



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:37 AM GMT

PDB ID : 1K83
Title : Crystal Structure of Yeast RNA Polymerase II Complexed with the Inhibitor Alpha Amanitin
Authors : Bushnell, D.A.; Cramer, P.; Kornberg, R.D.
Deposited on : 2001-10-22
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

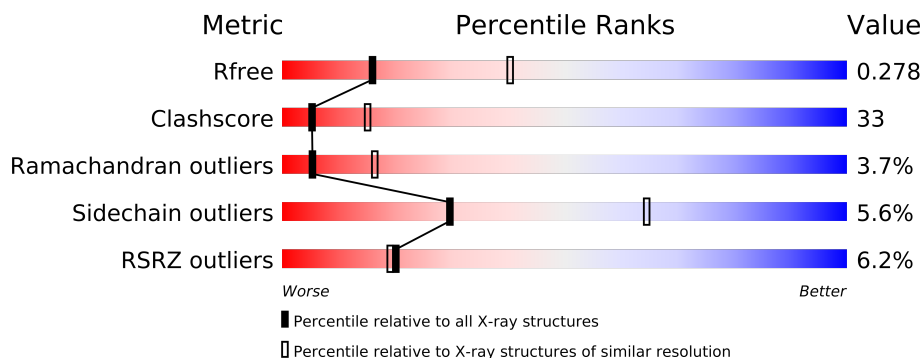
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	M	8	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
13	MN	A	3009	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27902 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1366	Total	C	N	O	S	0	0	0
			10751	6785	1871	2036	59			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1082	Total	C	N	O	S	0	0	0
			8616	5467	1503	1594	52			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

- Molecule 11 is a protein called ALPHA AMANITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total 1	Zn 1	0	0
12	B	1	Total 1	Zn 1	0	0
12	I	2	Total 2	Zn 2	0	0
12	C	1	Total 1	Zn 1	0	0
12	A	2	Total 2	Zn 2	0	0
12	L	1	Total 1	Zn 1	0	0

- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total 1	Mn 1	0	0

- Molecule 14 is water.

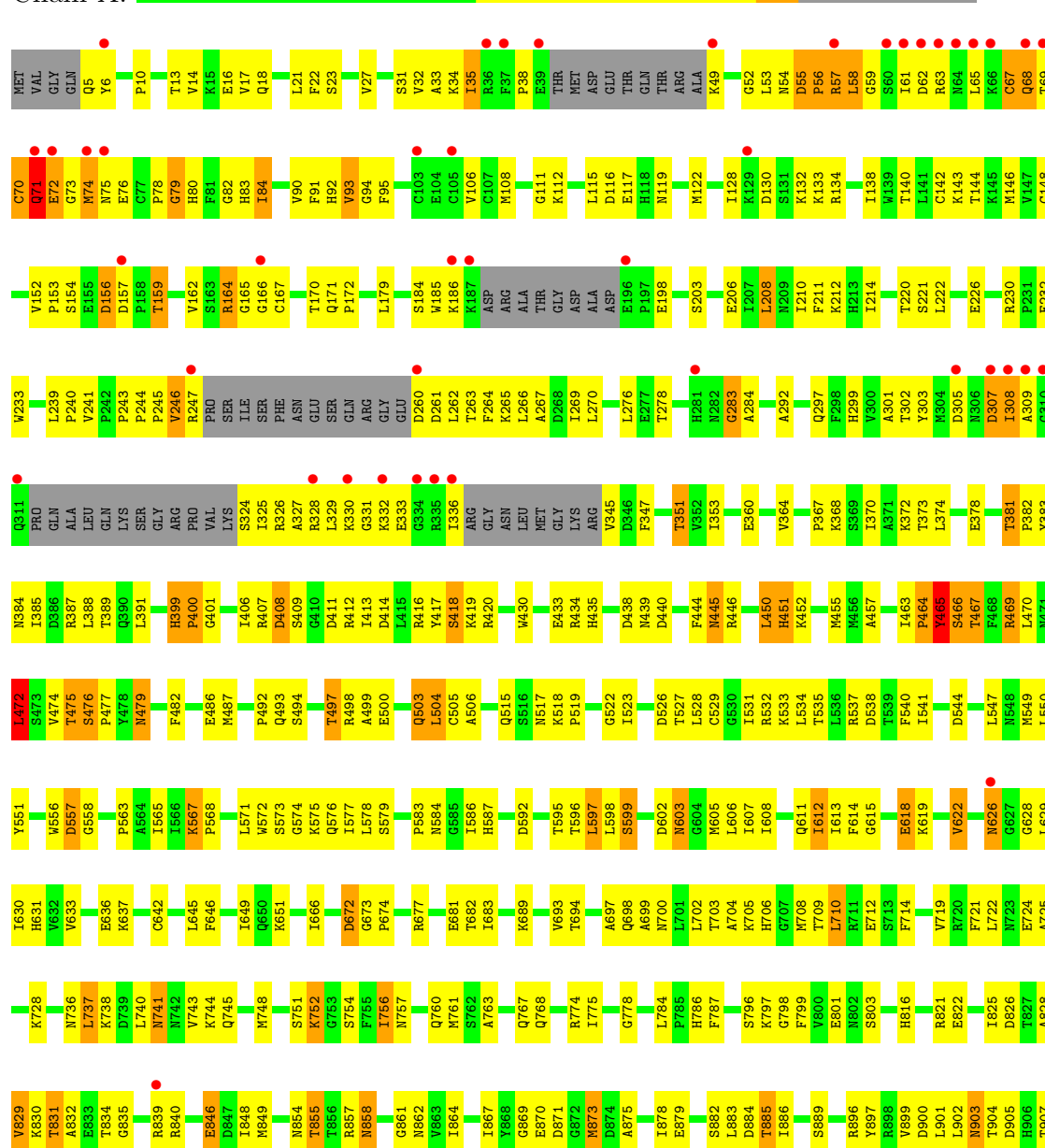
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	31	Total 31	O 31	0	0
14	B	23	Total 23	O 23	0	0
14	C	3	Total 3	O 3	0	0
14	E	6	Total 6	O 6	0	0
14	F	4	Total 4	O 4	0	0
14	J	1	Total 1	O 1	0	0
14	M	1	Total 1	O 1	0	0

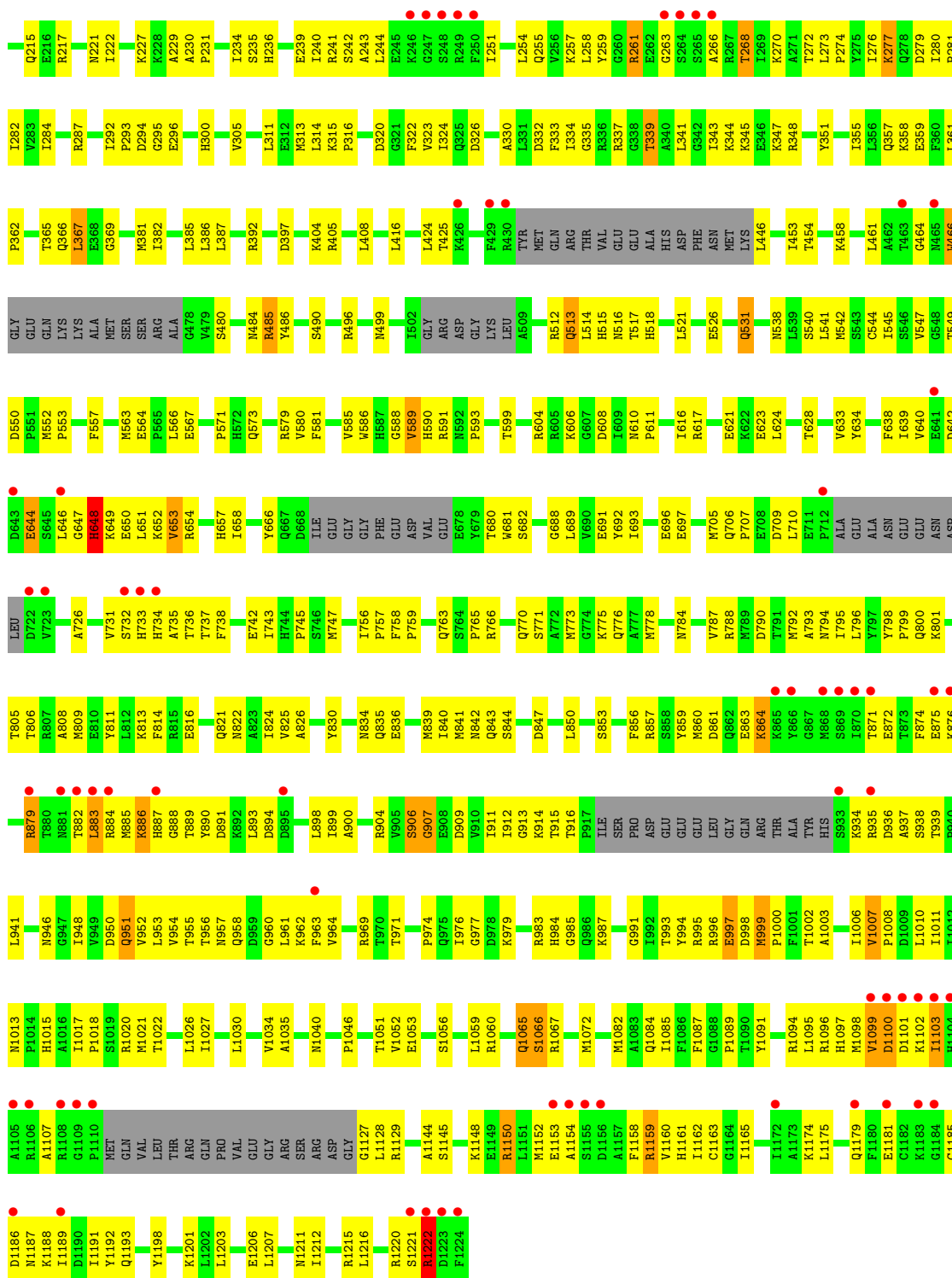
3 Residue-property plots

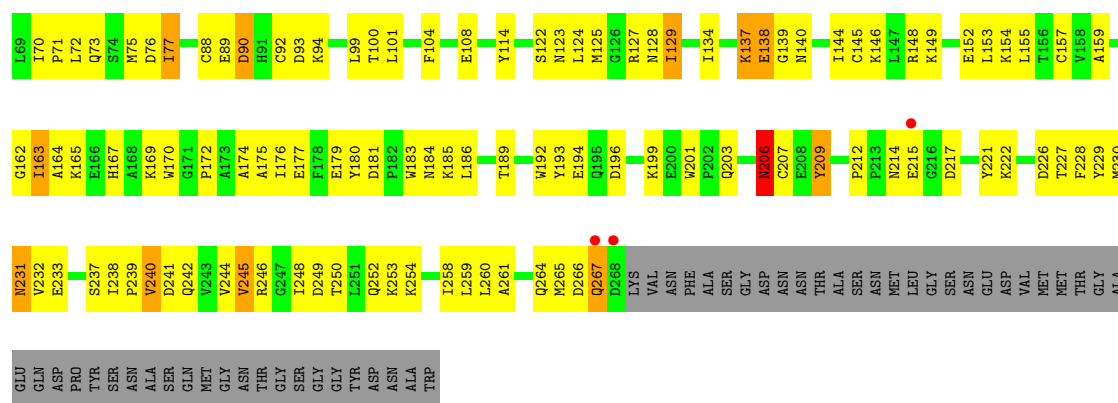
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 LARGEST SUBUNIT

Chain A:

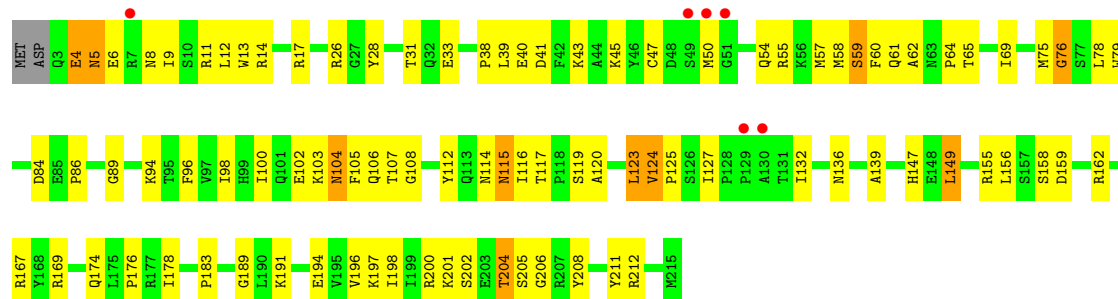






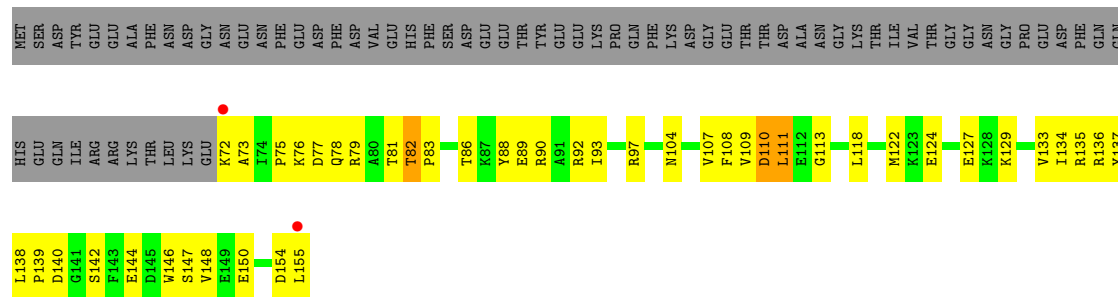
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

Chain E:



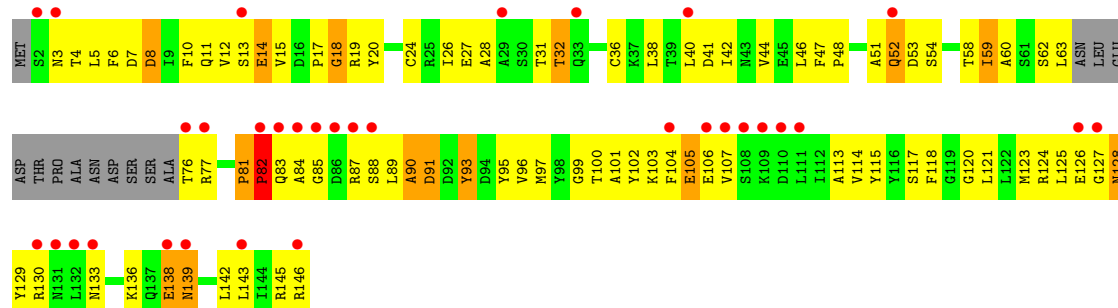
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F:



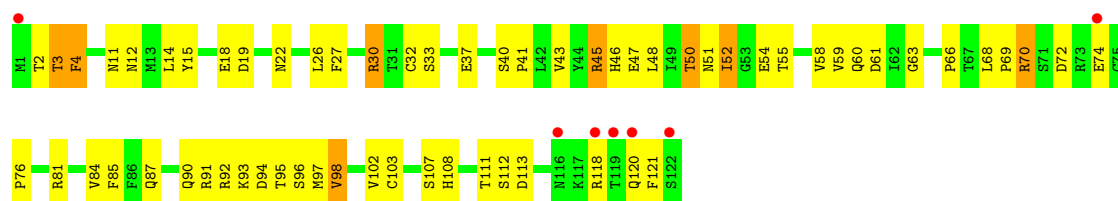
• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H:



- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I:



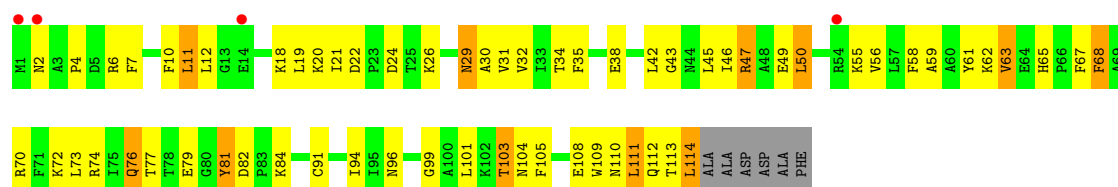
- Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J:



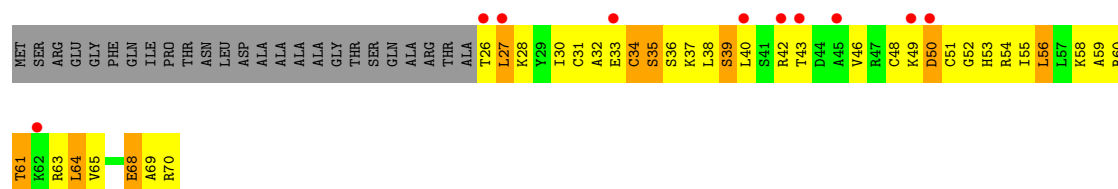
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

Chain K:



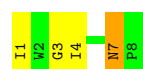
- Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

Chain L:



- Molecule 11: ALPHA AMANITIN

Chain M:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.51 Å 222.48 Å 374.23 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 93.4 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.79 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.280 0.228 , 0.278	Depositor DCC
R_{free} test set	3507 reflections (3.01%)	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 125151 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27902	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, HYP, TRX, CSX, ILX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/10940	0.68	2/14792 (0.0%)
2	B	0.42	0/8786	0.68	1/11847 (0.0%)
3	C	0.40	0/2133	0.66	0/2891
4	E	0.40	0/1780	0.67	0/2395
5	F	0.46	0/691	0.67	0/933
6	H	0.36	0/1086	0.68	0/1470
7	I	0.48	0/1016	0.68	0/1365
8	J	0.44	0/541	0.70	0/727
9	K	0.39	0/937	0.62	0/1265
10	L	0.47	0/361	0.71	0/478
11	M	2.39	1/22 (4.5%)	1.63	0/26
All	All	0.42	1/28293 (0.0%)	0.68	3/38189 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	7	ASN	CA-C	5.26	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	GLY	N-CA-C	5.82	127.64	113.10
1	A	798	GLY	N-CA-C	5.55	126.98	113.10
1	A	472	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10751	0	10819	759	0
2	B	8616	0	8645	586	0
3	C	2095	0	2051	165	0
4	E	1744	0	1772	87	0
5	F	679	0	701	55	0
6	H	1068	0	1040	115	0
7	I	997	0	953	75	0
8	J	532	0	542	56	0
9	K	919	0	929	71	0
10	L	359	0	382	61	1
11	M	64	0	51	7	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
13	A	1	0	0	0	0
14	A	31	0	0	1	0
14	B	23	0	0	5	0
14	C	3	0	0	0	0
14	E	6	0	0	1	0
14	F	4	0	0	0	0
14	J	1	0	0	0	0
14	M	1	0	0	0	0
All	All	27902	0	27885	1826	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (1826) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.09	1.15
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.17	1.09

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:871:THR:HG22	2:B:872:GLU:H	1.09	1.09
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.08
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.33	1.07
2:B:705:MET:HE3	2:B:742:GLU:HG3	1.37	1.07
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.10	1.06
2:B:800:GLN:HB3	8:J:52:THR:CG2	1.86	1.05
2:B:955:THR:HG22	2:B:956:THR:H	1.23	1.04
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.39	1.03
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.23	1.02
3:C:56:THR:HG23	3:C:58:LEU:H	1.15	1.02
1:A:672:ASP:HB2	1:A:736:ASN:ND2	1.73	1.02
2:B:29:ASP:HB3	2:B:658:ILE:CD1	1.88	1.02
1:A:470:LEU:HD11	1:A:487:MET:HE1	1.40	1.02
1:A:308:ILE:HG22	1:A:309:ALA:H	1.25	1.01
1:A:450:LEU:H	1:A:450:LEU:HD12	1.27	0.99
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.28	0.99
1:A:901:LEU:N	1:A:926:GLN:HE21	1.61	0.98
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.45	0.98
1:A:55:ASP:H	1:A:56:PRO:HD2	1.28	0.97
1:A:974:ASP:HB2	6:H:136:LYS:HZ3	1.27	0.97
7:I:111:THR:HG22	7:I:113:ASP:H	1.28	0.97
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.43	0.97
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.46	0.97
9:K:65:HIS:HD2	9:K:67:PHE:H	1.04	0.96
1:A:470:LEU:HD11	1:A:487:MET:CE	1.95	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.80	0.96
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.48	0.95
1:A:80:HIS:O	1:A:243:PRO:HB3	1.66	0.95
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.94	0.95
1:A:345:VAL:HG21	2:B:1129:ARG:HA	1.46	0.95
1:A:901:LEU:H	1:A:926:GLN:NE2	1.64	0.94
5:F:111:LEU:H	5:F:111:LEU:HD12	1.30	0.94
2:B:392:ARG:NH2	7:I:52:ILE:HD11	1.81	0.94
2:B:1153:GLU:HG2	2:B:1154:ALA:H	1.30	0.94
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.47	0.94
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.48	0.94
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.65	0.94
2:B:244:LEU:HD11	2:B:366:GLN:HE21	1.29	0.94
2:B:205:ILE:HD13	2:B:461:LEU:HB3	1.48	0.93
2:B:542:MET:HG3	2:B:747:MET:HE3	1.46	0.93
2:B:654:ARG:H	2:B:657:HIS:HD2	1.12	0.93
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.51	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:597:LEU:H	1:A:597:LEU:HD12	1.34	0.92
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	0.94	0.92
1:A:49:LYS:HD3	1:A:55:ASP:HB2	1.49	0.92
1:A:399:HIS:O	1:A:401:GLY:N	2.02	0.92
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.52	0.92
1:A:903:ASN:HD22	1:A:905:ASP:H	1.14	0.91
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.32	0.91
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.52	0.91
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.50	0.91
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.50	0.91
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.53	0.91
2:B:103:ASN:HB2	2:B:169:ARG:NH2	1.86	0.90
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.53	0.90
2:B:365:THR:HG22	2:B:367:LEU:H	1.35	0.90
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.36	0.90
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.31	0.90
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.53	0.90
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.53	0.90
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.69	0.89
1:A:567:LYS:HB3	6:H:96:VAL:N	1.88	0.89
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.51	0.89
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.69	0.89
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.55	0.88
1:A:33:ALA:O	1:A:83:HIS:HB3	1.74	0.88
1:A:179:LEU:HD21	1:A:308:ILE:HD13	1.56	0.87
3:C:148:ARG:NH1	8:J:64:ASN:HA	1.89	0.87
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.56	0.87
2:B:563:MET:CE	2:B:580:VAL:HB	2.05	0.87
6:H:100:THR:OG1	6:H:138:GLU:HG3	1.73	0.87
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.54	0.87
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.90	0.87
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.88	0.87
4:E:78:LEU:HD23	4:E:107:THR:HB	1.56	0.87
1:A:112:LYS:NZ	1:A:165:GLY:H	1.73	0.87
2:B:806:THR:HG22	2:B:808:ALA:H	1.39	0.86
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.54	0.86
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.56	0.86
2:B:130:VAL:HG12	2:B:131:ASP:H	1.41	0.86
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.10	0.86
2:B:205:ILE:CD1	2:B:461:LEU:HB3	2.06	0.86
4:E:159:ASP:HA	4:E:162:ARG:NH1	1.91	0.86
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	1.91	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:K:113:THR:O	9:K:114:LEU:HB2	1.74	0.85
1:A:305:ASP:HB3	1:A:326:ARG:CZ	2.06	0.85
10:L:61:THR:HB	10:L:63:ARG:HG2	1.58	0.85
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.59	0.85
3:C:73:GLN:HE21	3:C:75:MET:H	1.24	0.84
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.11	0.84
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.57	0.84
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.57	0.84
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.58	0.84
2:B:871:THR:HG22	2:B:872:GLU:N	1.92	0.84
2:B:268:THR:HG21	2:B:270:LYS:HE3	1.60	0.83
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.92	0.83
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.77	0.83
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.77	0.83
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.61	0.83
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.61	0.83
6:H:130:ARG:HA	6:H:133:ASN:HD22	1.41	0.83
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.13	0.83
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.61	0.83
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.59	0.83
1:A:132:LYS:HZ1	1:A:1411:GLU:HB3	1.44	0.82
1:A:901:LEU:H	1:A:926:GLN:HE21	0.85	0.82
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.44	0.82
2:B:324:ILE:HD11	2:B:333:PHE:CD1	2.15	0.82
1:A:587:HIS:NE2	1:A:969:GLN:HG2	1.94	0.81
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.62	0.81
1:A:1394:THR:HG22	1:A:1395:GLY:N	1.92	0.81
7:I:47:GLU:OE1	7:I:50:THR:HG23	1.79	0.81
1:A:709:THR:HG21	7:I:93:LYS:O	1.79	0.81
6:H:130:ARG:HA	6:H:133:ASN:ND2	1.95	0.81
1:A:32:VAL:HG11	1:A:68:GLN:HE22	1.44	0.81
3:C:174:ALA:O	8:J:10:CYS:HB2	1.79	0.81
2:B:914:LYS:HB3	2:B:937:ALA:O	1.81	0.81
1:A:982:THR:HG22	1:A:984:LYS:H	1.46	0.81
1:A:38:PRO:HA	1:A:270:LEU:HD13	1.63	0.80
1:A:1198:ASP:O	1:A:1202:MET:HG2	1.81	0.80
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.46	0.80
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.61	0.80
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.47	0.80
10:L:26:THR:HG22	10:L:27:LEU:H	1.47	0.80
1:A:503:GLN:HE21	5:F:90:ARG:NH2	1.80	0.80
5:F:109:VAL:HG12	5:F:110:ASP:N	1.96	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:109:VAL:HG12	5:F:110:ASP:H	1.46	0.80
1:A:913:LEU:HD11	1:A:981:LEU:O	1.81	0.79
3:C:51:VAL:HG22	3:C:155:LEU:HD12	1.64	0.79
1:A:55:ASP:O	1:A:57:ARG:N	2.14	0.79
9:K:65:HIS:CD2	9:K:67:PHE:H	1.96	0.79
1:A:567:LYS:NZ	6:H:46:LEU:HB2	1.98	0.79
2:B:244:LEU:HD11	2:B:366:GLN:NE2	1.96	0.79
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	1.64	0.79
1:A:55:ASP:N	1:A:56:PRO:HD2	1.97	0.79
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.47	0.79
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.12	0.79
1:A:347:PHE:H	2:B:1107:ALA:HA	1.47	0.79
3:C:56:THR:HG23	3:C:58:LEU:N	1.94	0.79
9:K:29:ASN:HD21	9:K:79:GLU:HA	1.48	0.79
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.65	0.79
2:B:889:THR:HG22	2:B:891:ASP:H	1.44	0.78
1:A:328:ARG:HD3	1:A:332:LYS:NZ	1.97	0.78
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.13	0.78
6:H:105:GLU:O	6:H:107:VAL:HG23	1.84	0.78
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.45	0.78
2:B:294:ASP:H	7:I:12:ASN:ND2	1.82	0.78
5:F:147:SER:OG	5:F:150:GLU:HG3	1.84	0.77
1:A:112:LYS:HZ2	1:A:165:GLY:H	1.30	0.77
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.67	0.77
2:B:871:THR:CG2	2:B:872:GLU:H	1.91	0.77
1:A:974:ASP:HB2	6:H:136:LYS:NZ	1.98	0.77
10:L:26:THR:HG22	10:L:27:LEU:N	2.00	0.77
2:B:652:LYS:HE3	2:B:688:GLY:O	1.85	0.77
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.49	0.77
7:I:50:THR:H	7:I:92:ARG:HH12	1.33	0.76
3:C:258:ILE:HD13	9:K:35:PHE:HE2	1.50	0.76
4:E:100:ILE:HD13	4:E:108:GLY:HA3	1.66	0.76
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.65	0.76
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.64	0.76
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.66	0.76
1:A:596:THR:HG22	1:A:597:LEU:H	1.51	0.76
1:A:677:ARG:O	1:A:681:GLU:HG3	1.85	0.76
1:A:1400:CYS:HB3	1:A:1405:THR:OG1	1.85	0.76
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.67	0.76
2:B:531:GLN:H	2:B:531:GLN:CD	1.87	0.76
1:A:276:LEU:HD13	1:A:292:ALA:HB3	1.67	0.76
6:H:15:VAL:HG22	6:H:26:ILE:HG12	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:94:LYS:HG3	4:E:123:LEU:HD11	1.65	0.75
6:H:101:ALA:H	6:H:138:GLU:HA	1.50	0.75
6:H:103:LYS:HZ2	6:H:114:VAL:HB	1.51	0.75
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.67	0.75
4:E:155:ARG:HD2	4:E:194:GLU:OE2	1.86	0.75
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.51	0.75
1:A:855:THR:HG21	1:A:857:ARG:NE	1.96	0.75
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.67	0.75
1:A:901:LEU:HA	1:A:907:THR:HG23	1.67	0.74
7:I:45:ARG:HH11	7:I:45:ARG:HG2	1.53	0.74
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.68	0.74
3:C:261:ALA:O	3:C:265:MET:HB2	1.86	0.74
1:A:760:GLN:HE22	11:M:1:ILX:HG23	1.53	0.74
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.03	0.74
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.69	0.74
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.18	0.74
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.68	0.74
8:J:48:ARG:HG2	8:J:48:ARG:HH11	1.51	0.73
1:A:567:LYS:HB3	6:H:96:VAL:H	1.52	0.73
10:L:32:ALA:HB2	10:L:55:ILE:HB	1.70	0.73
2:B:130:VAL:HG12	2:B:131:ASP:N	2.02	0.73
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.70	0.73
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.69	0.73
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.69	0.73
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.03	0.73
9:K:47:ARG:HB3	9:K:47:ARG:NH1	2.01	0.73
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.18	0.73
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.24	0.73
3:C:137:LYS:H	3:C:137:LYS:HD2	1.53	0.73
6:H:104:PHE:O	6:H:106:GLU:N	2.21	0.73
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.24	0.73
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.54	0.73
2:B:654:ARG:H	2:B:657:HIS:CD2	2.03	0.73
1:A:170:THR:HG21	1:A:186:LYS:O	1.89	0.73
6:H:36:CYS:HB2	6:H:129:TYR:OH	1.88	0.73
2:B:709:ASP:HB2	2:B:733:HIS:HB3	1.71	0.73
1:A:1128:GLN:O	1:A:1132:LYS:HG3	1.87	0.72
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.54	0.72
3:C:196:ASP:OD2	3:C:199:LYS:HG3	1.90	0.72
2:B:542:MET:HE1	2:B:747:MET:HG3	1.70	0.72
1:A:329:LEU:O	1:A:333:GLU:N	2.22	0.72
6:H:11:GLN:NE2	6:H:52:GLN:HA	2.04	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.72	0.72
1:A:903:ASN:ND2	1:A:905:ASP:H	1.86	0.72
1:A:108:MET:HG2	1:A:171:GLN:HE22	1.53	0.72
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.70	0.72
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.72	0.72
2:B:680:THR:HG22	2:B:681:TRP:N	2.05	0.71
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.72	0.71
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.70	0.71
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.54	0.71
3:C:250:THR:O	3:C:254:LYS:HG3	1.90	0.71
1:A:526:ASP:HB2	2:B:835:GLN:OE1	1.91	0.71
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.38	0.71
1:A:132:LYS:NZ	1:A:1411:GLU:HB3	2.04	0.71
2:B:879:ARG:HB3	2:B:883:LEU:CD2	2.21	0.71
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.25	0.71
1:A:5:GLN:HG2	1:A:6:TYR:H	1.55	0.71
3:C:66:ARG:NH2	8:J:3:VAL:O	2.23	0.71
1:A:907:THR:HG22	1:A:908:LEU:H	1.56	0.71
9:K:30:ALA:HB2	9:K:76:GLN:HG3	1.73	0.71
2:B:277:LYS:HD2	2:B:277:LYS:N	2.06	0.71
2:B:243:ALA:HB2	2:B:251:ILE:HG12	1.73	0.71
2:B:1097:HIS:HB3	2:B:1102:LYS:NZ	2.06	0.70
1:A:1398:MET:HG3	1:A:1426:GLU:OE2	1.92	0.70
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.21	0.70
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.30	0.70
1:A:567:LYS:CB	1:A:568:PRO:CD	2.69	0.70
1:A:308:ILE:HG22	1:A:309:ALA:N	2.04	0.70
1:A:55:ASP:C	1:A:57:ARG:H	1.95	0.70
1:A:573:SER:HB3	1:A:576:GLN:HG3	1.74	0.70
2:B:955:THR:HG23	10:L:54:ARG:O	1.92	0.70
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.73	0.70
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.56	0.70
2:B:705:MET:CE	2:B:742:GLU:HG3	2.17	0.70
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.74	0.70
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.07	0.70
7:I:111:THR:HG22	7:I:112:SER:N	2.07	0.70
1:A:329:LEU:HA	1:A:332:LYS:HB2	1.74	0.69
2:B:899:ILE:HG22	2:B:900:ALA:N	2.05	0.69
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.73	0.69
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.07	0.69
1:A:672:ASP:CB	1:A:736:ASN:HD21	2.03	0.69
6:H:130:ARG:HA	6:H:133:ASN:HB2	1.74	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:890:TYR:HB3	2:B:893:LEU:HD12	1.73	0.69
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.73	0.69
2:B:1181:GLU:HG3	2:B:1188:LYS:HE2	1.73	0.69
1:A:855:THR:CG2	1:A:857:ARG:HE	1.98	0.69
2:B:954:VAL:O	10:L:55:ILE:O	2.11	0.69
1:A:1398:MET:HG2	1:A:1425:SER:HB2	1.73	0.69
8:J:36:LEU:HB2	8:J:47:ARG:HH21	1.57	0.69
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.28	0.69
2:B:801:LYS:O	8:J:52:THR:HG23	1.93	0.69
10:L:38:LEU:HG	10:L:39:SER:H	1.58	0.69
1:A:56:PRO:O	1:A:57:ARG:HG3	1.93	0.69
2:B:542:MET:CE	2:B:747:MET:HG3	2.23	0.69
1:A:262:LEU:O	1:A:266:LEU:HG	1.93	0.69
5:F:76:LYS:O	5:F:79:ARG:HD2	1.93	0.69
1:A:1147:THR:HB	7:I:48:LEU:HD12	1.75	0.69
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.74	0.68
1:A:1336:MET:HE1	1:A:1381:LEU:H	1.58	0.68
2:B:1198:TYR:CE1	2:B:1201:LYS:HD3	2.28	0.68
6:H:125:LEU:C	6:H:130:ARG:HH12	1.97	0.68
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.74	0.68
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.57	0.68
1:A:974:ASP:CB	6:H:136:LYS:HZ3	2.05	0.68
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.75	0.68
2:B:737:THR:HG21	7:I:66:PRO:HA	1.76	0.68
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.28	0.68
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.09	0.68
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.75	0.68
1:A:1341:ILE:HD12	1:A:1379:GLY:HA2	1.76	0.68
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.74	0.68
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.75	0.67
1:A:140:THR:HA	1:A:143:LYS:HE2	1.76	0.67
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.74	0.67
1:A:445:ASN:CB	1:A:455:MET:HG2	2.19	0.67
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.28	0.67
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.77	0.67
1:A:1077:THR:HG22	1:A:1077:THR:O	1.94	0.67
1:A:465:TYR:HA	9:K:2:ASN:HB3	1.76	0.67
2:B:118:ARG:NH1	2:B:204:ILE:HD11	2.09	0.67
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.24	0.67
6:H:103:LYS:NZ	6:H:114:VAL:HB	2.09	0.67
3:C:196:ASP:CG	3:C:199:LYS:HG3	2.14	0.67
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.41	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.77	0.67
10:L:34:CYS:HB3	10:L:51:CYS:SG	2.34	0.67
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.30	0.67
3:C:265:MET:HE1	9:K:19:LEU:HB2	1.77	0.67
2:B:1181:GLU:CG	2:B:1188:LYS:HE2	2.25	0.67
1:A:1394:THR:CG2	1:A:1395:GLY:H	1.93	0.67
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.25	0.67
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.25	0.67
5:F:77:ASP:O	5:F:78:GLN:HB2	1.94	0.67
5:F:138:LEU:HD12	5:F:142:SER:OG	1.94	0.67
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.24	0.66
2:B:876:LYS:HE2	2:B:893:LEU:O	1.94	0.66
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.76	0.66
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.77	0.66
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.76	0.66
1:A:67:CYS:O	1:A:68:GLN:HB2	1.93	0.66
3:C:22:LEU:HD12	3:C:230:MET:CE	2.26	0.66
2:B:62:ILE:O	2:B:65:GLU:HG2	1.95	0.66
2:B:955:THR:HG22	2:B:956:THR:N	2.05	0.66
1:A:49:LYS:HD3	1:A:55:ASP:CB	2.22	0.66
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.77	0.66
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.60	0.66
8:J:2:ILE:HD11	8:J:57:ILE:HD13	1.78	0.66
1:A:597:LEU:N	1:A:597:LEU:HD12	2.07	0.66
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.10	0.66
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.44	0.66
1:A:263:THR:HA	1:A:266:LEU:HD12	1.78	0.66
1:A:834:THR:HG21	1:A:1077:THR:HA	1.78	0.66
1:A:689:LYS:O	1:A:693:VAL:HG23	1.96	0.66
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.56	0.66
7:I:50:THR:CG2	7:I:52:ILE:HG23	2.26	0.66
2:B:874:PHE:O	2:B:875:GLU:HG3	1.95	0.66
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	1.95	0.66
3:C:148:ARG:HD2	8:J:61:LEU:O	1.96	0.66
9:K:18:LYS:HZ3	9:K:38:GLU:HG2	1.61	0.66
1:A:464:PRO:O	1:A:465:TYR:O	2.14	0.66
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.11	0.66
1:A:23:SER:O	1:A:27:VAL:HG23	1.95	0.65
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.44	0.65
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.60	0.65
2:B:737:THR:HG21	7:I:66:PRO:O	1.96	0.65
3:C:249:ASP:OD1	3:C:253:LYS:HE3	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:J:1:MET:HG3	8:J:60:PHE:CE2	2.24	0.65
1:A:541:ILE:N	1:A:541:ILE:HD12	2.11	0.65
3:C:5:GLY:C	3:C:24:ASN:HD22	2.00	0.65
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.23	0.65
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.26	0.65
1:A:901:LEU:O	1:A:920:LEU:HD23	1.95	0.65
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.26	0.65
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.79	0.65
4:E:5:ASN:O	4:E:9:ILE:HG13	1.97	0.65
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.26	0.65
5:F:81:THR:HB	5:F:144:GLU:OE1	1.95	0.65
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.76	0.65
2:B:737:THR:CG2	7:I:66:PRO:HA	2.27	0.65
1:A:537:ARG:NH1	6:H:120:GLY:O	2.30	0.65
1:A:1390:ASN:O	1:A:1391:ARG:HB2	1.96	0.65
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.32	0.65
1:A:65:LEU:O	1:A:71:GLN:HA	1.97	0.65
2:B:806:THR:HG22	2:B:808:ALA:N	2.08	0.65
2:B:957:ASN:OD1	2:B:958:GLN:N	2.28	0.65
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.62	0.65
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.78	0.65
2:B:731:VAL:HG12	2:B:732:SER:N	2.12	0.65
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.79	0.65
1:A:387:ARG:O	1:A:391:LEU:HG	1.96	0.65
1:A:1140:HIS:CE1	1:A:1272:THR:HG23	2.32	0.65
2:B:515:HIS:HD2	2:B:517:THR:H	1.43	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.79	0.65
1:A:998:LEU:HD12	1:A:1001:ARG:NH1	2.11	0.64
2:B:864:LYS:CG	2:B:871:THR:HG23	2.25	0.64
6:H:103:LYS:HB3	6:H:105:GLU:OE2	1.97	0.64
3:C:265:MET:CE	9:K:19:LEU:HB2	2.27	0.64
1:A:666:ILE:HG12	2:B:1026:LEU:HB3	1.77	0.64
2:B:680:THR:CG2	2:B:681:TRP:N	2.61	0.64
1:A:768:GLN:HE21	1:A:816:HIS:HA	1.63	0.64
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.78	0.64
6:H:82:PRO:O	6:H:84:ALA:N	2.28	0.64
1:A:754:SER:OG	1:A:756:ILE:HG22	1.97	0.64
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.38	0.64
6:H:5:LEU:HD22	6:H:133:ASN:O	1.97	0.64
1:A:328:ARG:HD3	1:A:332:LYS:HZ1	1.61	0.64
1:A:826:ASP:O	1:A:830:LYS:HB2	1.97	0.64
3:C:73:GLN:HE21	3:C:75:MET:N	1.95	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:109:VAL:CG1	5:F:110:ASP:H	2.11	0.64
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.29	0.64
2:B:864:LYS:HB3	2:B:871:THR:HA	1.79	0.64
3:C:67:LEU:HD13	3:C:155:LEU:HD21	1.80	0.64
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.79	0.64
2:B:1022:THR:HG23	2:B:1022:THR:O	1.97	0.64
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.62	0.64
1:A:1395:GLY:C	1:A:1397:LEU:H	2.01	0.64
10:L:38:LEU:HD22	10:L:56:LEU:HD21	1.78	0.64
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.63	0.64
2:B:1159:ARG:CG	2:B:1193:GLN:HE21	2.11	0.64
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.79	0.64
1:A:70:CYS:O	1:A:72:GLU:HG3	1.98	0.63
1:A:595:THR:OG1	1:A:603:ASN:HB3	1.97	0.63
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.79	0.63
3:C:239:PRO:O	3:C:242:GLN:HB2	1.97	0.63
9:K:38:GLU:OE1	9:K:42:LEU:HD22	1.98	0.63
2:B:235:SER:HA	2:B:261:ARG:NH2	2.14	0.63
9:K:103:THR:HG22	9:K:104:ASN:N	2.13	0.63
1:A:469:ARG:NH2	2:B:991:GLY:O	2.31	0.63
2:B:956:THR:HA	2:B:961:LEU:O	1.97	0.63
6:H:11:GLN:HE21	6:H:52:GLN:HA	1.61	0.63
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.98	0.63
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.80	0.63
6:H:85:GLY:O	6:H:89:LEU:HD21	1.98	0.63
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.80	0.63
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.81	0.63
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.98	0.63
1:A:203:SER:OG	1:A:206:GLU:HG3	1.98	0.63
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.99	0.63
1:A:79:GLY:HA3	1:A:245:PRO:HG3	1.81	0.63
1:A:869:GLY:O	4:E:204:THR:HG21	1.97	0.63
4:E:204:THR:HG22	4:E:205:SER:N	2.11	0.63
1:A:535:THR:O	1:A:535:THR:HG22	1.98	0.63
4:E:4:GLU:O	4:E:6:GLU:N	2.32	0.63
1:A:596:THR:HG22	1:A:597:LEU:N	2.13	0.63
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.81	0.63
2:B:995:ARG:HD3	9:K:6:ARG:HH12	1.63	0.63
2:B:339:THR:HG21	2:B:348:ARG:HG2	1.80	0.63
1:A:1447:GLU:OE1	1:A:1447:GLU:HA	1.97	0.63
3:C:52:GLU:HA	10:L:64:LEU:CD2	2.29	0.63
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:103:ASN:CB	2:B:169:ARG:HH22	2.10	0.62
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.79	0.62
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.80	0.62
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.19	0.62
4:E:120:ALA:O	4:E:123:LEU:HB2	2.00	0.62
2:B:969:ARG:HH11	2:B:969:ARG:HB3	1.64	0.62
2:B:43:LEU:HD11	2:B:811:TYR:O	1.98	0.62
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.80	0.62
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.81	0.62
1:A:58:LEU:HD22	1:A:80:HIS:O	2.00	0.62
10:L:51:CYS:O	10:L:53:HIS:N	2.31	0.62
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.82	0.62
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.82	0.62
9:K:56:VAL:HA	9:K:77:THR:HG22	1.81	0.62
10:L:38:LEU:O	10:L:39:SER:HB2	2.00	0.62
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.81	0.62
10:L:26:THR:CG2	10:L:27:LEU:H	2.11	0.62
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.80	0.62
1:A:858:ASN:HD22	1:A:858:ASN:C	2.02	0.62
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.29	0.62
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.80	0.62
2:B:680:THR:HG22	2:B:682:SER:H	1.63	0.62
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.46	0.62
10:L:55:ILE:O	10:L:56:LEU:HB2	1.99	0.62
1:A:446:ARG:HB2	1:A:487:MET:SD	2.39	0.62
4:E:28:TYR:CZ	4:E:78:LEU:HG	2.35	0.62
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.97	0.62
1:A:704:ALA:HB2	1:A:710:LEU:CD1	2.27	0.61
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.30	0.61
4:E:40:GLU:OE1	4:E:43:LYS:HD2	2.00	0.61
2:B:705:MET:HE1	2:B:745:PRO:HB3	1.82	0.61
1:A:1394:THR:CG2	1:A:1398:MET:HB2	2.29	0.61
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.65	0.61
1:A:332:LYS:HD3	2:B:1206:GLU:OE2	2.00	0.61
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.65	0.61
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.61
6:H:130:ARG:CA	6:H:133:ASN:HD22	2.12	0.61
9:K:18:LYS:NZ	9:K:38:GLU:HG2	2.15	0.61
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.82	0.61
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.82	0.61
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.32	0.61
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.15	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:886:LYS:NZ	2:B:886:LYS:HB3	2.16	0.61
1:A:693:VAL:CG2	1:A:721:PHE:HE1	2.10	0.61
6:H:89:LEU:C	6:H:91:ASP:H	2.03	0.61
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.83	0.61
3:C:67:LEU:CD1	3:C:155:LEU:HD21	2.31	0.61
7:I:51:ASN:O	7:I:54:GLU:HG3	2.00	0.61
1:A:597:LEU:CD1	1:A:597:LEU:H	2.11	0.61
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.49	0.61
2:B:63:ILE:O	2:B:67:SER:HB3	2.01	0.61
2:B:879:ARG:HB3	2:B:883:LEU:HD22	1.81	0.61
1:A:825:ILE:CD1	2:B:512:ARG:HG3	2.30	0.61
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.83	0.61
3:C:51:VAL:HG22	3:C:155:LEU:CD1	2.30	0.61
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.83	0.61
2:B:164:LYS:O	2:B:165:VAL:HB	2.01	0.61
7:I:50:THR:HG22	7:I:52:ILE:HG23	1.82	0.61
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.03	0.60
1:A:724:GLU:O	1:A:728:LYS:HG2	2.01	0.60
1:A:32:VAL:HG11	1:A:68:GLN:NE2	2.16	0.60
2:B:1097:HIS:HB3	2:B:1102:LYS:HZ2	1.64	0.60
1:A:834:THR:HG21	1:A:1077:THR:CA	2.30	0.60
1:A:1111:MET:CE	1:A:1331:SER:HB2	2.31	0.60
7:I:95:THR:HG22	7:I:96:SER:N	2.15	0.60
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.83	0.60
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.16	0.60
10:L:58:LYS:O	10:L:58:LYS:HD3	2.01	0.60
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.82	0.60
1:A:903:ASN:HD22	1:A:905:ASP:N	1.94	0.60
2:B:731:VAL:HG12	2:B:732:SER:H	1.65	0.60
1:A:825:ILE:HD13	2:B:512:ARG:HG3	1.83	0.60
7:I:63:GLY:O	7:I:70:ARG:NH2	2.35	0.60
2:B:800:GLN:CB	8:J:52:THR:HG22	2.26	0.60
1:A:760:GLN:HB2	2:B:1021:MET:CE	2.31	0.60
5:F:154:ASP:O	5:F:155:LEU:HD23	2.01	0.60
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.37	0.60
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.31	0.60
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.37	0.60
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.37	0.60
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.02	0.60
7:I:98:VAL:HG21	7:I:113:ASP:CB	2.31	0.60
9:K:46:ILE:O	9:K:50:LEU:HB2	2.01	0.60
2:B:103:ASN:HB2	2:B:169:ARG:CZ	2.30	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:L:33:GLU:HB2	10:L:53:HIS:CD2	2.37	0.60
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.01	0.60
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.02	0.60
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.01	0.60
1:A:673:GLY:N	1:A:674:PRO:HD2	2.17	0.60
2:B:120:ARG:HG3	2:B:955:THR:HG21	1.84	0.60
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.01	0.60
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.37	0.60
1:A:283:GLY:O	1:A:284:ALA:HB2	2.02	0.60
4:E:124:VAL:HB	4:E:125:PRO:CD	2.32	0.60
1:A:1113:THR:HG22	1:A:1113:THR:O	2.02	0.60
2:B:1103:ILE:O	2:B:1103:ILE:HG22	2.02	0.59
6:H:130:ARG:CA	6:H:133:ASN:HB2	2.32	0.59
1:A:831:THR:HG22	1:A:832:ALA:N	2.17	0.59
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.83	0.59
3:C:8:VAL:HG12	3:C:9:LYS:N	2.16	0.59
1:A:378:GLU:CD	1:A:387:ARG:HH22	2.05	0.59
6:H:76:THR:HG22	6:H:76:THR:O	2.02	0.59
2:B:915:THR:HG21	2:B:934:LYS:HG2	1.84	0.59
1:A:523:ILE:HD13	1:A:649:ILE:HG21	1.83	0.59
1:A:276:LEU:HD13	1:A:292:ALA:CB	2.33	0.59
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.36	0.59
1:A:849:MET:CE	1:A:1436:ILE:HA	2.31	0.59
1:A:57:ARG:HB3	1:A:68:GLN:NE2	2.18	0.59
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.32	0.59
6:H:103:LYS:CD	6:H:114:VAL:HB	2.31	0.59
5:F:81:THR:HG21	5:F:136:ARG:CD	2.32	0.59
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.18	0.59
1:A:840:ARG:HG3	1:A:1385:THR:HG22	1.85	0.59
10:L:48:CYS:SG	10:L:49:LYS:N	2.75	0.59
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.17	0.59
2:B:98:THR:HG22	2:B:99:LYS:N	2.17	0.59
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.33	0.59
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.84	0.59
3:C:6:PRO:HB2	9:K:101:LEU:HB2	1.85	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.50	0.59
2:B:134:LYS:NZ	2:B:446:LEU:HD13	2.17	0.59
3:C:31:ASN:O	3:C:35:ARG:HG3	2.03	0.59
1:A:108:MET:HG2	1:A:171:GLN:NE2	2.16	0.58
1:A:608:ILE:HD12	1:A:613:ILE:HD12	1.84	0.58
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.85	0.58
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.24	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.38	0.58
1:A:1080:THR:O	1:A:1081:LEU:HG	2.03	0.58
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.18	0.58
1:A:63:ARG:HA	1:A:74:MET:HE2	1.83	0.58
9:K:12:LEU:HD11	9:K:18:LYS:HE2	1.86	0.58
10:L:34:CYS:O	10:L:36:SER:N	2.36	0.58
1:A:1265:ASN:HD21	2:B:263:GLY:C	2.06	0.58
2:B:35:SER:O	2:B:39:ARG:HG3	2.02	0.58
3:C:93:ASP:O	3:C:127:ARG:NH2	2.37	0.58
1:A:381:THR:CG2	1:A:383:TYR:H	2.16	0.58
1:A:763:ALA:O	1:A:803:SER:HB3	2.04	0.58
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.03	0.58
3:C:39:ALA:O	3:C:163:ILE:HG23	2.03	0.58
6:H:87:ARG:O	6:H:89:LEU:HG	2.04	0.58
1:A:208:LEU:CD2	1:A:212:LYS:HE3	2.33	0.58
6:H:40:LEU:HD12	6:H:41:ASP:H	1.69	0.58
2:B:563:MET:HE2	2:B:580:VAL:HB	1.81	0.58
4:E:158:SER:O	4:E:162:ARG:HG3	2.04	0.58
2:B:515:HIS:CD2	2:B:517:THR:H	2.22	0.58
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.33	0.58
2:B:1153:GLU:CG	2:B:1154:ALA:H	2.07	0.58
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.68	0.58
1:A:494:SER:OG	1:A:497:THR:HB	2.04	0.58
10:L:30:ILE:HG22	10:L:31:CYS:N	2.19	0.58
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.18	0.58
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.84	0.58
1:A:1341:ILE:HD12	1:A:1379:GLY:CA	2.34	0.58
6:H:87:ARG:O	6:H:89:LEU:N	2.37	0.58
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.44	0.58
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.19	0.58
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.34	0.58
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.85	0.58
2:B:889:THR:HG21	2:B:891:ASP:OD2	2.04	0.58
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.85	0.58
3:C:49:VAL:CG1	3:C:155:LEU:HD11	2.34	0.57
2:B:25:ILE:HD12	2:B:653:VAL:HB	1.85	0.57
1:A:760:GLN:HB2	2:B:1021:MET:HE1	1.85	0.57
2:B:229:ALA:C	2:B:231:PRO:HD2	2.23	0.57
4:E:117:THR:HG22	4:E:119:SER:H	1.69	0.57
8:J:12:LYS:NZ	8:J:17:LYS:NZ	2.52	0.57
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.04	0.57
2:B:860:MET:HG2	2:B:861:ASP:H	1.68	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:K:47:ARG:HH11	9:K:47:ARG:CB	2.06	0.57
2:B:1153:GLU:HG2	2:B:1154:ALA:N	2.12	0.57
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.39	0.57
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.86	0.57
2:B:98:THR:O	2:B:126:SER:HB3	2.04	0.57
1:A:184:SER:HA	1:A:198:GLU:O	2.04	0.57
2:B:341:LEU:O	2:B:341:LEU:HG	2.04	0.57
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.39	0.57
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.69	0.57
1:A:567:LYS:CB	6:H:96:VAL:H	2.16	0.57
5:F:107:VAL:HG12	5:F:109:VAL:H	1.69	0.57
4:E:38:PRO:HG2	4:E:41:ASP:OD2	2.04	0.57
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.29	0.57
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.05	0.57
1:A:244:PRO:N	1:A:245:PRO:HD2	2.19	0.57
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.86	0.57
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.34	0.57
2:B:130:VAL:CG1	2:B:131:ASP:H	2.15	0.57
1:A:381:THR:HG23	1:A:383:TYR:H	1.70	0.57
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.86	0.57
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.86	0.57
1:A:32:VAL:CG2	1:A:58:LEU:HD23	2.34	0.57
1:A:329:LEU:HB3	1:A:333:GLU:HB3	1.87	0.57
2:B:616:ILE:HD13	2:B:696:GLU:HG3	1.86	0.57
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.86	0.57
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.35	0.57
1:A:345:VAL:HG11	2:B:1128:LEU:O	2.05	0.57
6:H:103:LYS:HG2	6:H:115:TYR:N	2.19	0.57
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.40	0.57
4:E:116:ILE:HG22	4:E:117:THR:N	2.20	0.57
4:E:58:MET:O	4:E:59:SER:O	2.23	0.57
6:H:7:ASP:O	6:H:8:ASP:HB2	2.05	0.57
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.30	0.56
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.53	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.40	0.56
2:B:737:THR:O	2:B:737:THR:HG22	2.04	0.56
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.34	0.56
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.05	0.56
2:B:955:THR:CG2	2:B:956:THR:H	2.03	0.56
2:B:103:ASN:CB	2:B:169:ARG:HH12	2.18	0.56
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.05	0.56
1:A:32:VAL:HB	1:A:57:ARG:HB3	1.85	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:365:THR:HG22	2:B:366:GLN:N	2.20	0.56
2:B:654:ARG:N	2:B:657:HIS:HD2	1.93	0.56
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.69	0.56
2:B:284:ILE:CG1	2:B:324:ILE:HD12	2.35	0.56
7:I:2:THR:O	7:I:3:THR:C	2.43	0.56
1:A:537:ARG:HD2	6:H:20:TYR:CE1	2.41	0.56
1:A:1390:ASN:O	1:A:1391:ARG:CB	2.52	0.56
2:B:957:ASN:CG	2:B:958:GLN:H	2.08	0.56
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.18	0.56
1:A:613:ILE:HD13	6:H:102:TYR:HB3	1.87	0.56
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.40	0.56
1:A:112:LYS:NZ	1:A:164:ARG:HB2	2.20	0.56
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.05	0.56
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.40	0.56
1:A:1383:SER:HB3	1:A:1387:HIS:CD2	2.40	0.56
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.87	0.56
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.87	0.56
1:A:92:HIS:CD2	1:A:94:GLY:H	2.23	0.56
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.06	0.56
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.85	0.56
4:E:114:ASN:O	4:E:115:ASN:HB3	2.05	0.56
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.84	0.56
2:B:899:ILE:HG22	2:B:900:ALA:H	1.70	0.56
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.19	0.56
9:K:22:ASP:O	9:K:31:VAL:HG13	2.06	0.56
4:E:31:THR:C	4:E:33:GLU:N	2.58	0.56
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.38	0.56
2:B:860:MET:HG2	2:B:861:ASP:N	2.21	0.56
2:B:864:LYS:CB	2:B:871:THR:HA	2.36	0.56
2:B:884:ARG:O	2:B:936:ASP:HB2	2.06	0.56
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.86	0.56
6:H:103:LYS:HZ1	6:H:114:VAL:CG2	2.18	0.56
1:A:534:LEU:O	1:A:574:GLY:HA3	2.05	0.56
1:A:61:ILE:HG22	1:A:62:ASP:H	1.70	0.56
1:A:774:ARG:HB2	1:A:797:LYS:HG2	1.87	0.56
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.88	0.56
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.94	0.56
2:B:648:HIS:N	2:B:648:HIS:CD2	2.72	0.56
5:F:93:ILE:HD13	5:F:148:VAL:HG22	1.88	0.56
6:H:138:GLU:HG2	6:H:139:ASN:N	2.21	0.56
1:A:382:PRO:HD2	5:F:104:ASN:OD1	2.06	0.56
2:B:104:GLU:OE2	10:L:54:ARG:HD3	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:465:TYR:CA	9:K:2:ASN:HB3	2.36	0.56
2:B:35:SER:HA	2:B:811:TYR:HE2	1.70	0.56
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.87	0.56
2:B:953:LEU:HD21	2:B:955:THR:OG1	2.06	0.55
1:A:35:ILE:HG23	1:A:52:GLY:O	2.06	0.55
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.29	0.55
1:A:329:LEU:HD21	2:B:1203:LEU:HD13	1.87	0.55
1:A:388:LEU:HD23	1:A:391:LEU:HD12	1.88	0.55
1:A:694:THR:O	1:A:698:GLN:HG3	2.06	0.55
1:A:69:THR:O	1:A:71:GLN:HG3	2.06	0.55
7:I:111:THR:HG22	7:I:112:SER:H	1.70	0.55
1:A:540:PHE:C	1:A:541:ILE:HD12	2.26	0.55
3:C:22:LEU:HD12	3:C:230:MET:HE3	1.87	0.55
1:A:725:ALA:HA	1:A:728:LYS:CE	2.36	0.55
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.87	0.55
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.29	0.55
2:B:119:LEU:HD22	2:B:953:LEU:CD1	2.37	0.55
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.89	0.55
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.38	0.55
7:I:103:CYS:O	7:I:107:SER:HA	2.07	0.55
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.20	0.55
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.33	0.55
2:B:181:LEU:HD22	2:B:189:LEU:HD23	1.87	0.55
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.31	0.55
1:A:500:GLU:O	1:A:504:LEU:HB2	2.06	0.55
1:A:629:LEU:O	1:A:633:VAL:HG23	2.07	0.55
1:A:1216:ILE:O	1:A:1219:THR:HB	2.07	0.55
2:B:651:LEU:HD11	2:B:707:PRO:CB	2.32	0.55
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.89	0.55
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.42	0.55
4:E:156:LEU:HD21	4:E:197:LYS:HB2	1.89	0.55
1:A:1169:ILE:O	1:A:1173:HIS:HD2	1.89	0.55
1:A:1265:ASN:HD21	2:B:263:GLY:HA2	1.71	0.55
1:A:1167:GLU:O	1:A:1171:GLN:HG3	2.07	0.55
1:A:418:SER:O	1:A:420:ARG:N	2.40	0.55
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.47	0.55
6:H:13:SER:O	6:H:14:GLU:HB2	2.05	0.55
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.22	0.55
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.39	0.55
1:A:108:MET:HA	1:A:210:ILE:HD13	1.87	0.55
1:A:849:MET:HE3	1:A:1436:ILE:HA	1.87	0.55
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:I:111:THR:HG22	7:I:113:ASP:N	2.11	0.54
1:A:595:THR:HG23	1:A:599:SER:HB3	1.88	0.54
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.36	0.54
1:A:1277:GLU:H	1:A:1277:GLU:CD	2.10	0.54
1:A:157:ASP:C	1:A:159:THR:H	2.09	0.54
10:L:39:SER:O	10:L:40:LEU:HD23	2.07	0.54
1:A:919:ILE:HG12	1:A:925:LEU:HD12	1.89	0.54
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.42	0.54
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.89	0.54
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.89	0.54
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.72	0.54
2:B:1003:ALA:O	3:C:177:GLU:HA	2.06	0.54
1:A:1128:GLN:O	1:A:1128:GLN:HG3	2.07	0.54
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.08	0.54
1:A:551:TYR:CE2	9:K:62:LYS:HE2	2.42	0.54
1:A:579:SER:OG	1:A:612:ILE:HG23	2.07	0.54
1:A:1147:THR:HB	7:I:48:LEU:CD1	2.37	0.54
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.23	0.54
6:H:103:LYS:HD3	6:H:114:VAL:HB	1.88	0.54
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.32	0.54
1:A:267:ALA:O	1:A:270:LEU:HB2	2.07	0.54
2:B:843:GLN:N	2:B:994:TYR:O	2.35	0.54
2:B:861:ASP:OD2	2:B:914:LYS:HD2	2.08	0.54
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.89	0.54
1:A:450:LEU:N	1:A:450:LEU:HD12	2.08	0.54
1:A:767:GLN:O	11:M:3:GLY:HA2	2.07	0.54
2:B:1148:LYS:HG3	2:B:1152:MET:CE	2.38	0.54
9:K:20:LYS:HB2	9:K:34:THR:HB	1.88	0.54
1:A:470:LEU:HD11	1:A:487:MET:HE2	1.84	0.54
2:B:103:ASN:HB2	2:B:169:ARG:NH1	2.23	0.54
1:A:57:ARG:C	1:A:68:GLN:HE21	2.11	0.54
6:H:107:VAL:HG12	6:H:107:VAL:O	2.08	0.54
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.90	0.54
2:B:89:GLU:N	2:B:135:ARG:O	2.40	0.54
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.88	0.54
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.23	0.54
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.54
3:C:55:THR:O	3:C:55:THR:HG22	2.08	0.54
1:A:994:GLN:NE2	1:A:1023:ARG:HE	2.06	0.54
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.88	0.54
2:B:272:THR:HG22	2:B:272:THR:O	2.08	0.54
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.38	0.54
1:A:761:MET:O	1:A:803:SER:HB2	2.08	0.54
1:A:112:LYS:HZ1	1:A:165:GLY:H	1.54	0.53
5:F:75:PRO:O	5:F:77:ASP:O	2.25	0.53
1:A:1265:ASN:HD21	2:B:263:GLY:CA	2.20	0.53
1:A:239:LEU:HD23	1:A:240:PRO:N	2.22	0.53
2:B:1099:VAL:C	2:B:1101:ASP:H	2.12	0.53
1:A:327:ALA:HA	1:A:330:LYS:HD2	1.89	0.53
2:B:899:ILE:CG2	2:B:900:ALA:N	2.71	0.53
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.72	0.53
1:A:134:ARG:HD2	1:A:221:SER:O	2.09	0.53
1:A:736:ASN:O	1:A:737:LEU:C	2.46	0.53
2:B:1127:GLY:O	2:B:1128:LEU:HB3	2.08	0.53
1:A:399:HIS:O	1:A:400:PRO:C	2.44	0.53
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.91	0.53
1:A:1336:MET:HE1	1:A:1381:LEU:N	2.22	0.53
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.38	0.53
2:B:952:VAL:HB	10:L:58:LYS:CB	2.36	0.53
4:E:5:ASN:HA	4:E:8:ASN:HB3	1.90	0.53
2:B:230:ALA:N	2:B:231:PRO:HD2	2.24	0.53
1:A:911:SER:O	1:A:978:PRO:HG3	2.09	0.53
6:H:59:ILE:O	6:H:60:ALA:HB3	2.09	0.53
1:A:709:THR:HG23	7:I:94:ASP:HA	1.90	0.53
1:A:1328:TYR:CG	1:A:1329:THR:N	2.75	0.53
4:E:89:GLY:HA2	4:E:117:THR:OG1	2.08	0.53
2:B:313:MET:HE2	2:B:386:LEU:HD22	1.90	0.53
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.44	0.53
1:A:567:LYS:CG	6:H:96:VAL:H	2.21	0.53
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.90	0.53
6:H:89:LEU:O	6:H:91:ASP:N	2.39	0.53
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.44	0.53
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.90	0.53
1:A:907:THR:HG22	1:A:908:LEU:N	2.21	0.53
1:A:243:PRO:C	1:A:245:PRO:HD2	2.29	0.53
1:A:345:VAL:CG1	2:B:1150:ARG:HH22	2.21	0.53
1:A:146:MET:HA	1:A:171:GLN:HB3	1.91	0.53
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.44	0.53
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.39	0.53
2:B:496:ARG:NH2	2:B:541:LEU:HA	2.23	0.53
9:K:47:ARG:HD3	9:K:59:ALA:O	2.08	0.53
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.34	0.53
3:C:22:LEU:HD12	3:C:230:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:167:HIS:HD2	3:C:169:LYS:H	1.57	0.53
3:C:124:LEU:O	3:C:127:ARG:HG2	2.09	0.53
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.91	0.53
5:F:111:LEU:N	5:F:111:LEU:HD12	2.11	0.53
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.50	0.53
1:A:579:SER:HB3	1:A:611:GLN:HA	1.91	0.53
1:A:1392:SER:O	1:A:1393:ASN:HB2	2.09	0.53
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.90	0.53
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.07	0.53
7:I:45:ARG:NH1	7:I:45:ARG:HG2	2.20	0.53
1:A:1199:ARG:O	1:A:1202:MET:HB2	2.09	0.53
1:A:503:GLN:NE2	5:F:90:ARG:HH22	2.06	0.53
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.44	0.53
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.89	0.53
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.29	0.53
8:J:32:GLU:CD	8:J:32:GLU:H	2.13	0.53
6:H:97:MET:CE	6:H:142:LEU:HD23	2.38	0.53
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.07	0.53
1:A:1405:THR:HG23	1:A:1408:ILE:HD12	1.89	0.53
1:A:705:LYS:HD2	1:A:708:MET:HE1	1.91	0.53
4:E:112:TYR:CE1	4:E:115:ASN:HA	2.44	0.53
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.13	0.53
1:A:901:LEU:N	1:A:926:GLN:NE2	2.37	0.52
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.90	0.52
2:B:563:MET:HE3	2:B:580:VAL:HB	1.89	0.52
10:L:27:LEU:HD22	10:L:37:LYS:HD3	1.91	0.52
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.91	0.52
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.91	0.52
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.74	0.52
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.91	0.52
3:C:49:VAL:HG11	3:C:155:LEU:HD11	1.90	0.52
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.74	0.52
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.39	0.52
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.37	0.52
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.28	0.52
1:A:17:VAL:HA	2:B:1215:ARG:O	2.09	0.52
1:A:406:ILE:HA	1:A:411:ASP:O	2.10	0.52
2:B:884:ARG:O	2:B:936:ASP:CB	2.57	0.52
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.09	0.52
2:B:997:GLU:CG	3:C:39:ALA:HB2	2.39	0.52
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.44	0.52
1:A:1341:ILE:CD1	1:A:1376:THR:HG23	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:834:THR:CG2	1:A:1077:THR:OG1	2.57	0.52
2:B:65:GLU:HG3	2:B:65:GLU:O	2.10	0.52
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.40	0.52
2:B:164:LYS:O	2:B:165:VAL:CB	2.57	0.52
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.73	0.52
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.23	0.52
1:A:68:GLN:C	1:A:70:CYS:H	2.13	0.52
1:A:345:VAL:HG13	2:B:1150:ARG:HH12	1.74	0.52
2:B:167:ILE:HG22	2:B:167:ILE:O	2.09	0.52
4:E:176:PRO:O	4:E:212:ARG:HA	2.10	0.52
8:J:48:ARG:O	8:J:52:THR:HB	2.10	0.52
1:A:353:ILE:HG21	1:A:487:MET:CE	2.26	0.52
6:H:125:LEU:HB3	6:H:130:ARG:CZ	2.40	0.52
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.24	0.52
2:B:105:SER:O	2:B:106:ASP:HB2	2.10	0.52
3:C:237:SER:O	3:C:238:ILE:HG13	2.10	0.52
2:B:344:LYS:H	2:B:347:LYS:HZ1	1.57	0.52
2:B:1165:ILE:HG13	2:B:1187:ASN:HD21	1.75	0.52
1:A:1386:ARG:HG3	1:A:1386:ARG:O	2.10	0.52
2:B:906:SER:O	2:B:907:GLY:C	2.47	0.52
2:B:824:ILE:CG1	8:J:48:ARG:HH12	2.23	0.52
6:H:103:LYS:HG2	6:H:115:TYR:H	1.74	0.52
1:A:899:VAL:HG12	1:A:929:LEU:HD13	1.90	0.52
3:C:137:LYS:H	3:C:137:LYS:CD	2.21	0.52
2:B:130:VAL:CG1	2:B:131:ASP:N	2.73	0.52
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.57	0.52
5:F:77:ASP:O	5:F:78:GLN:CB	2.57	0.52
2:B:98:THR:HG22	2:B:99:LYS:H	1.74	0.52
2:B:484:ASN:ND2	2:B:486:TYR:HE1	2.08	0.52
1:A:262:LEU:HD11	1:A:328:ARG:HD2	1.92	0.52
6:H:18:GLY:O	6:H:20:TYR:N	2.42	0.52
2:B:272:THR:OG1	2:B:279:ASP:OD1	2.26	0.52
1:A:72:GLU:HB3	1:A:76:GLU:HB2	1.90	0.52
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.45	0.52
3:C:77:ILE:CA	3:C:129:ILE:HD11	2.38	0.52
10:L:26:THR:CG2	10:L:27:LEU:N	2.67	0.52
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.23	0.52
10:L:68:GLU:CD	10:L:68:GLU:H	2.12	0.52
9:K:111:LEU:N	9:K:111:LEU:HD23	2.24	0.52
1:A:479:ASN:HD22	1:A:479:ASN:C	2.12	0.52
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.92	0.51
3:C:18:VAL:O	3:C:20:PHE:HD2	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:L:51:CYS:C	10:L:53:HIS:H	2.10	0.51
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.91	0.51
1:A:606:LEU:HG	1:A:613:ILE:HB	1.92	0.51
4:E:59:SER:O	4:E:60:PHE:HB3	2.09	0.51
1:A:971:PHE:O	1:A:972:HIS:C	2.46	0.51
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.51
1:A:32:VAL:HB	1:A:57:ARG:CB	2.40	0.51
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.92	0.51
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.26	0.51
4:E:61:GLN:HG2	4:E:62:ALA:N	2.25	0.51
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.24	0.51
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.46	0.51
1:A:998:LEU:HD12	1:A:1001:ARG:HH12	1.74	0.51
1:A:751:SER:O	1:A:752:LYS:O	2.29	0.51
6:H:113:ALA:HB1	6:H:124:ARG:HE	1.74	0.51
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.74	0.51
7:I:72:ASP:O	7:I:81:ARG:HD2	2.10	0.51
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.75	0.51
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.39	0.51
1:A:1336:MET:O	1:A:1336:MET:HG2	2.09	0.51
2:B:737:THR:HG21	7:I:66:PRO:CA	2.41	0.51
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.09	0.51
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.24	0.51
6:H:62:SER:O	6:H:63:LEU:C	2.48	0.51
1:A:540:PHE:HB3	1:A:571:LEU:HG	1.93	0.51
7:I:51:ASN:HB2	7:I:118:ARG:NH1	2.26	0.51
6:H:130:ARG:HA	6:H:133:ASN:CB	2.40	0.51
1:A:328:ARG:HB3	1:A:332:LYS:NZ	2.25	0.51
10:L:34:CYS:C	10:L:36:SER:H	2.12	0.51
1:A:1191:TRP:CE2	1:A:1257:ASP:OD1	2.64	0.51
2:B:794:ASN:C	2:B:795:ILE:HD12	2.30	0.51
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.44	0.51
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.10	0.51
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.91	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.93	0.51
2:B:1006:ILE:HD12	14:B:2021:HOH:O	2.09	0.51
1:A:775:ILE:O	1:A:797:LYS:HE3	2.10	0.51
2:B:210:LYS:HE3	2:B:480:SER:OG	2.11	0.51
2:B:776:GLN:O	2:B:1095:LEU:HA	2.10	0.51
1:A:1395:GLY:C	1:A:1397:LEU:N	2.64	0.51
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.76	0.51
4:E:65:THR:O	4:E:69:ILE:HG13	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:55:ARG:HH11	4:E:55:ARG:HG3	1.75	0.51
1:A:1107:VAL:O	1:A:1107:VAL:HG12	2.09	0.51
1:A:857:ARG:HD3	1:A:861:GLY:O	2.11	0.51
9:K:43:GLY:O	9:K:47:ARG:HB2	2.11	0.51
9:K:21:ILE:CG2	9:K:31:VAL:HG11	2.40	0.51
2:B:1034:VAL:CG2	2:B:1059:LEU:HB2	2.41	0.51
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.51	0.51
10:L:46:VAL:O	10:L:54:ARG:HA	2.11	0.51
1:A:549:MET:SD	1:A:577:ILE:HD12	2.51	0.51
1:A:756:ILE:HD13	1:A:756:ILE:O	2.11	0.51
2:B:54:PHE:HA	2:B:58:THR:HB	1.92	0.51
2:B:847:ASP:O	3:C:65:HIS:HE1	1.93	0.51
1:A:1336:MET:HE1	1:A:1381:LEU:HG	1.92	0.51
1:A:871:ASP:OD2	4:E:204:THR:HG23	2.10	0.51
2:B:1002:THR:CG2	2:B:1006:ILE:H	2.23	0.51
2:B:174:LEU:HD22	2:B:202:TYR:CZ	2.46	0.51
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.92	0.51
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.92	0.51
1:A:961:ARG:O	1:A:965:GLN:HG3	2.10	0.51
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.25	0.51
10:L:38:LEU:O	10:L:39:SER:CB	2.59	0.51
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.26	0.51
1:A:329:LEU:C	1:A:331:GLY:H	2.13	0.51
2:B:1148:LYS:HG3	2:B:1152:MET:HE3	1.93	0.51
2:B:1165:ILE:HD12	2:B:1187:ASN:ND2	2.26	0.51
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.92	0.51
6:H:93:TYR:CD1	6:H:93:TYR:N	2.79	0.51
1:A:754:SER:H	1:A:757:ASN:HD22	1.59	0.50
1:A:869:GLY:O	1:A:870:GLU:HB2	2.12	0.50
1:A:61:ILE:O	1:A:62:ASP:HB2	2.11	0.50
1:A:157:ASP:C	1:A:159:THR:N	2.64	0.50
3:C:89:GLU:O	3:C:90:ASP:HB3	2.10	0.50
4:E:45:LYS:HG2	4:E:45:LYS:O	2.11	0.50
6:H:10:PHE:O	6:H:54:SER:HA	2.11	0.50
1:A:327:ALA:HA	1:A:330:LYS:CD	2.41	0.50
2:B:737:THR:CG2	7:I:66:PRO:CA	2.89	0.50
1:A:858:ASN:ND2	1:A:858:ASN:C	2.65	0.50
8:J:25:LEU:O	8:J:29:GLU:HA	2.12	0.50
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.92	0.50
1:A:1394:THR:HG23	1:A:1398:MET:CE	2.41	0.50
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.77	0.50
5:F:81:THR:CG2	5:F:82:THR:N	2.75	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:606:LEU:HD23	1:A:614:PHE:CE2	2.47	0.50
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.93	0.50
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.11	0.50
1:A:1187:GLN:CG	1:A:1188:GLN:H	2.24	0.50
3:C:175:ALA:O	3:C:176:ILE:HG12	2.12	0.50
1:A:848:ILE:HG12	1:A:864:ILE:CD1	2.41	0.50
1:A:73:GLY:C	1:A:75:ASN:H	2.15	0.50
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.41	0.50
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.25	0.50
2:B:999:MET:HA	2:B:999:MET:CE	2.41	0.50
3:C:258:ILE:HD13	9:K:35:PHE:CE2	2.38	0.50
2:B:733:HIS:O	2:B:735:ALA:N	2.38	0.50
2:B:900:ALA:HB2	10:L:58:LYS:NZ	2.26	0.50
3:C:7:GLN:HG2	9:K:104:ASN:ND2	2.26	0.50
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.11	0.50
2:B:1185:CYS:O	2:B:1186:ASP:HB2	2.12	0.50
2:B:18:PHE:N	2:B:18:PHE:CD2	2.80	0.50
3:C:148:ARG:HH12	8:J:64:ASN:CA	2.20	0.50
2:B:294:ASP:H	7:I:12:ASN:HD22	1.57	0.50
3:C:137:LYS:C	3:C:138:GLU:HG2	2.32	0.50
2:B:969:ARG:NH1	2:B:969:ARG:HB3	2.25	0.50
1:A:557:ASP:OD1	1:A:557:ASP:N	2.45	0.50
7:I:55:THR:O	7:I:58:VAL:HG23	2.11	0.50
1:A:1395:GLY:O	1:A:1397:LEU:N	2.45	0.50
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.47	0.50
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.11	0.50
1:A:128:ILE:HG22	1:A:130:ASP:H	1.77	0.50
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.11	0.50
2:B:357:GLN:OE1	2:B:358:LYS:HE3	2.11	0.50
3:C:179:GLU:CG	3:C:180:TYR:N	2.74	0.50
8:J:24:LEU:O	8:J:30:LEU:HB2	2.11	0.50
1:A:535:THR:O	1:A:575:LYS:HE3	2.12	0.50
2:B:680:THR:CG2	2:B:681:TRP:H	2.24	0.50
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.10	0.50
8:J:12:LYS:HZ1	8:J:17:LYS:HZ1	1.60	0.50
2:B:46:GLN:OE1	2:B:47:GLN:HG2	2.12	0.50
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.52	0.50
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.31	0.50
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.42	0.50
2:B:879:ARG:HE	2:B:885:MET:HE2	1.77	0.50
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.42	0.50
8:J:2:ILE:HG22	8:J:3:VAL:N	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:100:THR:HG23	6:H:138:GLU:CB	2.42	0.50
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.93	0.50
1:A:246:VAL:C	1:A:328:ARG:HH12	2.14	0.50
2:B:235:SER:OG	2:B:236:HIS:HD2	1.95	0.50
1:A:705:LYS:O	1:A:708:MET:HB2	2.11	0.50
8:J:12:LYS:NZ	8:J:17:LYS:HZ1	2.10	0.50
2:B:542:MET:HG3	2:B:747:MET:CE	2.29	0.49
2:B:969:ARG:HE	3:C:59:ALA:HB1	1.77	0.49
1:A:714:PHE:HB2	7:I:97:MET:CE	2.42	0.49
2:B:773:MET:HE3	2:B:985:GLY:HA2	1.93	0.49
2:B:621:GLU:O	2:B:623:GLU:HG3	2.12	0.49
10:L:32:ALA:HB2	10:L:55:ILE:CB	2.42	0.49
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49
10:L:30:ILE:HG22	10:L:31:CYS:H	1.77	0.49
2:B:126:SER:OG	2:B:172:ILE:HD12	2.12	0.49
1:A:1101:LEU:O	1:A:1105:LEU:HG	2.11	0.49
9:K:31:VAL:HG12	9:K:32:VAL:N	2.27	0.49
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.51	0.49
1:A:106:VAL:HG22	1:A:111:GLY:HA2	1.93	0.49
3:C:56:THR:HG23	3:C:57:VAL:N	2.26	0.49
1:A:185:TRP:O	1:A:186:LYS:HB2	2.12	0.49
2:B:134:LYS:HZ1	2:B:446:LEU:HD13	1.77	0.49
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.47	0.49
2:B:983:ARG:HD3	14:B:2018:HOH:O	2.12	0.49
3:C:128:ASN:O	3:C:129:ILE:HG13	2.12	0.49
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.94	0.49
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.52	0.49
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.61	0.49
2:B:735:ALA:HB3	2:B:738:PHE:CZ	2.47	0.49
1:A:767:GLN:HG2	11:M:4:ILE:CD1	2.42	0.49
2:B:305:VAL:O	2:B:305:VAL:HG12	2.12	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.76	0.49
6:H:126:GLU:N	6:H:130:ARG:HH12	2.11	0.49
2:B:241:ARG:HG2	2:B:251:ILE:CG2	2.41	0.49
2:B:979:LYS:CE	2:B:987:LYS:HD2	2.41	0.49
4:E:4:GLU:O	4:E:5:ASN:C	2.51	0.49
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.95	0.49
2:B:809:MET:HG2	2:B:814:PHE:HB3	1.93	0.49
3:C:244:VAL:HG12	3:C:248:ILE:HD11	1.94	0.49
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.94	0.49
2:B:103:ASN:HB2	2:B:169:ARG:HH12	1.77	0.49
7:I:111:THR:HG1	7:I:121:PHE:HE2	1.60	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.49
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.12	0.49
3:C:165:LYS:O	9:K:6:ARG:NH1	2.46	0.49
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.39	0.49
1:A:606:LEU:HD11	1:A:608:ILE:CD1	2.43	0.49
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.46	0.49
10:L:43:THR:O	10:L:43:THR:HG22	2.12	0.49
6:H:103:LYS:NZ	6:H:114:VAL:CG2	2.76	0.49
1:A:329:LEU:HD23	1:A:332:LYS:HB2	1.94	0.49
11:M:4:ILE:H	11:M:4:ILE:HD12	1.78	0.49
1:A:786:HIS:N	1:A:786:HIS:CD2	2.81	0.49
3:C:183:TRP:O	3:C:185:LYS:N	2.41	0.49
2:B:705:MET:CE	2:B:745:PRO:HB3	2.42	0.49
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.48	0.49
1:A:5:GLN:OE1	2:B:1175:LEU:HD12	2.13	0.49
1:A:705:LYS:HB2	1:A:708:MET:CE	2.42	0.49
2:B:784:ASN:OD1	2:B:788:ARG:HD2	2.12	0.49
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.13	0.49
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.28	0.49
1:A:220:THR:O	1:A:222:LEU:O	2.31	0.49
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.94	0.48
6:H:81:PRO:CB	6:H:82:PRO:CD	2.91	0.48
1:A:982:THR:HG22	1:A:984:LYS:N	2.22	0.48
5:F:109:VAL:CG1	5:F:110:ASP:N	2.64	0.48
1:A:332:LYS:O	1:A:336:ILE:HD12	2.13	0.48
2:B:241:ARG:HG2	2:B:251:ILE:HG23	1.93	0.48
7:I:95:THR:HG22	7:I:96:SER:O	2.13	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.95	0.48
1:A:1030:ARG:HD3	1:A:1034:GLU:OE1	2.12	0.48
9:K:82:ASP:OD1	9:K:84:LYS:N	2.44	0.48
1:A:1190:PRO:HG3	7:I:18:GLU:OE2	2.13	0.48
2:B:787:VAL:O	2:B:787:VAL:HG12	2.12	0.48
3:C:227:THR:HG22	3:C:229:TYR:CE1	2.47	0.48
2:B:40:GLU:OE1	2:B:680:THR:CG2	2.60	0.48
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.52	0.48
2:B:35:SER:HA	2:B:811:TYR:CE2	2.47	0.48
2:B:234:ILE:CD1	2:B:257:LYS:HD3	2.43	0.48
2:B:1162:ILE:HD11	2:B:1216:LEU:HD12	1.94	0.48
1:A:1384:VAL:O	1:A:1386:ARG:N	2.46	0.48
4:E:147:HIS:CD2	4:E:149:LEU:H	2.31	0.48
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.13	0.48
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:ASP:N	1:A:56:PRO:CD	2.74	0.48
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.48	0.48
4:E:98:ILE:O	4:E:102:GLU:HG3	2.13	0.48
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.23	0.48
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.43	0.48
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.43	0.48
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.96	0.48
3:C:209:TYR:N	3:C:209:TYR:CD1	2.80	0.48
2:B:1099:VAL:O	2:B:1101:ASP:N	2.45	0.48
2:B:365:THR:HG22	2:B:367:LEU:N	2.16	0.48
10:L:60:ARG:HG2	10:L:61:THR:N	2.27	0.48
1:A:535:THR:HG22	1:A:575:LYS:HE2	1.94	0.48
1:A:982:THR:HG22	1:A:983:ILE:N	2.28	0.48
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.93	0.48
1:A:1111:MET:HE3	1:A:1114:PRO:HA	1.94	0.48
1:A:849:MET:CE	1:A:1437:GLY:H	2.27	0.48
3:C:31:ASN:O	3:C:34:ARG:HB3	2.13	0.48
3:C:148:ARG:HG2	3:C:149:LYS:N	2.29	0.48
1:A:767:GLN:HG3	1:A:768:GLN:O	2.12	0.48
3:C:8:VAL:HG12	3:C:9:LYS:H	1.78	0.48
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.14	0.48
7:I:69:PRO:HG2	7:I:85:PHE:O	2.14	0.48
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.94	0.48
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.14	0.48
1:A:1016:THR:CG2	4:E:206:GLY:HA3	2.43	0.48
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.48	0.48
7:I:111:THR:CG2	7:I:112:SER:N	2.75	0.48
5:F:127:GLU:O	5:F:129:LYS:HG3	2.13	0.48
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.46	0.48
7:I:84:VAL:HG12	7:I:102:VAL:HB	1.94	0.48
9:K:96:ASN:O	9:K:99:GLY:N	2.46	0.48
2:B:882:THR:C	2:B:884:ARG:H	2.17	0.48
3:C:145:CYS:SG	3:C:146:LYS:N	2.86	0.48
1:A:55:ASP:C	1:A:57:ARG:N	2.63	0.48
2:B:859:TYR:CD1	2:B:859:TYR:N	2.82	0.48
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.41	0.48
2:B:969:ARG:HH11	2:B:969:ARG:CB	2.26	0.48
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.49	0.48
1:A:528:LEU:HD23	1:A:751:SER:N	2.29	0.48
6:H:63:LEU:C	6:H:90:ALA:CB	2.82	0.48
1:A:1159:ARG:O	1:A:1170:ILE:HG21	2.12	0.48
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:552:MET:N	2:B:553:PRO:HD2	2.28	0.48
9:K:70:ARG:O	9:K:70:ARG:HG3	2.12	0.48
2:B:339:THR:CG2	2:B:343:ILE:HB	2.44	0.48
2:B:731:VAL:CG1	2:B:732:SER:H	2.27	0.48
1:A:384:ASN:ND2	1:A:388:LEU:HD11	2.29	0.48
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.96	0.48
4:E:64:PRO:HG2	4:E:75:MET:O	2.14	0.48
1:A:179:LEU:HG	1:A:308:ILE:HG21	1.96	0.48
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.49	0.48
2:B:644:GLU:HG3	2:B:654:ARG:NH2	2.26	0.48
1:A:871:ASP:CB	4:E:204:THR:CG2	2.90	0.48
2:B:652:LYS:CE	2:B:688:GLY:O	2.61	0.48
2:B:1160:VAL:HG12	2:B:1161:HIS:H	1.79	0.48
2:B:842:ASN:OD1	2:B:844:SER:HB2	2.14	0.48
1:A:438:ASP:O	1:A:439:ASN:HB2	2.14	0.48
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.96	0.48
4:E:31:THR:C	4:E:33:GLU:H	2.16	0.48
7:I:103:CYS:HB3	7:I:108:HIS:H	1.79	0.48
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.79	0.48
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.49	0.48
2:B:326:ASP:C	2:B:326:ASP:OD2	2.52	0.48
1:A:78:PRO:O	1:A:79:GLY:C	2.52	0.47
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.44	0.47
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.44	0.47
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.95	0.47
4:E:12:LEU:HD21	4:E:58:MET:SD	2.54	0.47
3:C:186:LEU:HD12	3:C:186:LEU:N	2.28	0.47
2:B:332:ASP:OD2	2:B:345:LYS:HG3	2.14	0.47
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.48	0.47
1:A:968:GLN:NE2	1:A:1035:TYR:O	2.47	0.47
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.48	0.47
1:A:528:LEU:O	1:A:531:ILE:HG22	2.14	0.47
1:A:1127:ASP:C	1:A:1129:GLU:N	2.67	0.47
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.14	0.47
4:E:202:SER:O	4:E:205:SER:O	2.33	0.47
3:C:206:ASN:ND2	3:C:229:TYR:CB	2.78	0.47
2:B:235:SER:HA	2:B:261:ARG:HH21	1.79	0.47
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.44	0.47
2:B:221:ASN:O	2:B:222:ILE:HG13	2.14	0.47
2:B:824:ILE:CG1	8:J:48:ARG:NH1	2.77	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.92	0.47
4:E:96:PHE:CE1	4:E:100:ILE:HD11	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:PRO:HA	1:A:270:LEU:CD1	2.40	0.47
2:B:64:CYS:HA	2:B:67:SER:HB3	1.95	0.47
2:B:89:GLU:O	2:B:90:ILE:HB	2.14	0.47
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.49	0.47
2:B:123:THR:OG1	2:B:458:LYS:HE3	2.14	0.47
2:B:254:LEU:HD23	2:B:381:MET:CE	2.45	0.47
2:B:1065:GLN:O	2:B:1065:GLN:HG3	2.14	0.47
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.43	0.47
8:J:12:LYS:HZ1	8:J:17:LYS:NZ	2.11	0.47
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.14	0.47
2:B:46:GLN:H	2:B:46:GLN:HG3	1.30	0.47
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.79	0.47
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.96	0.47
2:B:557:PHE:HZ	2:B:599:THR:HG21	1.79	0.47
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.77	0.47
3:C:68:GLY:O	3:C:169:LYS:HB2	2.14	0.47
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.96	0.47
1:A:1220:PHE:O	1:A:1221:LYS:C	2.53	0.47
2:B:915:THR:HG22	2:B:916:THR:N	2.29	0.47
2:B:863:GLU:O	2:B:864:LYS:O	2.33	0.47
8:J:48:ARG:NH1	8:J:48:ARG:HG2	2.26	0.47
2:B:268:THR:CG2	2:B:270:LYS:HE3	2.36	0.47
2:B:997:GLU:H	2:B:997:GLU:HG3	1.52	0.47
1:A:264:PHE:O	1:A:267:ALA:HB3	2.15	0.47
9:K:7:PHE:HB2	9:K:11:LEU:CD2	2.44	0.47
1:A:537:ARG:HG2	1:A:537:ARG:HH11	1.80	0.47
2:B:581:PHE:HA	2:B:585:VAL:O	2.15	0.47
2:B:274:PRO:HG3	2:B:359:GLU:HB3	1.96	0.47
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.97	0.47
1:A:1295:THR:O	1:A:1295:THR:HG22	2.14	0.47
1:A:1169:ILE:O	1:A:1173:HIS:CD2	2.68	0.47
1:A:10:PRO:HG2	2:B:1192:TYR:CD2	2.49	0.47
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.97	0.47
1:A:532:ARG:NH2	1:A:748:MET:HE3	2.30	0.47
2:B:169:ARG:N	2:B:454:THR:OG1	2.48	0.47
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.36	0.47
3:C:206:ASN:ND2	3:C:229:TYR:HB2	2.30	0.47
1:A:1431:GLY:O	2:B:1148:LYS:HE3	2.15	0.47
2:B:351:TYR:O	2:B:355:ILE:HG13	2.15	0.47
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.96	0.47
2:B:882:THR:HG21	2:B:935:ARG:HA	1.97	0.47
2:B:392:ARG:HH22	7:I:52:ILE:HD11	1.75	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:LYS:NZ	1:A:165:GLY:N	2.54	0.47
7:I:95:THR:CG2	7:I:96:SER:N	2.78	0.47
2:B:315:LYS:N	2:B:316:PRO:HD2	2.29	0.47
1:A:602:ASP:O	1:A:615:GLY:HA2	2.14	0.47
1:A:54:ASN:O	1:A:55:ASP:HB2	2.15	0.47
1:A:517:ASN:HD22	1:A:1364:ASN:HB2	1.80	0.47
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.50	0.47
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.14	0.47
1:A:1400:CYS:SG	1:A:1405:THR:HG21	2.55	0.47
2:B:579:ARG:HG3	2:B:581:PHE:HE1	1.80	0.47
2:B:114:PRO:HD3	2:B:124:TYR:CZ	2.49	0.47
1:A:740:LEU:HD21	3:C:193:TYR:CE2	2.51	0.47
6:H:31:THR:O	6:H:32:THR:CB	2.62	0.47
2:B:882:THR:HG22	2:B:884:ARG:H	1.80	0.46
5:F:111:LEU:O	5:F:113:GLY:N	2.39	0.46
5:F:79:ARG:NH2	5:F:150:GLU:OE2	2.44	0.46
3:C:18:VAL:HG23	3:C:240:VAL:HG12	1.96	0.46
2:B:46:GLN:NE2	2:B:496:ARG:HD2	2.30	0.46
1:A:626:ASN:O	1:A:631:HIS:CD2	2.69	0.46
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.95	0.46
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.81	0.46
6:H:97:MET:HE2	6:H:142:LEU:HD23	1.97	0.46
10:L:60:ARG:HG2	10:L:61:THR:H	1.80	0.46
1:A:465:TYR:CE2	9:K:4:PRO:HD2	2.50	0.46
2:B:296:GLU:O	2:B:300:HIS:CD2	2.66	0.46
1:A:840:ARG:HG3	1:A:1385:THR:CG2	2.45	0.46
1:A:1206:ASP:HB2	1:A:1274:ARG:NH1	2.30	0.46
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.97	0.46
6:H:27:GLU:HA	6:H:38:LEU:O	2.15	0.46
6:H:6:PHE:O	6:H:58:THR:HG23	2.14	0.46
1:A:65:LEU:HD22	1:A:72:GLU:O	2.16	0.46
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.75	0.46
2:B:899:ILE:CG2	2:B:900:ALA:H	2.28	0.46
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.79	0.46
2:B:121:ASN:HA	2:B:207:GLY:CA	2.45	0.46
2:B:324:ILE:HD11	2:B:333:PHE:CG	2.50	0.46
1:A:417:TYR:O	1:A:418:SER:HB2	2.15	0.46
3:C:229:TYR:N	3:C:229:TYR:CD1	2.83	0.46
2:B:122:LEU:HD22	2:B:958:GLN:CG	2.45	0.46
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.96	0.46
6:H:63:LEU:C	6:H:90:ALA:HB3	2.35	0.46
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:266:ASP:O	3:C:267:GLN:HB2	2.15	0.46
1:A:418:SER:C	1:A:420:ARG:H	2.18	0.46
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.79	0.46
7:I:74:GLU:HB2	7:I:81:ARG:NH1	2.30	0.46
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.97	0.46
3:C:179:GLU:HG3	3:C:180:TYR:H	1.79	0.46
2:B:404:LYS:O	2:B:405:ARG:NH1	2.37	0.46
7:I:40:SER:HB2	7:I:41:PRO:HD2	1.97	0.46
1:A:353:ILE:HD13	1:A:487:MET:CE	2.42	0.46
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.72	0.46
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.96	0.46
1:A:416:ARG:HG3	1:A:417:TYR:CD1	2.51	0.46
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.45	0.46
1:A:854:ASN:ND2	1:A:999:VAL:O	2.48	0.46
10:L:33:GLU:C	10:L:35:SER:H	2.18	0.46
2:B:731:VAL:CG1	2:B:732:SER:N	2.77	0.46
1:A:939:ASP:OD1	1:A:1023:ARG:NH1	2.49	0.46
6:H:99:GLY:N	6:H:118:PHE:CD2	2.84	0.46
6:H:127:GLY:O	6:H:128:ASN:HB2	2.15	0.46
3:C:259:LEU:HD21	9:K:91:CYS:HB2	1.97	0.46
7:I:59:VAL:HG12	7:I:61:ASP:H	1.81	0.46
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.64	0.46
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.46
1:A:345:VAL:HG12	2:B:1150:ARG:HH22	1.80	0.46
6:H:100:THR:CB	6:H:138:GLU:HG3	2.46	0.46
2:B:651:LEU:HD23	2:B:710:LEU:HD11	1.96	0.46
3:C:248:ILE:H	3:C:248:ILE:HG13	1.40	0.46
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.46	0.46
1:A:345:VAL:HG13	2:B:1150:ARG:NH1	2.31	0.46
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.38	0.46
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.50	0.46
1:A:265:LYS:O	1:A:269:ILE:HG13	2.15	0.46
2:B:484:ASN:O	2:B:485:ARG:HD2	2.15	0.46
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.98	0.46
1:A:53:LEU:HB3	1:A:54:ASN:OD1	2.16	0.46
1:A:79:GLY:HA3	1:A:245:PRO:CG	2.46	0.46
3:C:20:PHE:HE1	3:C:22:LEU:HG	1.80	0.46
1:A:5:GLN:CG	1:A:6:TYR:H	2.21	0.46
1:A:834:THR:HG22	1:A:1077:THR:OG1	2.16	0.46
2:B:979:LYS:HE2	2:B:979:LYS:HB3	1.81	0.46
6:H:113:ALA:CB	6:H:124:ARG:HH21	2.29	0.46
1:A:786:HIS:CD2	1:A:786:HIS:H	2.34	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:101:MET:SD	2:B:109:THR:HG21	2.55	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.46
2:B:564:GLU:HB2	2:B:589:VAL:HG12	1.96	0.46
2:B:120:ARG:NH2	10:L:54:ARG:HH11	2.14	0.46
1:A:307:ASP:C	1:A:308:ILE:HG13	2.36	0.46
1:A:35:ILE:HB	1:A:83:HIS:O	2.16	0.46
6:H:105:GLU:H	6:H:105:GLU:CD	2.19	0.46
3:C:60:ASP:OD2	10:L:60:ARG:NH2	2.49	0.46
1:A:834:THR:HG21	1:A:1077:THR:OG1	2.16	0.46
2:B:47:GLN:HA	2:B:47:GLN:OE1	2.15	0.46
2:B:996:ARG:HD3	14:B:2017:HOH:O	2.16	0.46
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.15	0.46
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.46	0.45
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.51	0.45
1:A:1391:ARG:O	1:A:1392:SER:HB3	2.16	0.45
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.98	0.45
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.47	0.45
1:A:84:ILE:HG22	1:A:239:LEU:O	2.15	0.45
2:B:484:ASN:ND2	2:B:486:TYR:CE1	2.83	0.45
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.99	0.45
2:B:295:GLY:HA3	7:I:11:ASN:ND2	2.32	0.45
7:I:15:TYR:CD1	7:I:15:TYR:N	2.85	0.45
1:A:368:LYS:HB2	1:A:368:LYS:HE3	1.68	0.45
2:B:904:ARG:HH21	2:B:948:ILE:HD11	1.81	0.45
1:A:857:ARG:CZ	5:F:139:PRO:HG3	2.46	0.45
8:J:7:CYS:HA	8:J:49:MET:HG2	1.98	0.45
2:B:25:ILE:HD12	2:B:653:VAL:CB	2.46	0.45
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.98	0.45
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.52	0.45
1:A:261:ASP:O	1:A:264:PHE:HB2	2.17	0.45
2:B:339:THR:HG23	2:B:343:ILE:HB	1.98	0.45
1:A:738:LYS:NZ	3:C:194:GLU:O	2.42	0.45
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.51	0.45
7:I:59:VAL:HG12	7:I:60:GLN:N	2.31	0.45
1:A:148:CYS:O	1:A:167:CYS:O	2.35	0.45
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.51	0.45
9:K:108:GLU:O	9:K:112:GLN:HG2	2.17	0.45
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.51	0.45
6:H:103:LYS:HA	6:H:115:TYR:HB2	1.98	0.45
1:A:329:LEU:C	1:A:331:GLY:N	2.70	0.45
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.51	0.45
2:B:957:ASN:CG	2:B:958:GLN:N	2.70	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:LYS:NZ	1:A:302:THR:HB	2.30	0.45
6:H:4:THR:HA	6:H:60:ALA:HA	1.98	0.45
3:C:186:LEU:CD1	3:C:186:LEU:N	2.79	0.45
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.97	0.45
4:E:75:MET:O	4:E:76:GLY:O	2.34	0.45
10:L:46:VAL:CG1	10:L:56:LEU:HD12	2.43	0.45
6:H:95:TYR:HE2	6:H:97:MET:CG	2.29	0.45
1:A:381:THR:HG21	1:A:383:TYR:HD1	1.82	0.45
1:A:1431:GLY:HA2	2:B:1152:MET:HE2	1.99	0.45
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.16	0.45
3:C:179:GLU:HG3	3:C:180:TYR:N	2.32	0.45
3:C:231:ASN:C	3:C:231:ASN:OD1	2.54	0.45
1:A:78:PRO:O	1:A:79:GLY:O	2.35	0.45
1:A:541:ILE:HG12	1:A:549:MET:HE1	1.98	0.45
1:A:577:ILE:HG12	1:A:577:ILE:H	1.57	0.45
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.98	0.45
1:A:130:ASP:OD2	1:A:133:LYS:HG3	2.16	0.45
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.46	0.45
4:E:43:LYS:O	4:E:47:CYS:HB2	2.16	0.45
1:A:156:ASP:HB2	1:A:157:ASP:H	1.55	0.45
1:A:90:VAL:HG12	1:A:91:PHE:O	2.17	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.45
6:H:96:VAL:HG22	6:H:143:LEU:HD22	1.97	0.45
4:E:28:TYR:CE2	4:E:78:LEU:HG	2.51	0.45
1:A:982:THR:O	1:A:985:ASP:HB2	2.16	0.45
2:B:341:LEU:CG	2:B:341:LEU:O	2.64	0.45
3:C:100:THR:HG22	3:C:101:LEU:N	2.30	0.45
2:B:863:GLU:OE1	2:B:962:LYS:HD2	2.17	0.45
8:J:48:ARG:CG	8:J:48:ARG:HH11	2.24	0.45
1:A:1392:SER:O	1:A:1393:ASN:CB	2.65	0.45
5:F:140:ASP:C	5:F:140:ASP:OD1	2.56	0.45
6:H:100:THR:HG23	6:H:138:GLU:HB2	1.99	0.45
1:A:407:ARG:O	1:A:408:ASP:C	2.56	0.45
5:F:90:ARG:HD3	5:F:155:LEU:HD12	1.98	0.45
3:C:14:SER:O	3:C:240:VAL:HG21	2.16	0.45
5:F:72:LYS:N	5:F:142:SER:HA	2.31	0.45
9:K:110:ASN:C	9:K:112:GLN:H	2.20	0.45
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.52	0.45
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.99	0.45
9:K:63:VAL:O	9:K:63:VAL:HG22	2.17	0.45
3:C:22:LEU:O	3:C:227:THR:HA	2.17	0.45
2:B:99:LYS:HB3	2:B:180:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:766:ARG:NH1	2:B:985:GLY:O	2.44	0.45
2:B:315:LYS:HB2	2:B:315:LYS:HE3	1.72	0.45
2:B:950:ASP:O	2:B:951:GLN:HG3	2.17	0.45
2:B:771:SER:O	2:B:775:LYS:HE3	2.17	0.45
2:B:169:ARG:HB2	2:B:454:THR:CG2	2.43	0.45
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.47	0.45
1:A:327:ALA:O	1:A:330:LYS:N	2.50	0.45
1:A:1391:ARG:HH21	1:A:1417:GLU:CD	2.20	0.45
1:A:92:HIS:C	1:A:92:HIS:CD2	2.91	0.45
3:C:260:LEU:O	3:C:260:LEU:HD12	2.16	0.45
2:B:25:ILE:HD12	2:B:653:VAL:CG2	2.47	0.44
1:A:78:PRO:O	1:A:78:PRO:HG2	2.17	0.44
2:B:913:GLY:HA2	2:B:938:SER:HB3	2.00	0.44
1:A:164:ARG:HB2	1:A:165:GLY:H	1.60	0.44
1:A:329:LEU:O	1:A:333:GLU:HG2	2.18	0.44
8:J:11:GLY:O	8:J:12:LYS:C	2.55	0.44
1:A:774:ARG:CB	1:A:797:LYS:HG2	2.47	0.44
2:B:69:LEU:HD21	2:B:425:THR:CG2	2.47	0.44
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.99	0.44
4:E:114:ASN:OD1	4:E:115:ASN:N	2.50	0.44
3:C:175:ALA:O	3:C:176:ILE:CG1	2.65	0.44
2:B:805:THR:HB	2:B:809:MET:SD	2.57	0.44
1:A:476:SER:N	1:A:477:PRO:HD2	2.33	0.44
1:A:32:VAL:HG23	1:A:33:ALA:N	2.32	0.44
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.99	0.44
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.52	0.44
2:B:188:ASP:O	2:B:192:LEU:HD12	2.17	0.44
1:A:740:LEU:CD1	1:A:740:LEU:N	2.80	0.44
2:B:590:HIS:HD2	2:B:593:PRO:HA	1.83	0.44
3:C:71:PRO:O	3:C:72:LEU:HD23	2.18	0.44
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.47	0.44
1:A:31:SER:OG	1:A:83:HIS:HB2	2.18	0.44
2:B:276:ILE:HG21	2:B:280:ILE:HD11	2.00	0.44
3:C:226:ASP:O	3:C:227:THR:HB	2.18	0.44
2:B:1096:ARG:HA	2:B:1098:MET:HE2	1.99	0.44
3:C:66:ARG:NH1	3:C:144:ILE:O	2.47	0.44
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.48	0.44
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.51	0.44
1:A:38:PRO:HB3	1:A:270:LEU:CB	2.48	0.44
1:A:871:ASP:CG	4:E:204:THR:HG23	2.38	0.44
6:H:31:THR:O	6:H:32:THR:HB	2.17	0.44
3:C:221:TYR:HE1	3:C:222:LYS:HE3	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:THR:O	1:A:278:THR:HG22	2.18	0.44
6:H:42:ILE:HG23	6:H:95:TYR:CZ	2.53	0.44
7:I:50:THR:HG22	7:I:51:ASN:H	1.82	0.44
6:H:103:LYS:HZ1	6:H:114:VAL:HG21	1.81	0.44
1:A:499:ALA:O	1:A:503:GLN:HB2	2.18	0.44
2:B:876:LYS:HE2	2:B:893:LEU:C	2.37	0.44
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.33	0.44
8:J:12:LYS:NZ	8:J:17:LYS:HZ2	2.16	0.44
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.18	0.44
2:B:692:TYR:O	2:B:693:ILE:HG13	2.18	0.44
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.48	0.44
2:B:860:MET:O	2:B:861:ASP:HB2	2.18	0.44
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.53	0.44
7:I:2:THR:HG22	7:I:2:THR:O	2.17	0.44
1:A:829:VAL:O	1:A:830:LYS:C	2.54	0.44
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.99	0.44
1:A:1295:THR:CG2	1:A:1295:THR:O	2.66	0.44
1:A:642:CYS:O	1:A:645:LEU:HB3	2.18	0.44
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.36	0.44
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.53	0.44
1:A:1204:ASP:C	1:A:1206:ASP:H	2.20	0.44
4:E:26:ARG:NH1	4:E:189:GLY:HA3	2.33	0.44
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.31	0.44
2:B:650:GLU:HG3	2:B:651:LEU:N	2.33	0.44
1:A:666:ILE:CD1	2:B:1030:LEU:HB2	2.47	0.44
10:L:33:GLU:O	10:L:35:SER:N	2.51	0.44
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.99	0.44
3:C:114:TYR:HB3	3:C:140:ASN:O	2.18	0.44
2:B:653:VAL:HG13	2:B:689:LEU:HB3	1.99	0.44
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.83	0.44
1:A:756:ILE:HD13	1:A:756:ILE:C	2.37	0.44
9:K:61:TYR:HA	9:K:72:LYS:O	2.18	0.44
2:B:778:MET:SD	2:B:1094:ARG:HD3	2.57	0.44
2:B:864:LYS:HD3	2:B:871:THR:OG1	2.17	0.43
2:B:104:GLU:CG	10:L:54:ARG:NH1	2.80	0.43
1:A:67:CYS:O	1:A:68:GLN:CB	2.66	0.43
2:B:912:ILE:O	2:B:938:SER:HB2	2.18	0.43
1:A:1217:LYS:C	1:A:1219:THR:H	2.21	0.43
1:A:752:LYS:HD2	2:B:1015:HIS:O	2.18	0.43
7:I:55:THR:HG23	7:I:58:VAL:HG21	2.00	0.43
1:A:360:GLU:OE2	1:A:651:LYS:NZ	2.51	0.43
10:L:49:LYS:HD3	10:L:49:LYS:HA	1.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:J:44:TYR:HA	8:J:47:ARG:CG	2.35	0.43
1:A:709:THR:HB	1:A:712:GLU:HG3	1.99	0.43
3:C:137:LYS:N	3:C:137:LYS:HD2	2.27	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.43
4:E:124:VAL:HB	4:E:125:PRO:HD3	2.00	0.43
1:A:1431:GLY:HA2	2:B:1152:MET:CE	2.48	0.43
1:A:230:ARG:HB3	1:A:232:GLU:HG2	1.99	0.43
2:B:513:GLN:HG3	14:B:2008:HOH:O	2.17	0.43
3:C:17:ASN:N	3:C:17:ASN:HD22	2.16	0.43
4:E:106:GLN:O	4:E:106:GLN:HG2	2.17	0.43
2:B:872:GLU:HA	2:B:915:THR:O	2.18	0.43
6:H:12:VAL:HA	6:H:28:ALA:HB2	2.00	0.43
5:F:111:LEU:C	5:F:113:GLY:H	2.21	0.43
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.09	0.43
1:A:709:THR:HG22	1:A:710:LEU:N	2.33	0.43
1:A:622:VAL:HG13	1:A:622:VAL:O	2.17	0.43
1:A:492:PRO:CB	1:A:497:THR:CG2	2.96	0.43
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.19	0.43
1:A:1422:ARG:HA	1:A:1435:PRO:CG	2.48	0.43
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	2.00	0.43
1:A:367:PRO:CG	1:A:370:ILE:HD12	2.48	0.43
1:A:1127:ASP:C	1:A:1129:GLU:H	2.22	0.43
2:B:108:VAL:HG12	2:B:109:THR:N	2.34	0.43
1:A:1398:MET:O	1:A:1399:ARG:C	2.56	0.43
1:A:903:ASN:C	1:A:903:ASN:HD22	2.22	0.43
1:A:666:ILE:HD11	2:B:1026:LEU:O	2.17	0.43
3:C:241:ASP:O	3:C:245:VAL:HG23	2.19	0.43
1:A:1258:HIS:O	1:A:1259:MET:C	2.56	0.43
2:B:485:ARG:HG3	2:B:485:ARG:HH11	1.84	0.43
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.33	0.43
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.53	0.43
1:A:699:ALA:O	1:A:700:ASN:HB3	2.19	0.43
2:B:642:ASP:C	2:B:644:GLU:H	2.20	0.43
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.00	0.43
11:M:1:ILX:HB	11:M:7:ASN:OD1	2.17	0.43
4:E:94:LYS:O	4:E:98:ILE:HG13	2.18	0.43
1:A:1279:ILE:N	1:A:1279:ILE:HD12	2.32	0.43
1:A:849:MET:HE1	1:A:1436:ILE:HA	2.00	0.43
1:A:367:PRO:HB3	1:A:466:SER:HA	2.01	0.43
9:K:68:PHE:N	9:K:68:PHE:CD1	2.87	0.43
5:F:89:GLU:HB3	5:F:134:ILE:CD1	2.49	0.43
3:C:75:MET:CE	3:C:239:PRO:HG2	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.48	0.43
2:B:397:ASP:OD2	2:B:515:HIS:HE1	2.02	0.43
2:B:172:ILE:CD1	2:B:178:ASN:ND2	2.82	0.43
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.67	0.43
2:B:792:MET:SD	2:B:857:ARG:NH2	2.91	0.43
1:A:1402:PHE:C	1:A:1404:GLU:H	2.20	0.43
2:B:119:LEU:HD22	2:B:953:LEU:HD13	2.01	0.43
2:B:120:ARG:HG3	2:B:955:THR:CG2	2.47	0.43
7:I:50:THR:HG22	7:I:51:ASN:N	2.34	0.43
2:B:205:ILE:HD11	2:B:461:LEU:HB3	1.97	0.43
2:B:324:ILE:HG21	2:B:330:ALA:HA	2.00	0.43
5:F:107:VAL:HG12	5:F:108:PHE:N	2.34	0.43
1:A:324:SER:O	1:A:327:ALA:HB3	2.19	0.43
4:E:102:GLU:C	4:E:104:ASN:H	2.22	0.43
2:B:1002:THR:HG21	14:B:2021:HOH:O	2.18	0.43
2:B:397:ASP:OD2	2:B:515:HIS:CE1	2.72	0.43
2:B:221:ASN:OD1	2:B:242:SER:HA	2.19	0.43
10:L:46:VAL:HG12	10:L:46:VAL:O	2.19	0.43
6:H:103:LYS:HD3	6:H:114:VAL:CG1	2.48	0.43
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.78	0.43
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	2.00	0.43
1:A:73:GLY:O	1:A:75:ASN:N	2.51	0.43
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.52	0.43
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.53	0.43
1:A:987:VAL:O	1:A:991:LYS:HB2	2.19	0.43
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.43
2:B:175:ARG:HB3	2:B:175:ARG:HH11	1.84	0.43
9:K:113:THR:O	9:K:114:LEU:CB	2.55	0.43
9:K:103:THR:CG2	9:K:104:ASN:N	2.82	0.43
1:A:673:GLY:N	1:A:674:PRO:CD	2.82	0.43
8:J:6:ARG:HD3	8:J:11:GLY:O	2.18	0.43
4:E:31:THR:O	4:E:33:GLU:N	2.52	0.43
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.84	0.43
1:A:1161:THR:CG2	1:A:1162:VAL:N	2.81	0.43
10:L:32:ALA:CB	10:L:55:ILE:HB	2.44	0.43
1:A:915:SER:O	1:A:919:ILE:HB	2.18	0.43
1:A:535:THR:HG23	1:A:575:LYS:CG	2.40	0.43
2:B:889:THR:HG22	2:B:890:TYR:N	2.34	0.43
1:A:329:LEU:HD21	2:B:1203:LEU:CD1	2.48	0.43
3:C:169:LYS:NZ	10:L:69:ALA:HB3	2.34	0.43
1:A:1015:VAL:HG13	1:A:1015:VAL:O	2.18	0.43
2:B:544:CYS:HB2	2:B:634:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.39	0.43
2:B:1191:ILE:CG2	2:B:1192:TYR:N	2.82	0.43
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.53	0.43
1:A:1059:HIS:CD2	1:A:1059:HIS:N	2.87	0.43
2:B:887:HIS:O	2:B:888:GLY:C	2.58	0.43
6:H:40:LEU:HD12	6:H:41:ASP:N	2.33	0.42
4:E:117:THR:C	4:E:119:SER:N	2.72	0.42
1:A:16:GLU:HG3	2:B:1220:ARG:HA	2.01	0.42
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.19	0.42
8:J:7:CYS:SG	8:J:49:MET:HE3	2.59	0.42
1:A:179:LEU:CG	1:A:308:ILE:HG21	2.48	0.42
1:A:69:THR:C	1:A:71:GLN:H	2.21	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.54	0.42
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.54	0.42
1:A:13:THR:CA	1:A:1432:GLN:HE22	2.32	0.42
2:B:122:LEU:CD2	2:B:958:GLN:HG3	2.49	0.42
1:A:605:MET:HE2	1:A:607:ILE:HD11	2.01	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.54	0.42
1:A:1059:HIS:HB3	5:F:86:THR:HB	2.00	0.42
2:B:841:MET:O	2:B:993:THR:HA	2.19	0.42
1:A:618:GLU:HB2	1:A:619:LYS:H	1.72	0.42
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.84	0.42
7:I:90:GLN:O	7:I:91:ARG:HD3	2.18	0.42
1:A:500:GLU:OE2	2:B:1145:SER:OG	2.36	0.42
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.19	0.42
5:F:76:LYS:C	5:F:79:ARG:HD2	2.39	0.42
1:A:878:ILE:HG21	1:A:955:PRO:HB2	2.01	0.42
2:B:1165:ILE:CD1	2:B:1187:ASN:HD21	2.32	0.42
10:L:68:GLU:C	10:L:70:ARG:H	2.22	0.42
1:A:142:CYS:C	1:A:144:THR:N	2.73	0.42
2:B:34:ILE:O	2:B:37:PHE:HB3	2.18	0.42
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.18	0.42
2:B:872:GLU:OE1	2:B:914:LYS:HE2	2.19	0.42
2:B:900:ALA:HA	10:L:58:LYS:HD2	2.02	0.42
1:A:1061:GLY:O	1:A:1437:GLY:HA2	2.19	0.42
1:A:714:PHE:HB2	7:I:97:MET:HE2	2.00	0.42
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.52	0.42
1:A:1260:LEU:HA	1:A:1260:LEU:HD12	1.89	0.42
1:A:1394:THR:HG23	1:A:1398:MET:HE3	2.02	0.42
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.41	0.42
10:L:63:ARG:O	10:L:64:LEU:C	2.57	0.42
1:A:1336:MET:CE	1:A:1381:LEU:H	2.31	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:677:ARG:HB2	1:A:677:ARG:HE	1.67	0.42
1:A:464:PRO:HB2	1:A:465:TYR:H	1.67	0.42
1:A:1015:VAL:O	1:A:1015:VAL:CG1	2.67	0.42
7:I:15:TYR:CE1	7:I:30:ARG:HG3	2.55	0.42
1:A:980:ASP:OD2	1:A:1039:LYS:HB3	2.19	0.42
8:J:48:ARG:HG3	8:J:49:MET:N	2.34	0.42
3:C:146:LYS:HB2	8:J:57:ILE:CD1	2.49	0.42
3:C:64:ALA:HA	3:C:67:LEU:HD12	2.01	0.42
7:I:45:ARG:NH1	7:I:47:GLU:OE2	2.52	0.42
1:A:523:ILE:HG23	1:A:527:THR:HB	2.02	0.42
1:A:1201:ALA:O	1:A:1205:LYS:HG3	2.20	0.42
9:K:65:HIS:HD2	9:K:67:PHE:N	1.89	0.42
1:A:418:SER:C	1:A:420:ARG:N	2.73	0.42
2:B:763:GLN:HB2	2:B:1021:MET:CB	2.50	0.42
3:C:39:ALA:O	3:C:164:ALA:HB3	2.20	0.42
3:C:258:ILE:HD11	9:K:42:LEU:CD2	2.49	0.42
1:A:537:ARG:HD2	6:H:20:TYR:CZ	2.55	0.42
1:A:705:LYS:O	1:A:706:HIS:C	2.57	0.42
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.60	0.42
1:A:613:ILE:HG23	6:H:117:SER:HB2	2.01	0.42
1:A:633:VAL:HG21	1:A:645:LEU:HD22	2.02	0.42
2:B:906:SER:CB	2:B:946:ASN:HB2	2.50	0.42
3:C:209:TYR:HD1	3:C:209:TYR:H	1.68	0.42
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.34	0.42
5:F:118:LEU:O	5:F:122:MET:HG3	2.19	0.42
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	2.01	0.42
1:A:351:THR:O	1:A:486:GLU:HA	2.20	0.42
6:H:96:VAL:HG13	6:H:143:LEU:CD2	2.50	0.42
4:E:61:GLN:HB2	4:E:79:TRP:CZ3	2.54	0.42
1:A:324:SER:O	1:A:328:ARG:HG3	2.20	0.42
1:A:463:ILE:HD12	1:A:469:ARG:HD2	2.02	0.42
2:B:550:ASP:OD1	2:B:552:MET:HG3	2.20	0.42
1:A:1143:LEU:HD13	1:A:1273:LEU:HD11	2.00	0.42
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.02	0.42
2:B:287:ARG:HG2	2:B:292:ILE:HA	2.01	0.42
2:B:864:LYS:HD3	2:B:871:THR:HA	2.01	0.42
10:L:38:LEU:HD13	10:L:48:CYS:HA	2.01	0.42
10:L:49:LYS:O	10:L:50:ASP:HB2	2.19	0.42
1:A:93:VAL:HB	1:A:305:ASP:OD2	2.19	0.42
1:A:1438:THR:HG22	2:B:1144:ALA:CB	2.48	0.42
4:E:191:LYS:N	4:E:194:GLU:OE1	2.43	0.42
1:A:849:MET:HE1	1:A:1437:GLY:H	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:606:LEU:HD12	1:A:607:ILE:N	2.35	0.42
2:B:1165:ILE:CD1	2:B:1187:ASN:ND2	2.83	0.42
1:A:1157:ASP:O	1:A:1159:ARG:N	2.53	0.42
6:H:17:PRO:HA	6:H:24:CYS:SG	2.59	0.42
1:A:452:LYS:HG2	14:A:2026:HOH:O	2.18	0.42
2:B:120:ARG:CZ	10:L:54:ARG:HD2	2.49	0.42
1:A:903:ASN:O	1:A:907:THR:OG1	2.37	0.42
7:I:98:VAL:CG2	7:I:113:ASP:HB2	2.45	0.42
10:L:61:THR:HG21	10:L:63:ARG:HD3	2.02	0.42
2:B:1022:THR:CG2	2:B:1022:THR:O	2.67	0.42
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.50	0.42
4:E:124:VAL:CB	4:E:125:PRO:CD	2.98	0.42
1:A:977:LYS:HA	1:A:978:PRO:HD3	1.95	0.42
6:H:62:SER:O	6:H:63:LEU:O	2.37	0.42
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.83	0.42
1:A:106:VAL:CG2	1:A:111:GLY:HA2	2.50	0.42
3:C:264:GLN:C	3:C:266:ASP:H	2.24	0.42
3:C:17:ASN:HA	3:C:232:VAL:O	2.20	0.42
2:B:175:ARG:HB3	2:B:175:ARG:NH1	2.35	0.42
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.01	0.42
1:A:1155:ASP:HA	1:A:1156:PRO:HD2	1.87	0.41
1:A:34:LYS:HA	1:A:83:HIS:CD2	2.55	0.41
1:A:23:SER:CB	1:A:233:TRP:CE2	3.03	0.41
1:A:1111:MET:HE3	1:A:1114:PRO:CA	2.50	0.41
1:A:878:ILE:HG22	1:A:955:PRO:HB2	2.00	0.41
2:B:314:LEU:O	2:B:315:LYS:C	2.58	0.41
1:A:31:SER:CB	1:A:83:HIS:HB2	2.50	0.41
3:C:22:LEU:HA	3:C:22:LEU:HD23	1.87	0.41
2:B:335:GLY:O	2:B:339:THR:HB	2.19	0.41
1:A:829:VAL:O	1:A:832:ALA:N	2.53	0.41
2:B:566:LEU:HD11	2:B:586:TRP:CE2	2.55	0.41
4:E:54:GLN:HB3	4:E:57:MET:HE3	2.01	0.41
6:H:103:LYS:NZ	6:H:114:VAL:CB	2.79	0.41
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.83	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.02	0.41
1:A:140:THR:O	1:A:140:THR:HG22	2.20	0.41
1:A:1191:TRP:CZ3	7:I:43:VAL:HG21	2.48	0.41
1:A:1391:ARG:NH2	1:A:1417:GLU:HG3	2.34	0.41
7:I:59:VAL:CG1	7:I:60:GLN:N	2.83	0.41
2:B:461:LEU:HD12	2:B:466:TRP:HH2	1.85	0.41
2:B:642:ASP:C	2:B:644:GLU:N	2.74	0.41
1:A:760:GLN:HB2	2:B:1021:MET:HE3	2.00	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.56	0.41
1:A:883:LEU:O	1:A:886:ILE:HG22	2.21	0.41
1:A:529:CYS:HB2	2:B:1015:HIS:CE1	2.56	0.41
2:B:344:LYS:H	2:B:347:LYS:NZ	2.18	0.41
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.48	0.41
3:C:76:ASP:OD2	3:C:128:ASN:N	2.49	0.41
2:B:60:GLN:HA	2:B:95:ILE:HD12	2.02	0.41
3:C:167:HIS:CD2	3:C:169:LYS:H	2.36	0.41
2:B:65:GLU:O	2:B:66:ASP:HB2	2.20	0.41
1:A:1001:ARG:O	1:A:1002:GLY:C	2.59	0.41
1:A:858:ASN:ND2	1:A:862:ASN:H	2.18	0.41
7:I:4:PHE:H	7:I:4:PHE:HD2	1.68	0.41
2:B:322:PHE:CZ	7:I:30:ARG:HB2	2.55	0.41
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.20	0.41
1:A:1125:ALA:HB1	1:A:1303:GLU:HB2	2.03	0.41
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.55	0.41
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.92	0.41
7:I:32:CYS:SG	7:I:33:SER:N	2.92	0.41
1:A:778:GLY:HA3	2:B:516:ASN:ND2	2.36	0.41
1:A:1223:ASP:O	1:A:1224:LEU:HB2	2.21	0.41
7:I:111:THR:OG1	7:I:121:PHE:HE2	2.04	0.41
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.50	0.41
2:B:876:LYS:HE3	2:B:894:ASP:C	2.40	0.41
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.55	0.41
3:C:7:GLN:HG2	9:K:104:ASN:HD22	1.85	0.41
1:A:1277:GLU:N	1:A:1277:GLU:CD	2.73	0.41
2:B:1163:CYS:SG	2:B:1165:ILE:N	2.90	0.41
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.56	0.41
1:A:583:PRO:O	1:A:586:ILE:HG12	2.20	0.41
1:A:364:VAL:O	1:A:364:VAL:HG13	2.21	0.41
4:E:14:ARG:O	4:E:17:ARG:HB3	2.20	0.41
1:A:571:LEU:HD22	6:H:46:LEU:HD11	2.02	0.41
1:A:596:THR:C	1:A:598:LEU:H	2.24	0.41
1:A:1336:MET:CE	1:A:1381:LEU:N	2.83	0.41
2:B:616:ILE:O	2:B:624:LEU:HD12	2.21	0.41
9:K:31:VAL:CG1	9:K:32:VAL:N	2.83	0.41
1:A:211:PHE:HA	1:A:214:ILE:CD1	2.50	0.41
1:A:122:MET:CE	1:A:138:ILE:HG23	2.51	0.41
2:B:549:THR:HG22	2:B:628:THR:CG2	2.50	0.41
1:A:592:ASP:HB2	1:A:603:ASN:OD1	2.21	0.41
6:H:100:THR:HG23	6:H:138:GLU:HA	2.03	0.41
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:ASP:OD1	1:A:132:LYS:HB2	2.21	0.41
3:C:206:ASN:N	3:C:206:ASN:OD1	2.54	0.41
2:B:737:THR:CG2	2:B:737:THR:O	2.69	0.41
1:A:719:VAL:HG22	11:M:4:ILE:HD13	2.03	0.41
9:K:24:ASP:OD1	9:K:26:LYS:N	2.54	0.41
2:B:853:SER:OG	2:B:1094:ARG:NH1	2.53	0.41
6:H:145:ARG:O	6:H:146:ARG:OXT	2.39	0.41
2:B:813:LYS:HA	2:B:816:GLU:OE1	2.21	0.41
1:A:70:CYS:O	1:A:70:CYS:SG	2.79	0.41
1:A:1438:THR:O	5:F:92:ARG:HD2	2.20	0.41
6:H:126:GLU:N	6:H:130:ARG:HH22	2.18	0.41
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.36	0.41
2:B:883:LEU:O	2:B:885:MET:HG3	2.21	0.41
2:B:243:ALA:CB	2:B:251:ILE:HG12	2.46	0.41
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.51	0.41
10:L:31:CYS:SG	10:L:34:CYS:SG	3.19	0.41
1:A:1111:MET:HB2	1:A:1114:PRO:HG3	2.02	0.41
1:A:381:THR:CG2	1:A:383:TYR:CD1	3.04	0.41
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.21	0.41
1:A:1166:ASP:O	1:A:1169:ILE:HG22	2.21	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.03	0.41
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.03	0.41
1:A:846:GLU:HA	1:A:1066:VAL:HG23	2.03	0.41
2:B:571:PRO:C	2:B:573:GLN:N	2.73	0.41
1:A:1214:GLU:HA	1:A:1214:GLU:OE1	2.21	0.41
2:B:1221:SER:O	2:B:1222:ARG:O	2.39	0.41
1:A:1254:ALA:HB3	1:A:1256:GLU:HG2	2.02	0.41
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.03	0.41
2:B:915:THR:CG2	2:B:916:THR:N	2.84	0.41
7:I:120:GLN:O	7:I:121:PHE:HB2	2.21	0.41
7:I:2:THR:HG21	7:I:43:VAL:O	2.21	0.41
1:A:825:ILE:O	1:A:828:ALA:HB3	2.21	0.41
1:A:84:ILE:CG2	1:A:239:LEU:O	2.69	0.41
1:A:505:CYS:O	1:A:506:ALA:C	2.59	0.41
2:B:361:LEU:HD21	2:B:381:MET:HE1	2.02	0.41
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.21	0.41
4:E:200:ARG:HD2	14:E:2004:HOH:O	2.20	0.41
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.38	0.41
3:C:33:LEU:O	3:C:33:LEU:HD12	2.21	0.41
2:B:387:LEU:HA	2:B:387:LEU:HD12	1.76	0.41
2:B:882:THR:HB	2:B:934:LYS:O	2.21	0.40
8:J:52:THR:O	8:J:52:THR:HG22	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:25:ILE:HD13	2:B:658:ILE:CD1	2.50	0.40
5:F:111:LEU:H	5:F:111:LEU:CD1	2.06	0.40
1:A:596:THR:HG22	1:A:597:LEU:HD12	2.03	0.40
1:A:596:THR:CG2	1:A:597:LEU:H	2.28	0.40
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.21	0.40
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.02	0.40
1:A:260:ASP:OD1	1:A:261:ASP:N	2.53	0.40
6:H:89:LEU:C	6:H:91:ASP:N	2.72	0.40
1:A:265:LYS:HZ1	1:A:302:THR:HB	1.86	0.40
4:E:169:ARG:NE	5:F:140:ASP:OD2	2.54	0.40
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.21	0.40
4:E:84:ASP:O	4:E:86:PRO:HD3	2.21	0.40
1:A:584:ASN:O	1:A:637:LYS:HE3	2.21	0.40
6:H:12:VAL:HG13	6:H:26:ILE:HG23	2.04	0.40
2:B:1065:GLN:HE22	2:B:1067:ARG:CB	2.35	0.40
2:B:874:PHE:HA	2:B:913:GLY:O	2.21	0.40
3:C:108:GLU:HG2	3:C:149:LYS:HD2	2.01	0.40
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.76	0.40
1:A:867:ILE:HG22	4:E:208:TYR:HE1	1.86	0.40
6:H:36:CYS:HB2	6:H:129:TYR:HH	1.85	0.40
2:B:879:ARG:HE	2:B:885:MET:CE	2.33	0.40
1:A:1341:ILE:HD11	1:A:1376:THR:O	2.21	0.40
4:E:198:ILE:HD12	4:E:212:ARG:HG3	2.03	0.40
4:E:116:ILE:HG22	4:E:117:THR:H	1.85	0.40
3:C:209:TYR:N	3:C:209:TYR:HD1	2.19	0.40
1:A:835:GLY:O	1:A:839:ARG:HG3	2.21	0.40
6:H:51:ALA:O	6:H:53:ASP:N	2.54	0.40
6:H:10:PHE:HB3	6:H:28:ALA:HB1	2.04	0.40
1:A:112:LYS:HD2	1:A:165:GLY:HA3	2.03	0.40
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.03	0.40
1:A:535:THR:CG2	1:A:535:THR:O	2.66	0.40
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.52	0.40
2:B:788:ARG:CB	2:B:788:ARG:HH11	2.34	0.40
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.51	0.40
2:B:590:HIS:CD2	2:B:591:ARG:O	2.74	0.40
2:B:610:ASN:OD1	2:B:611:PRO:HD2	2.22	0.40
3:C:63:ILE:HD13	3:C:153:LEU:HD11	2.04	0.40
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	2.21	0.40
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.51	0.40
2:B:1153:GLU:CG	2:B:1154:ALA:N	2.77	0.40
3:C:73:GLN:NE2	3:C:75:MET:CB	2.84	0.40
3:C:39:ALA:HA	3:C:164:ALA:CB	2.41	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1434:ALA:C	1:A:1436:ILE:H	2.22	0.40
2:B:51:PHE:O	2:B:54:PHE:HB3	2.22	0.40
8:J:23:ASN:C	8:J:25:LEU:N	2.74	0.40
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.87	0.40
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.21	0.40
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.56	0.40
4:E:136:ASN:O	4:E:139:ALA:N	2.53	0.40
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.56	0.40
4:E:178:ILE:O	4:E:178:ILE:HG23	2.22	0.40
2:B:864:LYS:HB3	2:B:871:THR:CA	2.50	0.40
1:A:1394:THR:HG23	1:A:1398:MET:SD	2.62	0.40
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.49	0.40
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.74	0.40
1:A:767:GLN:HG2	11:M:4:ILE:HD12	2.03	0.40
1:A:84:ILE:O	1:A:84:ILE:HG23	2.22	0.40
2:B:242:SER:OG	2:B:362:PRO:HD2	2.22	0.40
1:A:787:PHE:CZ	1:A:796:SER:HA	2.56	0.40
3:C:99:LEU:HD12	3:C:99:LEU:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:L:28:LYS:NZ	10:L:28:LYS:NZ[3_655]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	1348/1733 (78%)	1160 (86%)	134 (10%)	54 (4%)	5 14
2	B	1062/1224 (87%)	931 (88%)	107 (10%)	24 (2%)	10 31
3	C	264/318 (83%)	223 (84%)	30 (11%)	11 (4%)	4 13
4	E	211/215 (98%)	180 (85%)	23 (11%)	8 (4%)	5 15
5	F	82/155 (53%)	71 (87%)	10 (12%)	1 (1%)	19 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	129/146 (88%)	88 (68%)	23 (18%)	18 (14%)	0	1
7	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	14	42
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	25	63
10	L	43/70 (61%)	23 (54%)	13 (30%)	7 (16%)	0	0
11	M	4/8 (50%)	4 (100%)	0	0	100	100
All	All	3438/4181 (82%)	2938 (86%)	374 (11%)	126 (4%)	5	16

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	56	PRO
1	A	399	HIS
1	A	464	PRO
1	A	465	TYR
1	A	466	SER
1	A	567	LYS
1	A	752	LYS
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1392	SER
1	A	1393	ASN
2	B	864	LYS
2	B	879	ARG
2	B	1100	ASP
2	B	1222	ARG
3	C	4	GLU
3	C	206	ASN
4	E	4	GLU
4	E	5	ASN
4	E	59	SER
6	H	19	ARG
6	H	52	GLN
6	H	81	PRO
6	H	88	SER
6	H	105	GLU
6	H	128	ASN
6	H	138	GLU

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Mol	Chain	Res	Type
10	L	39	SER
10	L	64	LEU
1	A	35	ILE
1	A	57	ARG
1	A	58	LEU
1	A	67	CYS
1	A	71	GLN
1	A	74	MET
1	A	79	GLY
1	A	84	ILE
1	A	400	PRO
1	A	419	LYS
1	A	626	ASN
1	A	628	GLY
1	A	846	GLU
1	A	885	THR
1	A	1202	MET
1	A	1221	LYS
1	A	1396	ALA
1	A	1399	ARG
1	A	1400	CYS
2	B	165	VAL
2	B	266	ALA
2	B	367	LEU
2	B	646	LEU
2	B	648	HIS
2	B	1066	SER
3	C	137	LYS
3	C	184	ASN
3	C	215	GLU
3	C	231	ASN
3	C	245	VAL
4	E	50	MET
4	E	76	GLY
6	H	18	GLY
6	H	90	ALA
10	L	34	CYS
10	L	35	SER
10	L	52	GLY
10	L	59	ALA
1	A	68	GLN
1	A	72	GLU

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Mol	Chain	Res	Type
1	A	308	ILE
1	A	408	ASP
1	A	409	SER
1	A	418	SER
1	A	467	THR
1	A	1278	ASN
2	B	666	TYR
2	B	734	HIS
2	B	906	SER
2	B	907	GLY
2	B	1099	VAL
3	C	90	ASP
4	E	115	ASN
5	F	73	ALA
6	H	32	THR
6	H	77	ARG
6	H	82	PRO
6	H	83	GLN
6	H	139	ASN
7	I	3	THR
9	K	111	LEU
1	A	599	SER
1	A	829	VAL
2	B	124	TYR
2	B	323	VAL
2	B	369	GLY
2	B	883	LEU
3	C	9	LYS
3	C	10	ILE
3	C	267	GLN
6	H	3	ASN
6	H	8	ASP
1	A	307	ASP
1	A	538	ASP
1	A	904	THR
1	A	958	VAL
1	A	1200	ALA
2	B	90	ILE
2	B	909	ASP
4	E	103	LYS
4	E	124	VAL
6	H	14	GLU

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Mol	Chain	Res	Type
10	L	56	LEU
1	A	283	GLY
1	A	737	LEU
1	A	1172	LEU
1	A	1257	ASP
2	B	464	GLY
2	B	1103	ILE
7	I	76	PRO
1	A	166	GLY
1	A	1002	GLY
1	A	246	VAL
2	B	647	GLY
6	H	59	ILE

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 X-ray entries followed by that with respect to entries of similar resolution. 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	1196/1520 (79%)	1116 (93%)	80 (7%)	23	55
2	B	940/1061 (89%)	899 (96%)	41 (4%)	39	75
3	C	234/274 (85%)	221 (94%)	13 (6%)	30	64
4	E	195/197 (99%)	190 (97%)	5 (3%)	59	90
5	F	74/137 (54%)	71 (96%)	3 (4%)	41	77
6	H	117/128 (91%)	114 (97%)	3 (3%)	59	90
7	I	116/116 (100%)	108 (93%)	8 (7%)	22	53
8	J	60/65 (92%)	57 (95%)	3 (5%)	34	70
9	K	99/102 (97%)	88 (89%)	11 (11%)	9	25
10	L	40/57 (70%)	34 (85%)	6 (15%)	4	12
11	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3073/3659 (84%)	2900 (94%)	173 (6%)	30	64

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	70	CYS
1	A	71	GLN
1	A	93	VAL
1	A	116	ASP
1	A	117	GLU
1	A	156	ASP
1	A	159	THR
1	A	164	ARG
1	A	208	LEU
1	A	226	GLU
1	A	247	ARG
1	A	351	THR
1	A	373	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	434	ARG
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	465	TYR
1	A	467	THR
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	479	ASN
1	A	493	GLN
1	A	497	THR
1	A	503	GLN
1	A	504	LEU
1	A	515	GLN
1	A	544	ASP
1	A	557	ASP
1	A	597	LEU
1	A	603	ASN
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	672	ASP
1	A	703	THR

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Mol	Chain	Res	Type
1	A	710	LEU
1	A	741	ASN
1	A	756	ILE
1	A	821	ARG
1	A	822	GLU
1	A	831	THR
1	A	855	THR
1	A	858	ASN
1	A	873	MET
1	A	882	SER
1	A	885	THR
1	A	903	ASN
1	A	919	ILE
1	A	920	LEU
1	A	969	GLN
1	A	1015	VAL
1	A	1030	ARG
1	A	1048	ASN
1	A	1060	PRO
1	A	1118	VAL
1	A	1122	PRO
1	A	1128	GLN
1	A	1240	CYS
1	A	1255	GLU
1	A	1257	ASP
1	A	1264	GLU
1	A	1297	GLU
1	A	1308	THR
1	A	1318	THR
1	A	1325	THR
1	A	1336	MET
1	A	1366	ARG
1	A	1385	THR
1	A	1387	HIS
1	A	1419	ASP
1	A	1426	GLU
1	A	1438	THR
2	B	18	PHE
2	B	20	ASP
2	B	46	GLN
2	B	131	ASP
2	B	183	GLU

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Mol	Chain	Res	Type
2	B	194	GLU
2	B	217	ARG
2	B	261	ARG
2	B	268	THR
2	B	277	LYS
2	B	337	ARG
2	B	339	THR
2	B	424	LEU
2	B	466	TRP
2	B	485	ARG
2	B	490	SER
2	B	513	GLN
2	B	531	GLN
2	B	540	SER
2	B	547	VAL
2	B	567	GLU
2	B	589	VAL
2	B	644	GLU
2	B	648	HIS
2	B	653	VAL
2	B	736	THR
2	B	886	LYS
2	B	939	THR
2	B	951	GLN
2	B	963	PHE
2	B	974	PRO
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1060	ARG
2	B	1065	GLN
2	B	1150	ARG
2	B	1159	ARG
2	B	1189	ILE
2	B	1211	ASN
2	B	1222	ARG
3	C	26	ASP
3	C	50	GLU
3	C	52	GLU
3	C	57	VAL
3	C	77	ILE
3	C	88	CYS

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Mol	Chain	Res	Type
3	C	129	ILE
3	C	138	GLU
3	C	163	ILE
3	C	206	ASN
3	C	209	TYR
3	C	233	GLU
3	C	240	VAL
4	E	104	ASN
4	E	123	LEU
4	E	149	LEU
4	E	196	VAL
4	E	204	THR
5	F	82	THR
5	F	110	ASP
5	F	111	LEU
6	H	82	PRO
6	H	91	ASP
6	H	93	TYR
7	I	4	PHE
7	I	30	ARG
7	I	45	ARG
7	I	50	THR
7	I	52	ILE
7	I	70	ARG
7	I	87	GLN
7	I	98	VAL
8	J	1	MET
8	J	28	ASP
8	J	48	ARG
9	K	11	LEU
9	K	29	ASN
9	K	47	ARG
9	K	50	LEU
9	K	63	VAL
9	K	68	PHE
9	K	73	LEU
9	K	76	GLN
9	K	81	TYR
9	K	103	THR
9	K	114	LEU
10	L	27	LEU
10	L	42	ARG

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Mol	Chain	Res	Type
10	L	50	ASP
10	L	61	THR
10	L	65	VAL
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	68	GLN
1	A	71	GLN
1	A	92	HIS
1	A	118	HIS
1	A	171	GLN
1	A	299	HIS
1	A	358	ASN
1	A	390	GLN
1	A	394	ASN
1	A	397	ASN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	631	HIS
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	854	ASN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1124	HIS
1	A	1173	HIS
1	A	1218	GLN
1	A	1265	ASN
1	A	1364	ASN

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Mol	Chain	Res	Type
1	A	1432	GLN
2	B	46	GLN
2	B	115	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	255	GLN
2	B	300	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	648	HIS
2	B	657	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	786	ASN
2	B	958	GLN
2	B	1015	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1176	ASN
2	B	1177	HIS
2	B	1187	ASN
2	B	1193	GLN
2	B	1211	ASN
3	C	17	ASN
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS

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Mol	Chain	Res	Type
3	C	140	ASN
3	C	167	HIS
3	C	203	GLN
3	C	242	GLN
3	C	252	GLN
4	E	101	GLN
4	E	104	ASN
4	E	147	HIS
6	H	11	GLN
6	H	128	ASN
6	H	133	ASN
7	I	11	ASN
7	I	12	ASN
7	I	114	GLN
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
11	ILX	M	1	11	9,9,10	5.11	4 (44%)	9,11,13	1.71	3 (33%)
11	TRX	M	2	11	16,16,17	5.37	8 (50%)	20,22,24	1.51	6 (30%)
11	CSX	M	6	11	4,6,7	14.45	3 (75%)	3,6,8	4.12	1 (33%)
11	HYP	M	8	11	8,8,9	6.96	3 (37%)	8,10,12	1.77	2 (25%)

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
11	ILX	M	1	11	-	0/10/12/14	0/0/0/0
11	TRX	M	2	11	-	0/4/6/8	0/0/2/2
11	CSX	M	6	11	-	0/2/5/7	0/0/0/0
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	6	CSX	O-C	27.81	1.30	1.11
11	M	2	TRX	O-C	18.83	1.24	1.11
11	M	8	HYP	O-C	18.44	1.24	1.11
11	M	1	ILX	O-C	13.82	1.20	1.11
11	M	6	CSX	CB-CA	6.24	1.63	1.53
11	M	8	HYP	CA-C	5.68	1.59	1.48
11	M	2	TRX	CZ2-CH2	5.00	1.47	1.37
11	M	6	CSX	CA-C	4.72	1.57	1.48
11	M	2	TRX	CA-C	4.34	1.56	1.48
11	M	1	ILX	CB-CA	4.14	1.60	1.53
11	M	1	ILX	CA-C	3.71	1.55	1.48
11	M	2	TRX	CZ2-CE2	3.52	1.49	1.39
11	M	8	HYP	CA-N	3.37	1.60	1.46
11	M	2	TRX	CD1-CG	3.37	1.43	1.37
11	M	2	TRX	CD2-CE2	3.21	1.46	1.41
11	M	2	TRX	CD1-NE1	2.95	1.42	1.37
11	M	1	ILX	OG1-CG1	2.84	1.49	1.43
11	M	2	TRX	CZ3-CH2	2.73	1.44	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	6	CSX	C-CA-N	-6.95	106.89	113.83
11	M	1	ILX	CG2-CB-CG1	-3.82	105.72	111.26
11	M	8	HYP	C-CA-N	3.19	116.77	110.86
11	M	2	TRX	OH2-CH2-CZ3	-2.89	111.82	120.05
11	M	2	TRX	C-CA-N	2.60	116.42	113.83
11	M	2	TRX	CH2-CZ2-CE2	-2.40	116.37	119.14
11	M	8	HYP	CB-CA-N	-2.39	100.92	104.59
11	M	1	ILX	OD1-CD1-CG1	2.35	116.32	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	2	TRX	CD1-CG-CD2	-2.22	104.56	107.29
11	M	1	ILX	C-CA-N	-2.09	108.54	111.94
11	M	2	TRX	OH2-CH2-CZ2	2.06	127.15	121.07
11	M	2	TRX	CB-CA-N	-2.05	102.49	112.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1366/1733 (78%)	-0.02	74 (5%)	25 25	18, 48, 107, 137	0
2	B	1082/1224 (88%)	0.01	77 (7%)	16 14	20, 46, 105, 128	0
3	C	266/318 (83%)	-0.08	3 (1%)	77 78	30, 53, 83, 124	0
4	E	213/215 (99%)	0.02	6 (2%)	50 52	22, 59, 99, 109	0
5	F	84/155 (54%)	-0.24	2 (2%)	56 57	24, 44, 67, 82	0
6	H	133/146 (91%)	1.21	33 (24%)	1 1	64, 94, 122, 125	0
7	I	122/122 (100%)	0.03	7 (5%)	23 23	30, 51, 89, 106	0
8	J	65/70 (92%)	-0.34	1 (1%)	70 71	26, 47, 76, 85	0
9	K	114/120 (95%)	-0.12	4 (3%)	42 42	31, 60, 79, 97	0
10	L	45/70 (64%)	1.12	10 (22%)	1 1	49, 86, 108, 110	0
11	M	8/8 (100%)	1.10	0	100 100	72, 78, 83, 84	0
All	All	3498/4181 (83%)	0.04	217 (6%)	20 19	18, 50, 105, 137	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	13.5
1	A	1390	ASN	10.8
2	B	882	THR	9.7
1	A	1402	PHE	8.8
2	B	866	TYR	8.3
2	B	247	GLY	8.3
1	A	1391	ARG	8.0
3	C	268	ASP	7.8
2	B	137	TYR	7.6
1	A	1389	PHE	7.5
2	B	643	ASP	7.0
1	A	1092	LYS	6.5

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Mol	Chain	Res	Type	RSRZ
6	H	131	ASN	6.5
3	C	267	GLN	6.5
1	A	62	ASP	6.4
1	A	1404	GLU	6.3
1	A	166	GLY	6.2
1	A	66	LYS	6.2
1	A	1388	GLY	6.1
2	B	883	LEU	6.1
2	B	869	SER	6.0
1	A	1393	ASN	5.9
2	B	1223	ASP	5.8
2	B	1221	SER	5.8
2	B	1184	GLY	5.8
2	B	1155	SER	5.8
6	H	104	PHE	5.8
2	B	1156	ASP	5.7
6	H	139	ASN	5.7
7	I	1	MET	5.6
6	H	146	ARG	5.3
2	B	246	LYS	5.2
1	A	49	LYS	5.1
1	A	1081	LEU	5.1
1	A	1386	ARG	5.1
2	B	734	HIS	5.1
2	B	1100	ASP	5.1
1	A	68	GLN	5.1
1	A	311	GLN	5.0
1	A	65	LEU	5.0
2	B	249	ARG	4.9
1	A	1403	GLU	4.7
1	A	1450	LEU	4.7
1	A	1175	SER	4.7
2	B	248	SER	4.7
2	B	1105	ALA	4.7
2	B	1106	ARG	4.7
1	A	1387	HIS	4.6
1	A	186	LYS	4.6
2	B	870	ILE	4.6
6	H	87	ARG	4.5
6	H	107	VAL	4.5
2	B	733	HIS	4.5
6	H	85	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	1080	THR	4.5
2	B	1109	GLY	4.4
2	B	722	ASP	4.4
2	B	868	MET	4.4
6	H	88	SER	4.3
2	B	265	SER	4.3
1	A	310	GLY	4.3
2	B	250	PHE	4.2
1	A	334	GLY	4.2
10	L	43	THR	4.2
4	E	50	MET	4.1
1	A	1392	SER	4.1
10	L	50	ASP	4.1
2	B	1103	ILE	4.1
2	B	1110	PRO	4.1
2	B	884	ARG	4.0
2	B	18	PHE	4.0
4	E	129	PRO	4.0
6	H	84	ALA	4.0
10	L	26	THR	4.0
8	J	65	PRO	4.0
1	A	260	ASP	3.9
1	A	64	ASN	3.9
7	I	119	THR	3.9
2	B	1104	HIS	3.8
2	B	1101	ASP	3.8
1	A	61	ILE	3.8
2	B	1154	ALA	3.8
10	L	27	LEU	3.8
2	B	70	ILE	3.7
6	H	108	SER	3.7
2	B	865	LYS	3.7
6	H	132	LEU	3.7
7	I	118	ARG	3.7
1	A	1399	ARG	3.7
2	B	1099	VAL	3.6
2	B	1102	LYS	3.6
2	B	1108	ARG	3.6
1	A	187	LYS	3.6
1	A	281	HIS	3.5
1	A	37	PHE	3.5
9	K	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1174	PHE	3.5
2	B	1224	PHE	3.5
6	H	83	GLN	3.5
1	A	1448	GLU	3.5
1	A	309	ALA	3.5
1	A	75	ASN	3.5
4	E	49	SER	3.4
1	A	330	LYS	3.4
2	B	136	THR	3.4
5	F	155	LEU	3.4
6	H	3	ASN	3.3
1	A	57	ARG	3.3
6	H	82	PRO	3.3
1	A	36	ARG	3.3
1	A	63	ARG	3.3
1	A	1401	SER	3.3
2	B	465	ASN	3.2
2	B	871	THR	3.2
6	H	2	SER	3.2
1	A	305	ASP	3.2
2	B	712	PRO	3.2
2	B	106	ASP	3.2
6	H	86	ASP	3.2
1	A	308	ILE	3.1
2	B	1181	GLU	3.1
2	B	1183	LYS	3.1
1	A	72	GLU	3.1
2	B	1153	GLU	3.1
2	B	103	ASN	3.1
10	L	62	LYS	3.0
7	I	122	SER	3.0
2	B	429	PHE	3.0
2	B	933	SER	3.0
1	A	332	LYS	3.0
2	B	935	ARG	2.9
2	B	135	ARG	2.9
1	A	336	ILE	2.9
1	A	157	ASP	2.9
5	F	72	LYS	2.9
2	B	1189	ILE	2.9
2	B	887	HIS	2.9
3	C	215	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	266	ALA	2.8
1	A	74	MET	2.8
1	A	247	ARG	2.8
2	B	89	GLU	2.8
6	H	110	ASP	2.8
6	H	127	GLY	2.8
7	I	120	GLN	2.8
4	E	130	ALA	2.8
1	A	196	GLU	2.8
4	E	7	ARG	2.7
2	B	895	ASP	2.7
1	A	328	ARG	2.7
1	A	307	ASP	2.7
2	B	875	GLU	2.7
10	L	40	LEU	2.6
1	A	60	SER	2.6
2	B	263	GLY	2.6
2	B	876	LYS	2.6
1	A	1094	VAL	2.5
1	A	1400	CYS	2.5
1	A	1222	ASN	2.5
1	A	129	LYS	2.5
6	H	109	LYS	2.5
2	B	723	VAL	2.5
1	A	1221	LYS	2.5
6	H	106	GLU	2.4
2	B	1186	ASP	2.4
6	H	111	LEU	2.4
10	L	33	GLU	2.4
6	H	130	ARG	2.4
2	B	264	SER	2.4
2	B	963	PHE	2.4
9	K	54	ARG	2.4
6	H	29	ALA	2.4
1	A	1256	GLU	2.3
9	K	2	ASN	2.3
2	B	426	LYS	2.3
2	B	1222	ARG	2.3
7	I	74	GLU	2.3
1	A	1188	GLN	2.3
2	B	881	ASN	2.2
6	H	133	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1449	SER	2.2
1	A	39	GLU	2.2
1	A	6	TYR	2.2
4	E	51	GLY	2.2
10	L	49	LYS	2.2
2	B	66	ASP	2.2
2	B	1179	GLN	2.2
10	L	45	ALA	2.2
6	H	76	THR	2.2
1	A	1359	ASP	2.2
9	K	14	GLU	2.2
2	B	1172	ILE	2.2
1	A	105	CYS	2.1
2	B	463	THR	2.1
2	B	646	LEU	2.1
2	B	732	SER	2.1
2	B	108	VAL	2.1
10	L	42	ARG	2.1
7	I	116	ASN	2.1
2	B	879	ARG	2.1
6	H	77	ARG	2.1
6	H	138	GLU	2.1
1	A	103	CYS	2.1
1	A	71	GLN	2.1
1	A	1112	LYS	2.1
6	H	40	LEU	2.1
1	A	335	ARG	2.1
2	B	430	ARG	2.1
1	A	1255	GLU	2.1
6	H	13	SER	2.1
1	A	839	ARG	2.0
1	A	626	ASN	2.0
6	H	33	GLN	2.0
6	H	52	GLN	2.0
6	H	126	GLU	2.0
2	B	641	GLU	2.0
6	H	143	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	ILX	M	1	10/11	0.34	5.55	72,74,79,80	0
11	TRX	M	2	15/16	0.23	0.85	75,77,79,80	0
11	HYP	M	8	8/9	0.20	0.02	70,72,72,73	0
11	CSX	M	6	7/8	0.22	-0.57	80,82,84,86	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	MN	A	3009	1/1	0.32	3.65	149,149,149,149	0
12	ZN	B	3007	1/1	0.06	-1.27	64,64,64,64	0
12	ZN	C	3002	1/1	0.09	-1.28	49,49,49,49	0
12	ZN	A	3008	1/1	0.13	-1.52	81,81,81,81	0
12	ZN	I	3004	1/1	0.07	-1.60	62,62,62,62	0
12	ZN	J	3001	1/1	0.12	-1.71	46,46,46,46	0
12	ZN	L	3005	1/1	0.05	-1.81	86,86,86,86	0
12	ZN	I	3003	1/1	0.09	-1.98	45,45,45,45	0
12	ZN	A	3006	1/1	0.09	-2.14	64,64,64,64	0

6.5 Other polymers

There are no such residues in this entry.