.43
6:H:26:ILE:O	6:H:40:LEU:N	2.37	0.43
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.00	0.43
1:A:732:ILE:O	1:A:735:VAL:HB	2.17	0.43
2:B:698:SER:HB2	16:B:1301:SO4:O3	2.18	0.43
2:B:222:PHE:HB2	2:B:231:HIS:HA	1.99	0.43
2:B:361:HIS:CE1	2:B:362:LEU:HG	2.54	0.43
2:B:464:PHE:O	2:B:468:GLY:N	2.50	0.43
2:B:587:GLN:HE21	2:B:592:ILE:HG12	1.84	0.43
3:C:240:LYS:HA	3:C:244:ALA:HB2	1.99	0.43
4:E:42:PHE:O	4:E:46:TYR:N	2.50	0.43
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.83	0.43
4:E:55:ARG:HD2	4:E:82:PHE:HB3	1.99	0.43
1:A:1162:ASN:ND2	1:A:1164:LYS:HB2	2.34	0.43
1:A:507:TYR:CD1	1:A:508:PRO:HD2	2.54	0.43
2:B:181:VAL:HG13	8:J:63:TYR:HE1	1.83	0.43
2:B:315:LYS:HB3	2:B:315:LYS:HE3	1.83	0.43
2:B:343:ASP:OD1	2:B:344:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:LEU:HD22	2:B:663:ILE:HG22	2.00	0.43
4:E:40:GLU:HA	4:E:43:LYS:CE	2.49	0.43
5:F:146:TRP:HA	5:F:150:GLU:OE2	2.18	0.43
9:K:63:PHE:O	9:K:102:ASN:HA	2.19	0.43
1:A:1303:SER:O	1:A:1307:ASP:HA	2.18	0.43
1:A:1501:ILE:CG2	1:A:1502:PRO:CD	2.94	0.43
1:A:589:MET:SD	1:A:635:MET:HA	2.59	0.43
1:A:975:ASP:OD1	1:A:977:MET:N	2.48	0.43
2:B:1073:GLU:HB3	2:B:1076:ARG:HH21	1.83	0.43
2:B:1128:CYS:SG	2:B:1130:ARG:HB3	2.59	0.43
4:E:78:LEU:HD21	4:E:109:ILE:HD12	2.00	0.43
1:A:446:ARG:NH2	1:A:450:LYS:HB3	2.33	0.43
2:B:1134:ARG:HD3	2:B:1167:PHE:CE1	2.52	0.43
2:B:718:GLN:O	2:B:721:MET:N	2.52	0.43
3:C:60:ASP:HB3	3:C:63:ILE:CD1	2.49	0.43
1:A:1108:HIS:O	1:A:1111:GLU:HG2	2.18	0.43
1:A:1148:LEU:HB3	1:A:1163:GLU:OE2	2.18	0.43
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	2.01	0.43
1:A:1263:LEU:CB	1:A:1496:SER:CB	2.97	0.43
1:A:12:THR:O	1:A:1634:LEU:HD12	2.18	0.43
1:A:735:VAL:O	1:A:739:VAL:HG22	2.19	0.43
2:B:552:SER:O	2:B:647:SER:N	2.40	0.43
2:B:57:ASP:HB2	2:B:63:LEU:HD11	2.01	0.43
2:B:910:THR:HB	2:B:911:PRO:HD2	2.00	0.43
3:C:123:ASP:OD1	3:C:124:GLU:N	2.49	0.43
4:E:99:HIS:HA	4:E:102:GLU:CD	2.39	0.43
12:N:81:THR:HG22	12:N:86:ASP:HB3	2.01	0.43
1:A:1463:ASP:HB2	1:A:1469:TRP:CD1	2.54	0.42
1:A:1510:PRO:HG3	1:A:1520:VAL:HG23	2.01	0.42
1:A:510:PRO:HA	1:A:576:LYS:HG2	2.01	0.42
1:A:522:ALA:HA	1:A:525:ASN:HB2	2.01	0.42
1:A:805:VAL:O	1:A:809:VAL:HG23	2.19	0.42
2:B:345:SER:O	2:B:349:VAL:HG23	2.19	0.42
2:B:501:ARG:NH2	2:B:549:CYS:HB3	2.34	0.42
2:B:700:LEU:HD13	16:B:1301:SO4:O1	2.19	0.42
4:E:159:ASP:HA	4:E:162:ARG:HG2	2.00	0.42
1:A:1511:GLU:OE1	7:I:73:LYS:HD2	2.20	0.42
8:J:7:CYS:HB3	8:J:10:CYS:HB2	1.99	0.42
1:A:1504:ILE:CD1	1:A:1529:MET:CE	2.97	0.42
1:A:1657:LEU:HB2	5:F:133:VAL:O	2.20	0.42
1:A:731:ILE:O	1:A:735:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:GLN:HE21	1:A:982:VAL:CG2	2.32	0.42
2:B:698:SER:OG	16:B:1301:SO4:O4	2.23	0.42
2:B:282:HIS:N	2:B:323:ARG:HD2	2.34	0.42
2:B:156:ARG:CZ	2:B:450:LEU:HD13	2.49	0.42
3:C:137:ASN:OD1	3:C:203:SER:HA	2.19	0.42
3:C:213:GLY:HA2	3:C:216:HIS:O	2.19	0.42
3:C:60:ASP:HB3	3:C:63:ILE:HD12	2.01	0.42
4:E:68:SER:HB3	4:E:75:MET:SD	2.59	0.42
5:F:57:ASP:OD1	5:F:58:PHE:N	2.47	0.42
14:G:160:ASN:N	14:G:160:ASN:OD1	2.52	0.42
3:C:37:LYS:HG3	9:K:130:VAL:HG13	2.00	0.42
1:A:1442:VAL:O	1:A:1446:ARG:N	2.29	0.42
1:A:1559:ARG:HG3	1:A:1586:ALA:HB1	2.01	0.42
1:A:875:LEU:O	1:A:879:LEU:HG	2.19	0.42
1:A:908:VAL:CG1	1:A:941:SER:HB2	2.49	0.42
2:B:407:PHE:O	2:B:411:MET:HG3	2.19	0.42
2:B:611:TRP:C	2:B:620:LEU:HD21	2.40	0.42
2:B:789:ILE:HD12	2:B:927:CYS:SG	2.58	0.42
4:E:182:ASP:OD2	4:E:184:VAL:HB	2.19	0.42
7:I:84:GLU:HG2	7:I:94:MET:HB2	2.01	0.42
9:K:55:SER:N	9:K:60:SER:O	2.37	0.42
12:N:78:THR:HB	12:N:79:THR:H	1.56	0.42
1:A:1573:TYR:HA	7:I:122:ARG:NH2	2.31	0.42
1:A:254:THR:HA	1:A:312:SER:N	2.34	0.42
1:A:824:THR:HB	2:B:1023:ARG:HH11	1.83	0.42
1:A:946:LEU:HA	1:A:984:GLY:O	2.19	0.42
2:B:107:PRO:HG2	2:B:133:TYR:CE2	2.54	0.42
4:E:16:PHE:CZ	4:E:20:LYS:HE3	2.55	0.42
5:F:76:LYS:HG3	5:F:79:ARG:CZ	2.50	0.42
8:J:45:CYS:O	8:J:48:ARG:HG2	2.20	0.42
12:N:94:ASP:HB3	12:N:99:LEU:HG	2.00	0.42
1:A:1005:GLY:HA2	1:A:1008:ASP:HB2	2.02	0.42
1:A:54:LEU:HA	1:A:75:HIS:HB2	2.00	0.42
1:A:586:VAL:HB	1:A:648:LEU:HD21	2.01	0.42
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.86	0.42
1:A:826:PHE:CG	1:A:827:THR:N	2.88	0.42
1:A:885:ASP:CG	1:A:888:LYS:H	2.22	0.42
2:B:314:LYS:O	2:B:315:LYS:HB3	2.19	0.42
2:B:528:LEU:HA	2:B:528:LEU:HD23	1.76	0.42
2:B:534:PRO:HB2	2:B:538:PRO:HG2	2.01	0.42
2:B:893:ASN:O	2:B:895:PHE:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:LYS:O	2:B:896:GLN:N	2.53	0.42
2:B:936:MET:HA	2:B:937:PRO:HD2	1.87	0.42
3:C:31:TRP:CE3	9:K:82:LYS:HD2	2.53	0.42
3:C:31:TRP:HA	3:C:35:LYS:NZ	2.35	0.42
4:E:98:ILE:O	4:E:102:GLU:HG3	2.19	0.42
1:A:1204:THR:HG22	1:A:1205:PHE:N	2.34	0.42
1:A:465:GLY:O	1:A:469:LYS:N	2.32	0.42
1:A:844:THR:O	1:A:848:LYS:HG3	2.19	0.42
2:B:1105:ARG:H	2:B:1173:THR:HA	1.84	0.42
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.54	0.42
2:B:327:LEU:HD23	2:B:330:LEU:HD12	2.01	0.42
1:A:967:PRO:HB3	2:B:674:ILE:HD12	2.02	0.42
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.55	0.42
3:C:128:ASP:OD1	3:C:129:GLU:N	2.52	0.42
1:A:652:ASN:OD1	1:A:652:ASN:N	2.53	0.42
2:B:343:ASP:OD1	2:B:344:GLN:N	2.53	0.42
2:B:675:ALA:HB2	2:B:686:HIS:CG	2.54	0.42
4:E:55:ARG:HG3	4:E:84:ASP:HA	2.01	0.42
9:K:134:LYS:HA	9:K:137:GLU:OE1	2.20	0.42
1:A:1055:ILE:HD11	1:A:1174:TYR:CE1	2.54	0.42
1:A:372:LYS:HD2	1:A:374:GLY:O	2.20	0.42
4:E:53:PRO:HG2	4:E:55:ARG:HH12	1.85	0.42
5:F:59:GLN:O	5:F:63:GLN:HG3	2.19	0.42
8:J:54:VAL:HG12	8:J:56:LEU:H	1.84	0.42
1:A:711:LYS:HG3	9:K:106:GLN:NE2	2.35	0.42
1:A:1188:ILE:O	1:A:1192:SER:OG	2.25	0.42
1:A:1456:PHE:CD1	1:A:1476:LEU:HD23	2.54	0.42
1:A:253:GLU:O	1:A:312:SER:N	2.53	0.42
1:A:428:VAL:O	1:A:432:ASN:N	2.51	0.42
1:A:733:THR:O	1:A:737:LEU:N	2.47	0.42
1:A:836:THR:CG2	1:A:839:GLY:H	2.33	0.42
1:A:908:VAL:HG11	1:A:941:SER:HB2	2.02	0.42
2:B:1031:VAL:HG12	2:B:1032:TYR:O	2.19	0.42
2:B:527:PHE:HE2	2:B:669:GLN:OE1	2.02	0.42
4:E:151:PRO:HG2	4:E:153:HIS:CE1	2.54	0.42
6:H:10:PHE:O	6:H:54:SER:HA	2.20	0.42
6:H:104:PHE:CE2	6:H:137:GLN:HB2	2.54	0.42
1:A:1112:PRO:HG2	1:A:1115:LYS:HG2	2.01	0.42
1:A:1162:ASN:HB3	1:A:1165:LYS:HD3	2.01	0.42
1:A:1215:VAL:HG22	1:A:1216:THR:N	2.35	0.42
1:A:579:ARG:NH1	1:A:582:LYS:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:HIS:HB3	2:B:1091:ARG:HH22	1.85	0.42
2:B:240:ARG:HH11	2:B:360:VAL:HG21	1.85	0.42
4:E:24:LYS:HE2	4:E:32:GLN:HE22	1.85	0.42
2:B:1152:PHE:HZ	14:G:235:ASN:CG	2.22	0.42
9:K:111:THR:HB	9:K:115:ASP:OD2	2.19	0.42
1:A:1006:LEU:CD1	2:B:716:MET:HE3	2.50	0.41
1:A:125:LEU:C	1:A:128:GLY:H	2.24	0.41
1:A:1588:MET:O	1:A:1591:ARG:NH1	2.49	0.41
1:A:572:THR:HA	14:G:52:MET:CE	2.49	0.41
1:A:744:MET:HG3	1:A:745:PRO:HD2	2.01	0.41
2:B:361:HIS:NE2	2:B:362:LEU:HG	2.34	0.41
2:B:894:LYS:C	2:B:896:GLN:N	2.72	0.41
2:B:939:SER:OG	2:B:943:ILE:N	2.51	0.41
2:B:714:ARG:HH21	2:B:957:ARG:HG2	1.85	0.41
4:E:26:ARG:HE	4:E:188:LEU:HA	1.85	0.41
5:F:132:LEU:O	5:F:148:VAL:HG23	2.19	0.41
1:A:1240:LEU:O	1:A:1519:LEU:N	2.37	0.41
1:A:1293:HIS:ND1	1:A:1471:GLU:OE1	2.53	0.41
1:A:116:HIS:HB3	1:A:185:ARG:NH1	2.35	0.41
1:A:749:LEU:O	1:A:770:LEU:HD12	2.21	0.41
1:A:812:VAL:HG22	1:A:815:ARG:HH21	1.84	0.41
2:B:74:PHE:CE2	2:B:343:ASP:HB3	2.55	0.41
2:B:556:SER:HB3	2:B:621:PRO:HG3	2.02	0.41
3:C:105:PRO:HG3	8:J:6:ARG:NH2	2.34	0.41
3:C:165:ARG:HB3	3:C:189:PRO:CB	2.37	0.41
7:I:112:TYR:N	7:I:121:PHE:O	2.54	0.41
7:I:20:PRO:O	7:I:39:LYS:NZ	2.52	0.41
12:N:148:ILE:HD13	12:N:150:TYR:OH	2.20	0.41
1:A:734:THR:O	1:A:737:LEU:HB3	2.20	0.41
1:A:751:SER:OG	1:A:752:LYS:N	2.53	0.41
1:A:793:ILE:O	1:A:797:LEU:HG	2.20	0.41
2:B:1107:CYS:HB2	2:B:1195:ARG:NH2	2.35	0.41
2:B:349:VAL:O	2:B:352:GLU:HB3	2.19	0.41
2:B:372:ARG:NH2	2:B:574:SER:HA	2.36	0.41
2:B:470:LEU:N	2:B:481:VAL:O	2.28	0.41
2:B:828:GLY:N	2:B:869:THR:OG1	2.36	0.41
3:C:80:ALA:HB3	3:C:102:GLY:HA2	2.02	0.41
4:E:13:TRP:NE1	4:E:39:LEU:HA	2.35	0.41
2:B:894:LYS:HB3	10:L:45:ALA:HB1	2.02	0.41
1:A:1020:GLN:NE2	1:A:1191:GLN:HA	2.35	0.41
1:A:1268:ASP:H	1:A:1296:PHE:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1483:LEU:HD23	1:A:1483:LEU:HA	1.86	0.41
1:A:1600:ARG:HB2	1:A:1616:GLU:OE2	2.20	0.41
1:A:1:MET:HA	2:B:1098:TYR:CE2	2.55	0.41
1:A:126:GLN:HB3	1:A:343:PRO:CD	2.51	0.41
1:A:596:HIS:NE2	1:A:598:ALA:HB3	2.34	0.41
1:A:747:ILE:HG13	1:A:748:ASN:N	2.36	0.41
1:A:476:VAL:HG22	2:B:1069:ILE:O	2.20	0.41
2:B:325:GLN:HA	2:B:328:GLN:OE1	2.20	0.41
2:B:712:SER:O	2:B:715:ASN:N	2.53	0.41
2:B:743:ARG:HG2	2:B:744:LEU:O	2.21	0.41
4:E:48:ASP:CG	4:E:50:MET:HB3	2.41	0.41
1:A:248:PHE:O	1:A:249:THR:OG1	2.32	0.41
2:B:1189:LEU:HD12	2:B:1196:LEU:HD11	2.03	0.41
4:E:24:LYS:HE2	4:E:32:GLN:NE2	2.36	0.41
5:F:116:ASP:OD2	5:F:119:ARG:HG2	2.20	0.41
5:F:77:ASP:OD1	5:F:78:GLN:HG3	2.21	0.41
14:G:106:LYS:HE3	14:G:106:LYS:HB2	1.82	0.41
14:G:29:ASP:OD1	14:G:30:GLU:N	2.52	0.41
7:I:88:GLN:OE1	7:I:119:TYR:HB2	2.21	0.41
7:I:23:VAL:HB	7:I:39:LYS:NZ	2.34	0.41
8:J:7:CYS:O	8:J:11:GLY:N	2.48	0.41
1:A:1154:LEU:HA	1:A:1157:SER:OG	2.20	0.41
1:A:1031:HIS:HA	1:A:1184:ALA:HA	2.03	0.41
1:A:1245:ASP:OD1	1:A:1246:VAL:N	2.53	0.41
1:A:1643:VAL:O	1:A:1643:VAL:HG12	2.20	0.41
1:A:407:GLN:O	1:A:411:VAL:HG23	2.21	0.41
1:A:485:SER:HB2	1:A:615:ARG:NE	2.36	0.41
1:A:618:TYR:OH	2:B:783:MET:HB2	2.21	0.41
2:B:253:LEU:HD22	2:B:257:GLN:HB2	2.01	0.41
2:B:323:ARG:O	2:B:327:LEU:HG	2.20	0.41
3:C:140:CYS:O	3:C:198:PRO:HA	2.20	0.41
3:C:230:LEU:HD22	3:C:297:HIS:ND1	2.35	0.41
13:D:82:LEU:O	13:D:86:ILE:HG23	2.20	0.41
4:E:147:HIS:HB3	4:E:150:VAL:CG2	2.50	0.41
7:I:110:VAL:O	7:I:123:THR:N	2.37	0.41
9:K:89:CYS:SG	9:K:90:GLY:N	2.94	0.41
1:A:440:SER:OG	1:A:458:GLN:NE2	2.54	0.41
2:B:584:CYS:HB2	2:B:598:HIS:HA	2.02	0.41
2:B:555:GLN:HB2	2:B:646:HIS:HE1	1.85	0.41
2:B:915:ASP:H	2:B:927:CYS:CB	2.29	0.41
5:F:89:GLU:O	5:F:93:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:327:TYR:HE2	9:K:46:LYS:HE2	1.85	0.41
1:A:1268:ASP:HA	1:A:1297:PHE:CZ	2.56	0.41
1:A:1300:ASN:OD1	1:A:1301:GLU:N	2.53	0.41
1:A:693:GLN:HE22	9:K:88:PHE:HA	1.85	0.41
2:B:457:ILE:O	2:B:460:LYS:N	2.54	0.41
2:B:699:ILE:O	2:B:703:LEU:HG	2.20	0.41
3:C:216:HIS:HB3	3:C:219:PHE:CD2	2.56	0.41
3:C:85:PHE:HB2	10:L:65:VAL:HB	2.02	0.41
4:E:165:LEU:HD22	4:E:170:LEU:O	2.21	0.41
4:E:33:GLU:OE1	4:E:33:GLU:N	2.40	0.41
6:H:12:VAL:N	6:H:53:ASP:O	2.49	0.41
2:B:307:GLU:HG3	7:I:7:LEU:HD21	2.02	0.41
1:A:800:VAL:O	1:A:1079:LYS:HD2	2.21	0.41
1:A:399:LEU:HD11	1:A:422:ARG:HD2	2.03	0.41
1:A:76:GLN:HB2	1:A:362:VAL:O	2.20	0.41
2:B:790:ASN:HD21	2:B:944:GLN:HB3	1.85	0.41
3:C:84:TYR:O	3:C:204:LEU:HA	2.21	0.41
4:E:109:ILE:HG12	4:E:133:GLU:HB2	2.03	0.41
6:H:15:VAL:HG13	6:H:26:ILE:HG12	2.03	0.41
1:A:233:CYS:SG	1:A:235:ASN:HB2	2.61	0.41
1:A:717:PRO:HB3	1:A:726:TRP:CE2	2.55	0.41
1:A:736:LEU:HD23	1:A:736:LEU:HA	1.81	0.41
1:A:878:ARG:O	1:A:882:ILE:N	2.33	0.41
2:B:1079:LEU:HD12	2:B:1088:LEU:HD13	2.03	0.41
2:B:1116:SER:O	2:B:1124:SER:OG	2.21	0.41
2:B:225:ARG:HB2	2:B:229:TYR:CD2	2.56	0.41
2:B:252:TYR:CE1	2:B:256:GLY:HA2	2.56	0.41
2:B:285:ASP:O	2:B:289:PHE:N	2.40	0.41
1:A:826:PHE:HB3	2:B:777:SER:HB2	2.03	0.41
4:E:158:SER:O	4:E:161:LYS:HB3	2.21	0.41
7:I:85:LYS:HA	7:I:91:ASN:O	2.21	0.41
9:K:133:SER:OG	9:K:137:GLU:OE2	2.35	0.41
1:A:697:TYR:HE2	9:K:91:TYR:C	2.24	0.41
1:A:1263:LEU:C	1:A:1265:GLU:N	2.74	0.41
1:A:487:ASP:OD2	1:A:489:ASN:HB2	2.21	0.41
2:B:581:PRO:HB3	2:B:637:TYR:CE1	2.56	0.41
2:B:706:PHE:HE2	2:B:752:VAL:HG11	1.85	0.41
2:B:707:SER:O	2:B:710:ASN:N	2.43	0.41
4:E:127:ILE:HD11	4:E:132:ILE:HD11	2.02	0.41
7:I:120:LYS:HB3	7:I:120:LYS:HE3	1.90	0.41
10:L:48:CYS:HB3	10:L:52:GLY:N	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:ILE:HA	1:A:1321:PHE:CB	2.44	0.40
1:A:1648:ASN:O	1:A:1652:GLY:HA3	2.19	0.40
1:A:244:ARG:HH21	1:A:252:PHE:HD2	1.68	0.40
1:A:706:HIS:CG	1:A:808:LYS:HE2	2.55	0.40
2:B:1084:THR:HB	2:B:1087:LEU:HD12	2.03	0.40
2:B:161:LEU:O	2:B:163:VAL:HG23	2.20	0.40
2:B:885:VAL:HG22	2:B:903:ILE:HG23	2.02	0.40
3:C:165:ARG:HH12	3:C:190:ASP:HA	1.85	0.40
1:A:102:CYS:SG	1:A:104:PHE:HD2	2.45	0.40
1:A:1459:LYS:HB2	1:A:1473:LYS:HB3	2.02	0.40
1:A:141:LEU:HD13	1:A:181:LEU:HD13	2.03	0.40
1:A:402:ASP:O	1:A:406:LEU:HG	2.21	0.40
1:A:396:ILE:HG12	1:A:426:ALA:HB1	2.03	0.40
1:A:803:PRO:O	1:A:807:ALA:N	2.30	0.40
1:A:808:LYS:NZ	1:A:815:ARG:HH22	2.19	0.40
1:A:8:GLY:CA	14:G:115:PHE:CZ	3.05	0.40
2:B:359:LEU:HD22	2:B:361:HIS:HE1	1.85	0.40
2:B:445:TYR:O	2:B:449:VAL:HG23	2.21	0.40
2:B:538:PRO:HB2	2:B:542:LEU:HD12	2.03	0.40
2:B:886:ASN:HB2	2:B:902:SER:OG	2.22	0.40
7:I:8:ILE:O	7:I:16:LEU:HD12	2.21	0.40
12:N:70:LEU:HA	12:N:71:PRO:HD3	1.84	0.40
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.02	0.40
1:A:904:THR:C	1:A:906:GLN:H	2.25	0.40
2:B:1152:PHE:CZ	14:G:129:VAL:HG21	2.56	0.40
2:B:306:LEU:O	2:B:309:LEU:HB3	2.21	0.40
2:B:492:ASN:OD1	2:B:494:TYR:N	2.54	0.40
3:C:224:THR:HG23	3:C:225:ALA:N	2.36	0.40
4:E:195:VAL:HG13	4:E:212:ARG:O	2.21	0.40
4:E:48:ASP:OD2	4:E:50:MET:HB3	2.21	0.40
14:G:50:ALA:HA	14:G:113:PHE:CD2	2.56	0.40
14:G:35:SER:OG	14:G:132:VAL:N	2.46	0.40
11:M:11:GLU:O	11:M:87:SER:HA	2.22	0.40
1:A:1246:VAL:HG12	1:A:1247:SER:O	2.21	0.40
1:A:1316:VAL:HG13	1:A:1320:GLN:NE2	2.36	0.40
1:A:557:LEU:O	1:A:561:LEU:HG	2.20	0.40
1:A:25:ARG:NH2	1:A:80:GLU:OE1	2.52	0.40
1:A:854:GLY:HA3	1:A:974:THR:O	2.22	0.40
2:B:330:LEU:HD23	2:B:330:LEU:HA	1.87	0.40
2:B:331:GLY:O	2:B:335:ARG:HB2	2.20	0.40
3:C:319:ARG:HB2	3:C:319:ARG:CZ	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:73:TYR:CZ	14:G:238:THR:HG21	2.57	0.40
6:H:27:GLU:HA	6:H:39:THR:HA	2.04	0.40
2:B:569:GLY:HA3	12:N:90:MET:HE1	2.04	0.40
1:A:110:LEU:HD12	1:A:111:LYS:H	1.86	0.40
1:A:1148:LEU:HD21	1:A:1166:PHE:CD2	2.56	0.40
1:A:1250:GLN:O	1:A:1254:PHE:N	2.39	0.40
1:A:1615:TYR:CE2	1:A:1616:GLU:HG3	2.57	0.40
1:A:493:ASN:HA	1:A:653:THR:HG21	2.02	0.40
1:A:495:ILE:HD12	1:A:615:ARG:O	2.21	0.40
2:B:562:PRO:HA	2:B:565:LEU:HD12	2.04	0.40
2:B:588:ILE:O	2:B:591:LYS:N	2.54	0.40
2:B:61:LEU:HG	2:B:61:LEU:H	1.70	0.40
3:C:88:ASN:OD1	3:C:202:ILE:HG12	2.20	0.40
13:D:37:LEU:HD23	13:D:37:LEU:HA	1.88	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	1448/1664 (87%)	1364 (94%)	75 (5%)	9 (1%)	30	73
2	B	1158/1203 (96%)	1110 (96%)	41 (4%)	7 (1%)	30	73
3	C	303/335 (90%)	283 (93%)	19 (6%)	1 (0%)	46	82
4	E	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
5	F	96/155 (62%)	94 (98%)	2 (2%)	0	100	100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
7	I	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
8	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
9	K	99/142 (70%)	95 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
11	M	95/415 (23%)	86 (90%)	7 (7%)	2 (2%)	9	53
12	N	125/233 (54%)	108 (86%)	13 (10%)	4 (3%)	5	44
13	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	4	40
14	G	186/326 (57%)	171 (92%)	13 (7%)	2 (1%)	17	64
All	All	4122/5236 (79%)	3894 (94%)	201 (5%)	27 (1%)	31	71

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	LEU
2	B	657	PRO
2	B	658	LEU
2	B	659	ASP
3	C	226	SER
12	N	149	ASP
13	D	99	LEU
2	B	891	GLU
13	D	98	GLY
1	A	652	ASN
1	A	1649	VAL
2	B	892	SER
11	M	85	LYS
14	G	99	ASP
2	B	656	LEU
11	M	36	THR
12	N	115	SER
14	G	100	THR
1	A	905	SER
1	A	1264	SER
2	B	655	TYR
1	A	1050	TYR
1	A	1061	SER
12	N	70	LEU
1	A	1225	ILE
12	N	39	PRO
1	A	1569	VAL

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	1292/1465 (88%)	1288 (100%)	4 (0%)	94	97
2	B	1022/1053 (97%)	1020 (100%)	2 (0%)	95	97
3	C	269/296 (91%)	268 (100%)	1 (0%)	93	97
4	E	194/197 (98%)	194 (100%)	0	100	100
5	F	88/137 (64%)	88 (100%)	0	100	100
6	H	115/128 (90%)	115 (100%)	0	100	100
7	I	103/110 (94%)	103 (100%)	0	100	100
8	J	64/65 (98%)	64 (100%)	0	100	100
9	K	91/130 (70%)	91 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
11	M	88/371 (24%)	79 (90%)	9 (10%)	9	41
12	N	124/220 (56%)	120 (97%)	4 (3%)	46	78
13	D	55/116 (47%)	49 (89%)	6 (11%)	8	38
14	G	170/291 (58%)	158 (93%)	12 (7%)	18	58
All	All	3714/4636 (80%)	3676 (99%)	38 (1%)	83	92

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	905	SER
1	A	942	GLN
1	A	944	MET
1	A	1499	ARG
2	B	655	TYR
2	B	658	LEU
3	C	226	SER
11	M	17	ASP
11	M	18	GLN
11	M	31	ARG
11	M	44	LYS

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Mol	Chain	Res	Type
11	M	48	LYS
11	M	65	TYR
11	M	77	VAL
11	M	84	GLU
11	M	98	SER
12	N	51	GLN
12	N	124	THR
12	N	135	LYS
12	N	145	ILE
13	D	15	THR
13	D	29	GLN
13	D	38	GLN
13	D	46	GLU
13	D	80	THR
13	D	99	LEU
14	G	18	LYS
14	G	24	VAL
14	G	35	SER
14	G	39	VAL
14	G	139	ILE
14	G	147	LEU
14	G	167	THR
14	G	169	VAL
14	G	223	GLU
14	G	230	ARG
14	G	239	THR
14	G	243	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	224	HIS
1	A	263	ASN
1	A	378	HIS
1	A	458	GLN
1	A	489	ASN
1	A	537	GLN
1	A	730	GLN
1	A	880	GLN
1	A	942	GLN
1	A	950	GLN

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Mol	Chain	Res	Type
1	A	1031	HIS
1	A	1108	HIS
1	A	1116	GLN
1	A	1315	ASN
1	A	1319	ASN
1	A	1320	GLN
1	A	1447	GLN
2	B	27	ASN
2	B	43	GLN
2	B	183	HIS
2	B	246	GLN
2	B	248	ASN
2	B	254	ASN
2	B	267	ASN
2	B	427	GLN
2	B	504	HIS
2	B	547	HIS
2	B	587	GLN
2	B	686	HIS
2	B	695	ASN
2	B	893	ASN
2	B	1008	HIS
2	B	1034	GLN
2	B	1171	ASN
3	C	58	ASN
3	C	99	HIS
3	C	130	ASN
3	C	172	GLN
3	C	237	GLN
3	C	297	HIS
4	E	5	ASN
4	E	32	GLN
4	E	146	HIS
4	E	179	GLN
6	H	11	GLN
6	H	35	GLN
6	H	52	GLN
7	I	32	GLN
9	K	99	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	SO4	B	1301	-	4,4,4	0.46	0	6,6,6	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SO4	B	1301	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	SO4	8	0

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.