



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:40 pm BST

PDB ID : 1I50
Title : RNA POLYMERASE II CRYSTAL FORM II AT 2.8 Å RESOLUTION
Authors : Cramer, P.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2001-02-23
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

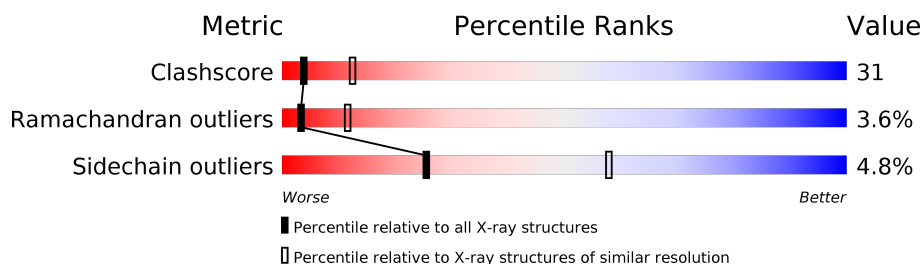
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

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	

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Mol	Chain	Length	Quality of chain
9	K	120	<div><div></div><div>52%</div><div>39%</div><div>• 5%</div></div>
10	L	70	<div><div></div><div>16%</div><div>37%</div><div>11%</div><div>•</div><div>34%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28366 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1419	Total	C	N	O	S	0	0	0
			11154	7023	1952	2118	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1094	Total	C	N	O	S	0	0	0
			8711	5525	1519	1614	53			

- 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	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- 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	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total 2	Zn 2	0	0
11	L	1	Total 1	Zn 1	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 13 is water.

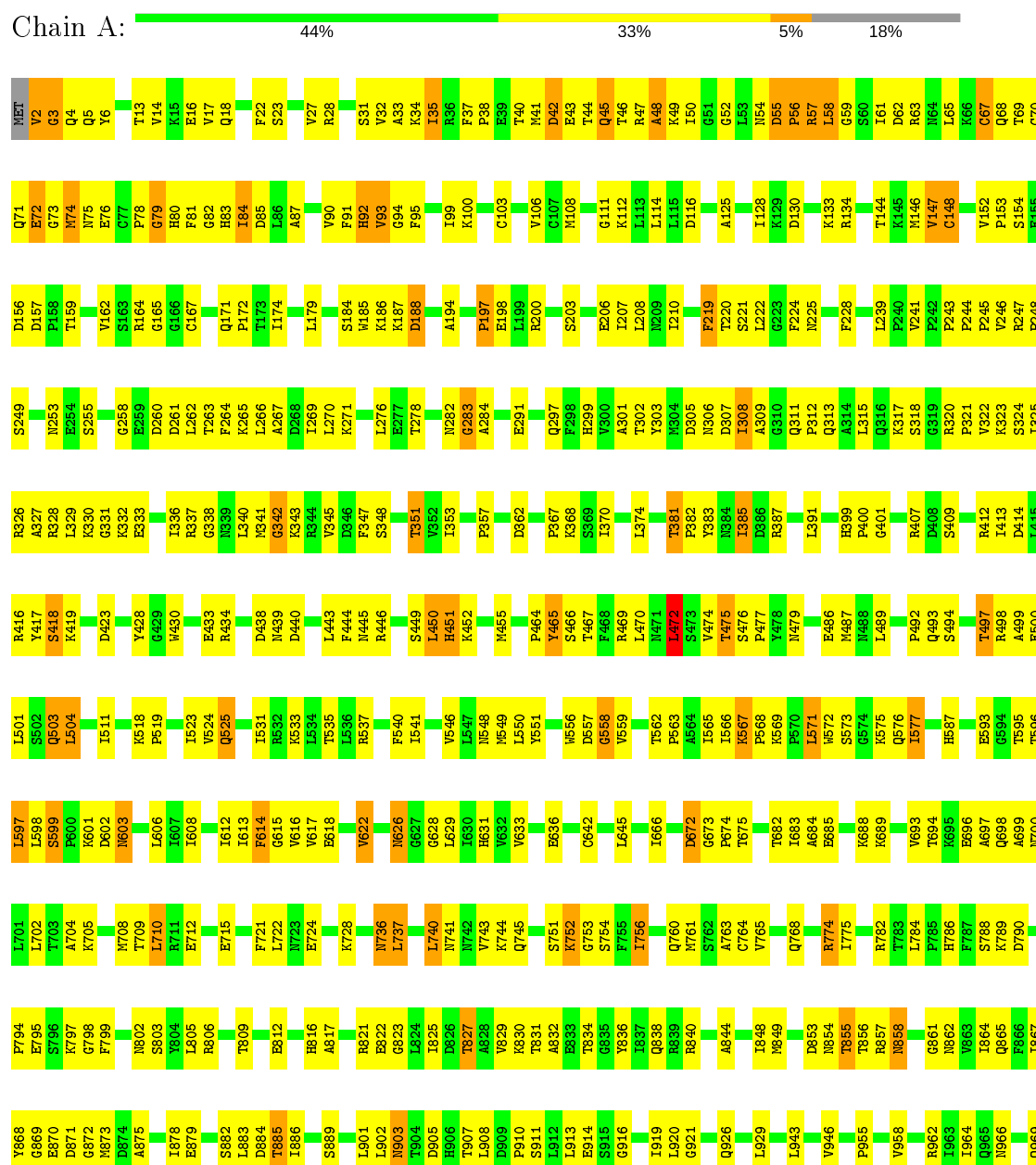
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	35	Total 35	O 35	0	0
13	B	23	Total 23	O 23	0	0
13	C	4	Total 4	O 4	0	0
13	E	7	Total 7	O 7	0	0
13	F	5	Total 5	O 5	0	0
13	I	2	Total 2	O 2	0	0
13	K	2	Total 2	O 2	0	0

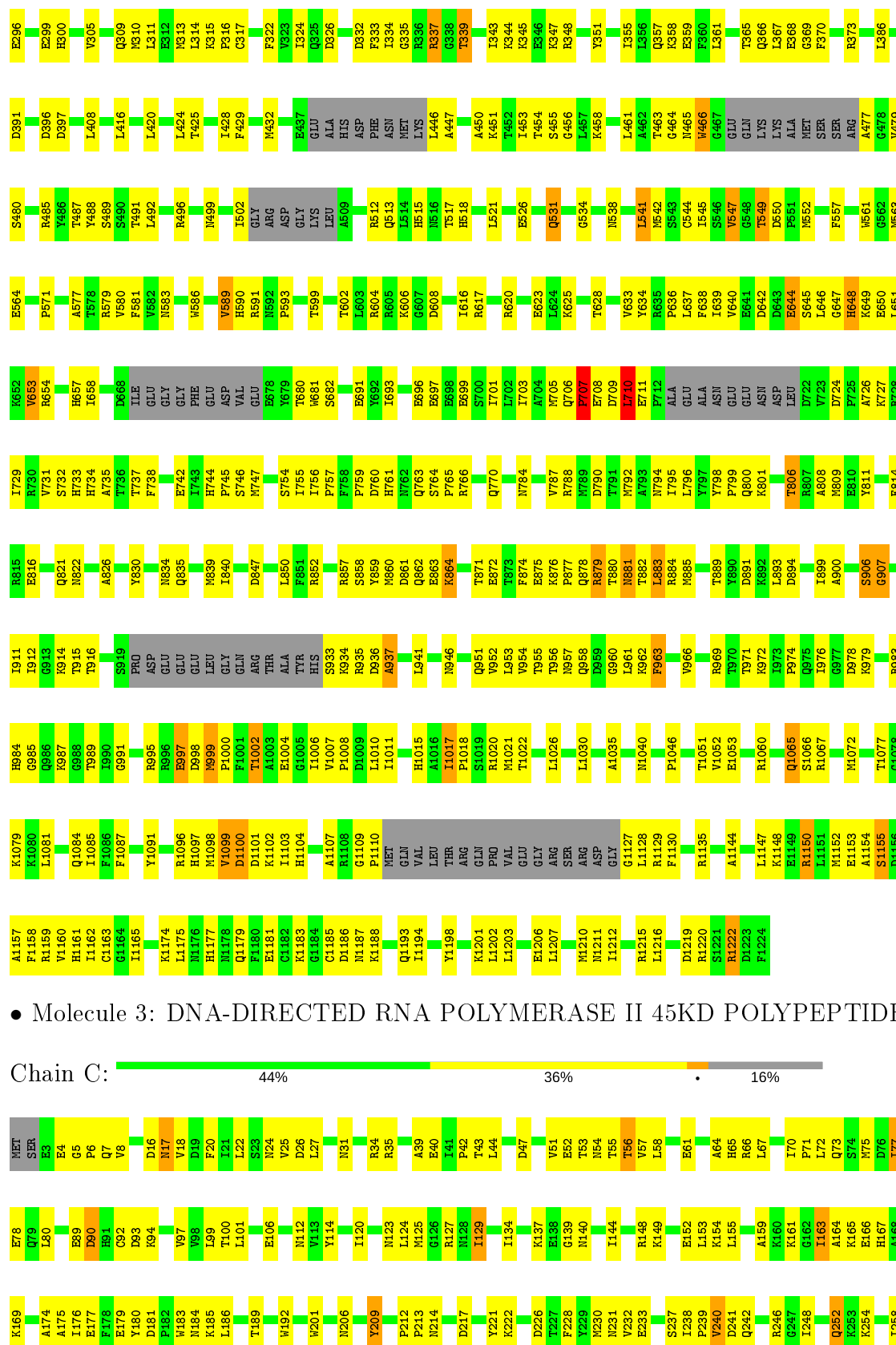
3 Residue-property plots

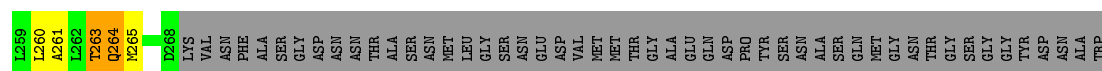
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

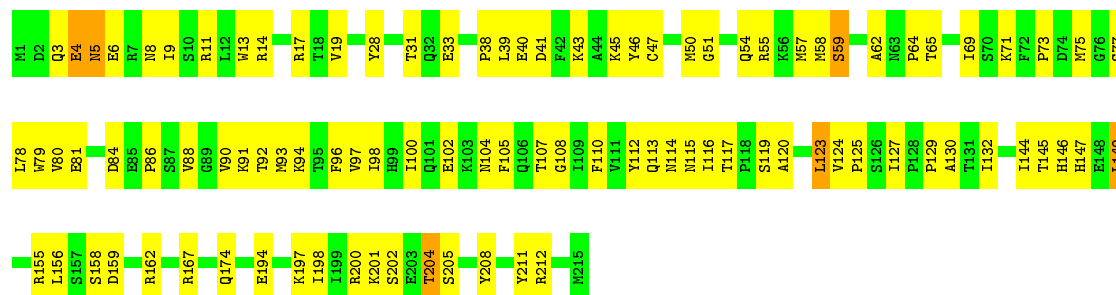






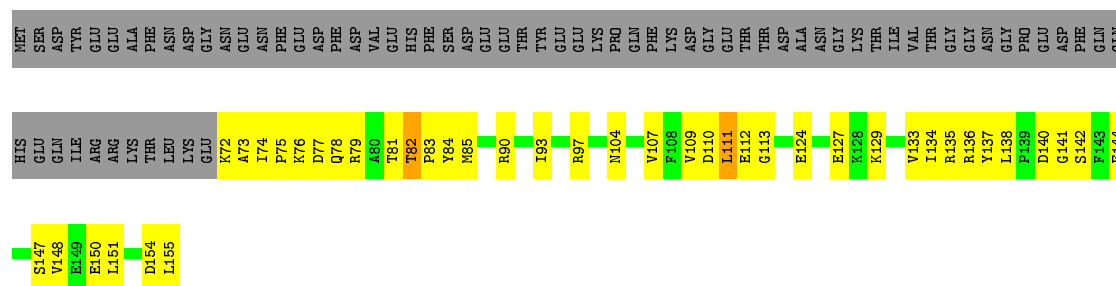
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

Chain E: 55% 42%



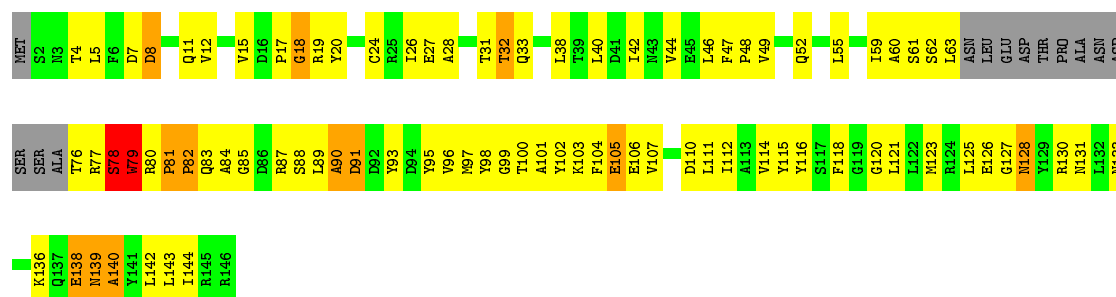
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F: 27% 26% 46%



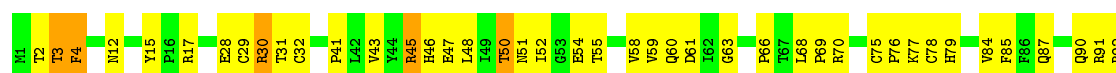
• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H: 32% 49% 8% 9%



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

Chain I: 52% 43% 5%

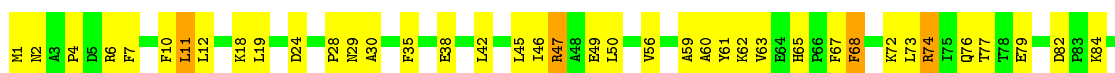




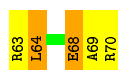
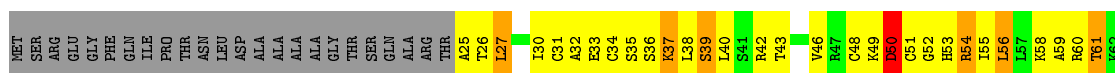
- Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE



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



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



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.70 Å 223.00 Å 376.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28366	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

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

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	0.39	1/11352 (0.0%)	0.68	2/15352 (0.0%)
2	B	0.42	2/8882 (0.0%)	0.70	5/11976 (0.0%)
3	C	0.37	0/2133	0.65	0/2891
4	E	0.37	0/1796	0.64	0/2416
5	F	0.40	0/691	0.63	0/933
6	H	0.88	1/1086 (0.1%)	1.23	3/1470 (0.2%)
7	I	0.40	0/1016	0.63	0/1365
8	J	0.41	0/541	0.70	0/727
9	K	0.38	0/937	0.60	0/1265
10	L	0.42	0/366	0.72	0/485
All	All	0.43	4/28800 (0.0%)	0.71	10/38880 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
6	H	0	3
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	79	TRP	C-N	-26.78	0.72	1.34
2	B	707	PRO	C-N	-11.27	1.08	1.34
2	B	710	LEU	C-N	-7.44	1.17	1.34
1	A	3	GLY	C-N	-5.20	1.22	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	78	SER	O-C-N	-31.77	71.87	122.70
6	H	78	SER	CA-C-N	20.38	162.03	117.20
2	B	707	PRO	O-C-N	-13.53	101.05	122.70
6	H	78	SER	C-N-CA	12.14	152.06	121.70
1	A	472	LEU	CA-CB-CG	-6.84	99.57	115.30
2	B	710	LEU	O-C-N	6.16	132.56	122.70
2	B	710	LEU	CA-C-N	-5.83	104.37	117.20
1	A	798	GLY	N-CA-C	5.36	126.49	113.10
2	B	937	ALA	N-CA-C	-5.26	96.80	111.00
2	B	707	PRO	C-N-CA	5.19	134.66	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	707	PRO	Mainchain
2	B	710	LEU	Mainchain
6	H	78	SER	Mainchain,Peptide
6	H	79	TRP	Mainchain

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11154	0	11222	754	0
2	B	8711	0	8734	539	0
3	C	2095	0	2051	141	0
4	E	1760	0	1788	87	0
5	F	679	0	701	50	0
6	H	1068	0	1038	121	0
7	I	997	0	956	64	0
8	J	532	0	542	47	0
9	K	919	0	929	65	0
10	L	364	0	387	68	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	1	0	0	0	0
13	A	35	0	0	2	0
13	B	23	0	0	2	0
13	C	4	0	0	0	0
13	E	7	0	0	1	0
13	F	5	0	0	0	0
13	I	2	0	0	0	0
13	K	2	0	0	0	0
All	All	28366	0	28348	1743	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1743) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:79:TRP:C	6:H:80:ARG:CA	1.90	1.41
2:B:708:GLU:O	2:B:711:GLU:HG3	1.20	1.34
6:H:79:TRP:CA	6:H:80:ARG:N	1.94	1.29
6:H:79:TRP:O	6:H:80:ARG:N	1.67	1.26
3:C:56:THR:HG23	3:C:58:LEU:H	1.14	1.13
1:A:855:THR:HG21	1:A:857:ARG:HE	1.02	1.11
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.32	1.10
1:A:308:ILE:HG22	1:A:309:ALA:H	1.14	1.09
1:A:47:ARG:HH12	1:A:255:SER:HA	1.17	1.09
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.21	1.08
1:A:672:ASP:HB2	1:A:736:ASN:HD21	0.94	1.08
1:A:1161:THR:HG22	1:A:1163:ILE:H	0.98	1.08
1:A:901:LEU:H	1:A:926:GLN:NE2	1.51	1.08
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	1.69	1.08
2:B:955:THR:HG22	2:B:956:THR:H	1.11	1.08
6:H:79:TRP:O	6:H:80:ARG:CA	1.98	1.07
2:B:710:LEU:CD2	2:B:738:PHE:CD1	2.38	1.07
1:A:345:VAL:HG21	2:B:1129:ARG:HA	1.33	1.07
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.35	1.06
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.14	1.06
7:I:111:THR:HG22	7:I:113:ASP:H	1.16	1.06
1:A:974:ASP:HB2	6:H:136:LYS:HZ3	1.15	1.06
2:B:800:GLN:HB3	8:J:52:THR:CG2	1.84	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:THR:HG22	2:B:872:GLU:H	1.21	1.05
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.16	1.04
1:A:672:ASP:HB2	1:A:736:ASN:ND2	1.72	1.03
1:A:264:PHE:HB3	1:A:315:LEU:HD22	1.39	1.03
1:A:313:GLN:HG2	1:A:322:VAL:HB	1.36	1.03
2:B:705:MET:HE1	2:B:742:GLU:HG3	1.41	1.03
2:B:29:ASP:HB3	2:B:658:ILE:CD1	1.88	1.02
3:C:148:ARG:NH1	8:J:64:ASN:HA	1.73	1.02
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.26	1.01
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.76	1.01
2:B:708:GLU:O	2:B:711:GLU:CG	2.08	1.01
2:B:542:MET:HG3	2:B:747:MET:HE3	1.40	1.00
6:H:130:ARG:HA	6:H:133:ASN:HD22	1.24	1.00
1:A:524:VAL:HG12	1:A:525:GLN:H	1.24	1.00
9:K:65:HIS:HD2	9:K:67:PHE:H	1.10	1.00
6:H:79:TRP:O	6:H:80:ARG:HA	1.62	0.99
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.45	0.99
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.45	0.98
1:A:3:GLY:O	1:A:5:GLN:N	1.98	0.97
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.44	0.96
1:A:597:LEU:H	1:A:597:LEU:HD12	1.28	0.96
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.80	0.95
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.46	0.95
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.31	0.95
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.31	0.95
1:A:567:LYS:HB3	6:H:96:VAL:H	1.30	0.95
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.49	0.95
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.00	0.95
1:A:901:LEU:H	1:A:926:GLN:HE21	1.05	0.95
1:A:913:LEU:HD11	1:A:981:LEU:O	1.68	0.94
1:A:855:THR:HG21	1:A:857:ARG:NE	1.84	0.93
2:B:737:THR:HG21	7:I:66:PRO:O	1.67	0.93
2:B:710:LEU:HD21	2:B:738:PHE:CD1	2.04	0.92
2:B:710:LEU:CD2	2:B:738:PHE:HD1	1.78	0.92
1:A:49:LYS:HD3	1:A:55:ASP:HB2	1.49	0.92
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.49	0.92
1:A:524:VAL:HG12	1:A:525:GLN:N	1.81	0.91
2:B:244:LEU:HD11	2:B:366:GLN:HE21	1.34	0.91
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.52	0.91
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.52	0.90
2:B:806:THR:HG22	2:B:809:MET:H	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.52	0.90
2:B:654:ARG:H	2:B:657:HIS:HD2	1.14	0.90
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.18	0.90
5:F:111:LEU:H	5:F:111:LEU:HD12	1.34	0.90
4:E:78:LEU:HD23	4:E:107:THR:HB	1.54	0.89
1:A:672:ASP:CB	1:A:736:ASN:HD21	1.84	0.89
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.51	0.89
1:A:903:ASN:ND2	1:A:905:ASP:H	1.70	0.89
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.56	0.88
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.38	0.88
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.03	0.88
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.53	0.88
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.55	0.88
1:A:470:LEU:HD11	1:A:487:MET:CE	2.05	0.87
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.87	0.87
1:A:567:LYS:HB3	6:H:96:VAL:N	1.90	0.86
1:A:855:THR:CG2	1:A:857:ARG:HE	1.87	0.86
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.57	0.86
2:B:889:THR:HG22	2:B:891:ASP:H	1.39	0.86
1:A:302:THR:HG21	1:A:312:PRO:CG	2.05	0.86
1:A:42:ASP:OD1	1:A:47:ARG:HG2	1.76	0.86
2:B:955:THR:HG22	2:B:956:THR:N	1.91	0.85
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.56	0.85
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.74	0.85
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.41	0.85
6:H:105:GLU:O	6:H:107:VAL:HG23	1.75	0.85
2:B:955:THR:HG23	10:L:54:ARG:O	1.77	0.85
10:L:38:LEU:HG	10:L:39:SER:H	1.41	0.85
6:H:103:LYS:HG2	6:H:115:TYR:H	1.41	0.84
1:A:381:THR:HG23	1:A:383:TYR:H	1.42	0.84
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.58	0.84
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.58	0.84
1:A:40:THR:HG22	1:A:41:MET:HG3	1.60	0.84
1:A:47:ARG:NH1	1:A:255:SER:HA	1.93	0.84
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.59	0.84
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.60	0.83
1:A:470:LEU:HD11	1:A:487:MET:HE1	1.59	0.83
2:B:25:ILE:HD12	2:B:653:VAL:HB	1.60	0.83
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	1.59	0.83
6:H:15:VAL:HG22	6:H:26:ILE:HG12	1.59	0.83
2:B:731:VAL:HG12	2:B:732:SER:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.77	0.83
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.42	0.83
7:I:45:ARG:HH11	7:I:45:ARG:HG2	1.44	0.82
7:I:50:THR:H	7:I:92:ARG:HH12	1.26	0.82
2:B:365:THR:HG22	2:B:367:LEU:H	1.43	0.82
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.77	0.82
2:B:464:GLY:O	2:B:477:ALA:HB3	1.78	0.82
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.58	0.82
1:A:503:GLN:HE21	5:F:90:ARG:NH2	1.76	0.82
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.61	0.82
6:H:103:LYS:HG2	6:H:115:TYR:N	1.94	0.82
1:A:1383:SER:HB3	1:A:1387:HIS:CE1	2.14	0.82
1:A:903:ASN:HD22	1:A:905:ASP:H	1.25	0.82
1:A:982:THR:HG22	1:A:984:LYS:H	1.44	0.82
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.62	0.82
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.60	0.82
2:B:277:LYS:HD2	2:B:277:LYS:N	1.93	0.82
2:B:583:ASN:HD21	2:B:628:THR:HB	1.45	0.81
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.62	0.81
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.94	0.81
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.10	0.81
1:A:597:LEU:N	1:A:597:LEU:HD12	1.96	0.81
1:A:399:HIS:O	1:A:401:GLY:N	2.14	0.81
2:B:130:VAL:HG12	2:B:131:ASP:H	1.45	0.81
1:A:33:ALA:O	1:A:83:HIS:HB3	1.82	0.80
2:B:1153:GLU:HG2	2:B:1154:ALA:H	1.47	0.80
1:A:567:LYS:NZ	6:H:46:LEU:HB2	1.97	0.80
1:A:1124:HIS:HB3	1:A:1130:GLN:OE1	1.81	0.80
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.81	0.79
1:A:1394:THR:HG22	1:A:1395:GLY:N	1.94	0.79
6:H:130:ARG:HA	6:H:133:ASN:ND2	1.96	0.79
1:A:313:GLN:HG2	1:A:322:VAL:CB	2.12	0.79
1:A:55:ASP:H	1:A:56:PRO:HD2	1.47	0.79
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.65	0.79
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.65	0.79
6:H:103:LYS:HG3	6:H:115:TYR:O	1.82	0.78
3:C:7:GLN:HG2	9:K:104:ASN:ND2	1.98	0.78
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.63	0.78
1:A:903:ASN:C	1:A:903:ASN:HD22	1.86	0.78
1:A:308:ILE:HG22	1:A:309:ALA:N	1.96	0.78
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:100:THR:OG1	6:H:138:GLU:HG3	1.84	0.78
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.66	0.78
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.65	0.78
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.18	0.78
2:B:914:LYS:HB3	2:B:937:ALA:O	1.83	0.78
1:A:565:ILE:HG21	1:A:567:LYS:HE2	1.66	0.77
1:A:1398:MET:HG3	1:A:1426:GLU:HG2	1.66	0.77
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.18	0.77
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.66	0.77
1:A:179:LEU:HD21	1:A:308:ILE:HD13	1.66	0.77
2:B:705:MET:CE	2:B:742:GLU:HG3	2.15	0.77
6:H:79:TRP:C	6:H:80:ARG:N	0.72	0.77
1:A:524:VAL:CG1	1:A:525:GLN:H	1.95	0.77
1:A:317:LYS:HD3	1:A:321:PRO:HD2	1.65	0.77
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.66	0.77
3:C:66:ARG:NH2	8:J:3:VAL:O	2.18	0.77
1:A:596:THR:HG22	1:A:597:LEU:H	1.50	0.77
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.67	0.77
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.77
1:A:1400:CYS:HB3	1:A:1405:THR:OG1	1.85	0.76
4:E:94:LYS:HG3	4:E:123:LEU:HD11	1.66	0.76
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.16	0.76
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.85	0.76
1:A:869:GLY:O	4:E:204:THR:HG21	1.83	0.76
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.01	0.76
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.16	0.76
5:F:76:LYS:O	5:F:79:ARG:HD2	1.86	0.76
9:K:29:ASN:HD21	9:K:79:GLU:HA	1.48	0.75
2:B:268:THR:HG21	2:B:270:LYS:HE3	1.69	0.75
1:A:974:ASP:CB	6:H:136:LYS:HZ3	1.96	0.75
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.50	0.75
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.68	0.75
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.50	0.75
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.33	0.75
5:F:109:VAL:HG12	5:F:110:ASP:N	2.00	0.75
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.68	0.75
3:C:124:LEU:O	3:C:127:ARG:HG2	1.86	0.75
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.00	0.75
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.87	0.75
2:B:955:THR:CG2	2:B:956:THR:H	1.95	0.75
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.17	0.74
1:A:768:GLN:HE21	1:A:816:HIS:HA	1.52	0.74
2:B:235:SER:HA	2:B:261:ARG:HH21	1.50	0.74
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.52	0.74
9:K:18:LYS:HZ2	9:K:38:GLU:HG2	1.51	0.74
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.70	0.74
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.52	0.74
5:F:147:SER:OG	5:F:150:GLU:HG3	1.88	0.74
9:K:65:HIS:CD2	9:K:67:PHE:H	2.01	0.74
1:A:613:ILE:HD13	6:H:102:TYR:HB3	1.69	0.74
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.03	0.73
4:E:100:ILE:HD13	4:E:108:GLY:HA3	1.70	0.73
1:A:345:VAL:HA	2:B:1150:ARG:HH12	1.52	0.73
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.70	0.73
1:A:225:ASN:ND2	1:A:228:PHE:HD1	1.86	0.73
2:B:954:VAL:O	10:L:55:ILE:O	2.07	0.73
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.68	0.73
6:H:100:THR:HG23	6:H:138:GLU:HA	1.69	0.73
1:A:225:ASN:HD21	1:A:228:PHE:HD1	1.36	0.73
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.52	0.73
2:B:563:MET:CE	2:B:580:VAL:HB	2.19	0.73
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.68	0.73
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.23	0.73
2:B:205:ILE:HD13	2:B:461:LEU:HB3	1.71	0.73
2:B:531:GLN:H	2:B:531:GLN:CD	1.92	0.73
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.52	0.73
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.19	0.72
3:C:261:ALA:O	3:C:265:MET:HB2	1.89	0.72
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.24	0.72
1:A:741:ASN:HD22	1:A:744:LYS:H	1.34	0.72
2:B:871:THR:HG22	2:B:872:GLU:N	2.02	0.72
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.36	0.72
1:A:907:THR:HG22	1:A:908:LEU:H	1.54	0.72
6:H:103:LYS:HD3	6:H:114:VAL:HB	1.70	0.72
1:A:1336:MET:HE1	1:A:1381:LEU:N	2.04	0.72
2:B:680:THR:HG22	2:B:682:SER:H	1.53	0.72
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.04	0.72
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.54	0.72
9:K:113:THR:O	9:K:114:LEU:HB2	1.90	0.72
1:A:573:SER:HB3	1:A:576:GLN:HG3	1.72	0.72
2:B:205:ILE:CD1	2:B:461:LEU:HB3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:125:LEU:C	6:H:130:ARG:HH12	1.93	0.72
1:A:32:VAL:HG11	1:A:68:GLN:HE22	1.55	0.71
1:A:752:LYS:HD2	2:B:1015:HIS:O	1.89	0.71
3:C:22:LEU:HD12	3:C:230:MET:CE	2.20	0.71
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.72	0.71
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.25	0.71
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.37	0.71
1:A:72:GLU:HB3	1:A:76:GLU:HB2	1.71	0.71
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.20	0.71
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.06	0.71
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.20	0.71
9:K:47:ARG:HB3	9:K:47:ARG:NH1	2.05	0.71
1:A:5:GLN:OE1	2:B:1175:LEU:HD12	1.91	0.71
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.20	0.71
2:B:710:LEU:HD23	2:B:738:PHE:CD1	2.24	0.70
1:A:55:ASP:O	1:A:57:ARG:N	2.24	0.70
2:B:800:GLN:CB	8:J:52:THR:HG22	2.18	0.70
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.04	0.70
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.72	0.70
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.05	0.70
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.73	0.70
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.74	0.70
1:A:1336:MET:HE1	1:A:1381:LEU:HG	1.72	0.70
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.07	0.70
1:A:565:ILE:CG2	1:A:567:LYS:HE2	2.21	0.70
2:B:731:VAL:HG12	2:B:732:SER:N	2.06	0.70
2:B:199:MET:HE3	2:B:492:LEU:HD23	1.74	0.70
2:B:654:ARG:H	2:B:657:HIS:CD2	2.04	0.70
3:C:56:THR:CG2	3:C:58:LEU:H	2.00	0.70
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.73	0.69
1:A:329:LEU:O	1:A:333:GLU:N	2.25	0.69
4:E:155:ARG:HD2	4:E:194:GLU:OE2	1.92	0.69
10:L:55:ILE:O	10:L:56:LEU:HB2	1.91	0.69
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.21	0.69
10:L:60:ARG:HG2	10:L:61:THR:H	1.58	0.69
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.74	0.69
1:A:80:HIS:O	1:A:243:PRO:HB3	1.92	0.69
2:B:1153:GLU:HG2	2:B:1154:ALA:N	2.06	0.69
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.74	0.69
3:C:20:PHE:HE1	3:C:22:LEU:HG	1.55	0.69
1:A:901:LEU:N	1:A:926:GLN:NE2	2.35	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:THR:HA	2:B:961:LEU:O	1.93	0.69
10:L:61:THR:HG21	10:L:63:ARG:HD3	1.74	0.69
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.72	0.69
1:A:302:THR:HG21	1:A:312:PRO:HG2	1.75	0.69
1:A:55:ASP:N	1:A:56:PRO:HD2	2.05	0.69
1:A:345:VAL:HG11	2:B:1128:LEU:O	1.93	0.69
2:B:120:ARG:HD2	2:B:955:THR:HG21	1.75	0.69
7:I:63:GLY:O	7:I:70:ARG:NH2	2.26	0.69
1:A:61:ILE:HG22	1:A:62:ASP:H	1.57	0.69
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.74	0.69
2:B:864:LYS:HD3	2:B:871:THR:HA	1.75	0.69
3:C:174:ALA:O	8:J:10:CYS:HB2	1.93	0.69
1:A:313:GLN:HE21	1:A:322:VAL:HG12	1.58	0.69
5:F:111:LEU:N	5:F:111:LEU:HD12	2.07	0.68
2:B:872:GLU:HG2	2:B:916:THR:OG1	1.94	0.68
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.74	0.68
2:B:130:VAL:HG12	2:B:131:ASP:N	2.08	0.68
6:H:104:PHE:O	6:H:106:GLU:N	2.25	0.68
5:F:77:ASP:O	5:F:78:GLN:HB2	1.92	0.68
1:A:1113:THR:HG22	1:A:1113:THR:O	1.93	0.68
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.59	0.68
5:F:109:VAL:HG12	5:F:110:ASP:H	1.58	0.68
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.74	0.68
2:B:680:THR:CG2	2:B:681:TRP:N	2.56	0.68
1:A:974:ASP:HB2	6:H:136:LYS:NZ	2.00	0.68
1:A:911:SER:O	1:A:978:PRO:HB3	1.94	0.68
2:B:1162:ILE:HD11	2:B:1216:LEU:HD12	1.75	0.68
3:C:258:ILE:HD13	9:K:35:PHE:HE2	1.58	0.68
1:A:1390:ASN:O	1:A:1391:ARG:HB2	1.94	0.67
1:A:23:SER:O	1:A:27:VAL:HG23	1.94	0.67
7:I:98:VAL:HG21	7:I:113:ASP:CB	2.23	0.67
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.29	0.67
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.58	0.67
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.75	0.67
2:B:120:ARG:CZ	10:L:54:ARG:HD2	2.25	0.67
1:A:1128:GLN:O	1:A:1132:LYS:HG3	1.94	0.67
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.76	0.67
2:B:235:SER:HA	2:B:261:ARG:NH2	2.08	0.67
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.25	0.67
3:C:39:ALA:O	3:C:163:ILE:HG23	1.95	0.67
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:879:ARG:HB3	2:B:883:LEU:CD2	2.25	0.67
1:A:317:LYS:HD3	1:A:321:PRO:CD	2.25	0.67
2:B:550:ASP:OD1	2:B:552:MET:HG3	1.94	0.67
2:B:542:MET:CE	2:B:747:MET:HG3	2.24	0.67
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.77	0.67
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.77	0.67
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.25	0.67
5:F:127:GLU:O	5:F:129:LYS:HG3	1.96	0.66
1:A:128:ILE:HG22	1:A:130:ASP:H	1.59	0.66
1:A:597:LEU:CD1	1:A:597:LEU:H	2.04	0.66
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.08	0.66
5:F:82:THR:HG22	5:F:84:TYR:H	1.60	0.66
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.76	0.66
4:E:117:THR:HG22	4:E:119:SER:H	1.60	0.66
7:I:47:GLU:OE1	7:I:50:THR:HG23	1.96	0.66
2:B:103:ASN:HB2	2:B:169:ARG:NH2	2.10	0.66
2:B:193:LYS:HD2	2:B:787:VAL:HG11	1.78	0.66
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.76	0.66
6:H:87:ARG:O	6:H:89:LEU:HG	1.95	0.66
6:H:11:GLN:NE2	6:H:52:GLN:HA	2.10	0.66
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.78	0.66
1:A:92:HIS:HD2	1:A:94:GLY:H	1.42	0.66
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.77	0.66
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.31	0.66
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.10	0.66
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.78	0.65
1:A:63:ARG:HA	1:A:74:MET:HE2	1.78	0.65
2:B:120:ARG:HH12	10:L:54:ARG:NH1	1.93	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.78	0.65
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.77	0.65
1:A:44:THR:O	1:A:45:GLN:HB2	1.97	0.65
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.62	0.65
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.77	0.65
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	1.96	0.65
1:A:470:LEU:HD11	1:A:487:MET:HE2	1.79	0.65
1:A:1383:SER:CB	1:A:1387:HIS:NE2	2.54	0.65
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.78	0.65
1:A:1111:MET:HB2	1:A:1114:PRO:HG3	1.78	0.65
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.77	0.65
1:A:320:ARG:N	1:A:321:PRO:HD3	2.12	0.65
4:E:204:THR:HG22	4:E:205:SER:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:O	1:A:475:THR:HB	1.97	0.65
1:A:595:THR:OG1	1:A:603:ASN:HB3	1.96	0.65
1:A:31:SER:CB	1:A:83:HIS:HB2	2.26	0.65
2:B:35:SER:O	2:B:39:ARG:HG3	1.97	0.65
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.61	0.65
1:A:901:LEU:HD13	1:A:919:ILE:HG23	1.77	0.65
2:B:322:PHE:HZ	7:I:30:ARG:HB2	1.62	0.65
2:B:801:LYS:O	8:J:52:THR:HG23	1.97	0.65
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.59	0.65
10:L:49:LYS:O	10:L:50:ASP:HB2	1.95	0.65
1:A:705:LYS:O	1:A:708:MET:HB2	1.97	0.64
2:B:54:PHE:HA	2:B:58:THR:HB	1.79	0.64
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.62	0.64
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.61	0.64
1:A:567:LYS:CB	1:A:568:PRO:CD	2.71	0.64
2:B:1198:TYR:CE1	2:B:1201:LYS:HD3	2.32	0.64
6:H:126:GLU:N	6:H:130:ARG:HH12	1.95	0.64
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.79	0.64
6:H:103:LYS:CD	6:H:114:VAL:HB	2.27	0.64
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.13	0.64
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.11	0.64
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.28	0.64
10:L:58:LYS:O	10:L:58:LYS:HD3	1.98	0.64
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.78	0.64
1:A:1167:GLU:O	1:A:1171:GLN:HG3	1.98	0.64
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.95	0.64
1:A:907:THR:HG22	1:A:908:LEU:N	2.12	0.64
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.28	0.64
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.96	0.64
4:E:112:TYR:CE1	4:E:115:ASN:HA	2.33	0.64
1:A:1295:THR:HB	1:A:1297:GLU:OE1	1.97	0.64
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.12	0.64
1:A:709:THR:HG21	7:I:93:LYS:O	1.98	0.64
4:E:158:SER:O	4:E:162:ARG:HG3	1.98	0.64
1:A:666:ILE:HG12	2:B:1026:LEU:HB3	1.80	0.63
2:B:784:ASN:OD1	2:B:788:ARG:HD2	1.97	0.63
6:H:103:LYS:HZ1	6:H:114:VAL:HG23	1.64	0.63
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.63	0.63
2:B:616:ILE:HD11	2:B:696:GLU:HB3	1.80	0.63
2:B:644:GLU:HG3	2:B:654:ARG:NH2	2.13	0.63
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.80	0.63
1:A:184:SER:HA	1:A:198:GLU:O	1.98	0.63
1:A:313:GLN:NE2	1:A:322:VAL:HG12	2.13	0.63
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.19	0.63
6:H:103:LYS:NZ	6:H:114:VAL:HG23	2.13	0.63
8:J:2:ILE:HG12	8:J:57:ILE:HG21	1.80	0.63
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.14	0.63
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.46	0.63
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.80	0.63
3:C:7:GLN:HG2	9:K:104:ASN:HD22	1.63	0.63
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.32	0.63
8:J:2:ILE:HG22	8:J:3:VAL:N	2.13	0.63
3:C:52:GLU:HA	10:L:64:LEU:CD2	2.28	0.63
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.80	0.63
6:H:4:THR:HA	6:H:60:ALA:HA	1.79	0.63
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.62	0.63
1:A:134:ARG:HD2	1:A:221:SER:O	1.97	0.63
1:A:317:LYS:CD	1:A:321:PRO:HD2	2.28	0.63
1:A:329:LEU:HA	1:A:332:LYS:HB2	1.81	0.63
3:C:5:GLY:C	3:C:24:ASN:HD22	2.00	0.63
7:I:50:THR:HG22	7:I:51:ASN:H	1.63	0.63
8:J:2:ILE:HD11	8:J:57:ILE:HD13	1.80	0.63
1:A:825:ILE:HD13	2:B:512:ARG:HG3	1.81	0.63
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.29	0.62
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.14	0.62
10:L:38:LEU:O	10:L:39:SER:HB2	1.99	0.62
1:A:322:VAL:HG22	1:A:323:LYS:N	2.14	0.62
1:A:32:VAL:HG11	1:A:68:GLN:NE2	2.13	0.62
1:A:1206:ASP:HB2	1:A:1274:ARG:NH1	2.14	0.62
1:A:566:ILE:O	1:A:567:LYS:O	2.17	0.62
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.14	0.62
6:H:82:PRO:O	6:H:84:ALA:N	2.32	0.62
7:I:45:ARG:NH1	7:I:45:ARG:HG2	2.11	0.62
1:A:601:LYS:HD2	1:A:603:ASN:ND2	2.13	0.62
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.99	0.62
10:L:30:ILE:HG22	10:L:31:CYS:N	2.14	0.62
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.97	0.62
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.81	0.62
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.80	0.62
9:K:18:LYS:NZ	9:K:38:GLU:HG2	2.14	0.62
1:A:1080:THR:O	1:A:1081:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1395:GLY:C	1:A:1397:LEU:H	2.02	0.62
1:A:853:ASP:O	1:A:854:ASN:HB2	1.99	0.62
2:B:563:MET:HE2	2:B:580:VAL:HB	1.81	0.62
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.82	0.62
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.81	0.62
2:B:322:PHE:CZ	7:I:30:ARG:HB2	2.35	0.62
2:B:294:ASP:H	7:I:12:ASN:ND2	1.97	0.62
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.47	0.62
2:B:35:SER:HA	2:B:811:TYR:HE2	1.65	0.62
1:A:47:ARG:O	1:A:48:ALA:HB2	2.00	0.61
1:A:1398:MET:CG	1:A:1426:GLU:HG2	2.28	0.61
1:A:56:PRO:O	1:A:57:ARG:HG3	2.00	0.61
2:B:1165:ILE:CD1	2:B:1187:ASN:HD21	2.13	0.61
2:B:164:LYS:O	2:B:165:VAL:HB	2.00	0.61
2:B:210:LYS:HE3	2:B:480:SER:OG	2.00	0.61
8:J:48:ARG:HG2	8:J:48:ARG:HH11	1.63	0.61
1:A:203:SER:OG	1:A:206:GLU:HG3	2.00	0.61
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.15	0.61
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.80	0.61
2:B:46:GLN:HG3	2:B:47:GLN:H	1.66	0.61
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.82	0.61
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.35	0.61
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.65	0.61
2:B:251:ILE:HG22	2:B:251:ILE:O	2.00	0.61
2:B:276:ILE:HD13	2:B:334:ILE:HG23	1.82	0.61
3:C:73:GLN:HE21	3:C:75:MET:H	1.47	0.61
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.80	0.61
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.81	0.61
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.14	0.61
5:F:111:LEU:O	5:F:113:GLY:N	2.31	0.61
7:I:103:CYS:O	7:I:107:SER:HA	2.01	0.61
9:K:12:LEU:HD11	9:K:18:LYS:HE2	1.82	0.61
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.82	0.61
1:A:387:ARG:O	1:A:391:LEU:HG	2.01	0.61
1:A:541:ILE:HG12	1:A:549:MET:HE1	1.83	0.61
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.66	0.61
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.24	0.61
2:B:602:THR:HG22	2:B:606:LYS:HE3	1.82	0.61
1:A:1064:VAL:HG13	13:A:3010:HOH:O	2.00	0.61
1:A:302:THR:HG21	1:A:312:PRO:HG3	1.80	0.61
3:C:179:GLU:HG3	3:C:180:TYR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:65:THR:O	4:E:69:ILE:HG13	2.01	0.61
4:E:28:TYR:CZ	4:E:78:LEU:HG	2.36	0.61
1:A:883:LEU:O	1:A:886:ILE:HG22	2.01	0.61
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.82	0.61
7:I:17:ARG:HG3	7:I:28:GLU:CD	2.21	0.61
7:I:4:PHE:H	7:I:4:PHE:HD2	1.48	0.61
1:A:345:VAL:HG12	2:B:1150:ARG:HH22	1.65	0.61
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.82	0.61
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.82	0.61
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.83	0.61
6:H:5:LEU:HD22	6:H:133:ASN:O	2.00	0.61
7:I:95:THR:HG22	7:I:96:SER:N	2.15	0.61
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.21	0.60
1:A:597:LEU:HD23	6:H:104:PHE:CD1	2.35	0.60
1:A:78:PRO:O	1:A:79:GLY:O	2.19	0.60
3:C:137:LYS:HD2	3:C:137:LYS:H	1.65	0.60
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.83	0.60
1:A:345:VAL:CG1	2:B:1150:ARG:HH22	2.13	0.60
1:A:1111:MET:HE3	1:A:1114:PRO:HA	1.83	0.60
1:A:689:LYS:O	1:A:693:VAL:HG23	2.01	0.60
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.83	0.60
1:A:903:ASN:HD22	1:A:905:ASP:N	1.97	0.60
2:B:680:THR:HG22	2:B:681:TRP:N	2.16	0.60
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.01	0.60
2:B:1181:GLU:CG	2:B:1188:LYS:HE2	2.31	0.60
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.37	0.60
2:B:706:GLN:NE2	2:B:709:ASP:OD2	2.34	0.60
1:A:849:MET:CE	1:A:1437:GLY:H	2.14	0.60
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.84	0.60
1:A:466:SER:O	1:A:467:THR:HG23	2.02	0.60
1:A:541:ILE:N	1:A:541:ILE:HD12	2.17	0.60
1:A:751:SER:O	1:A:752:LYS:O	2.19	0.60
3:C:22:LEU:HD12	3:C:230:MET:HE1	1.84	0.60
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.16	0.60
4:E:43:LYS:O	4:E:47:CYS:HB2	2.02	0.60
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.84	0.60
1:A:901:LEU:N	1:A:926:GLN:HE21	1.88	0.60
2:B:884:ARG:O	2:B:936:ASP:CB	2.50	0.60
1:A:79:GLY:HA3	1:A:245:PRO:HG3	1.84	0.59
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.83	0.59
2:B:1127:GLY:O	2:B:1128:LEU:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:879:ARG:HE	2:B:885:MET:HE2	1.66	0.59
1:A:1077:THR:HG22	1:A:1077:THR:O	2.02	0.59
1:A:1064:VAL:CG1	1:A:1370:LEU:HD22	2.32	0.59
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.02	0.59
2:B:62:ILE:O	2:B:65:GLU:HG2	2.03	0.59
2:B:899:ILE:HG22	2:B:900:ALA:N	2.17	0.59
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.02	0.59
2:B:542:MET:HE1	2:B:747:MET:HG3	1.85	0.59
3:C:52:GLU:HG2	10:L:64:LEU:HD11	1.84	0.59
5:F:81:THR:HB	5:F:144:GLU:OE1	2.03	0.59
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.29	0.59
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.37	0.59
1:A:1215:ARG:HA	1:A:1218:GLN:HE21	1.67	0.59
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.50	0.59
2:B:710:LEU:HD22	2:B:738:PHE:HD1	1.63	0.59
10:L:51:CYS:O	10:L:53:HIS:N	2.36	0.59
1:A:499:ALA:O	1:A:503:GLN:HB2	2.03	0.59
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.42	0.59
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.82	0.59
6:H:26:ILE:CD1	6:H:49:VAL:HG11	2.32	0.59
1:A:844:ALA:CB	1:A:1384:VAL:HG13	2.29	0.59
1:A:67:CYS:O	1:A:68:GLN:HB2	2.01	0.59
2:B:549:THR:O	2:B:628:THR:HG22	2.02	0.59
3:C:31:ASN:O	3:C:35:ARG:HG3	2.03	0.59
3:C:56:THR:HG23	3:C:58:LEU:N	2.00	0.59
3:C:6:PRO:HG3	3:C:25:VAL:HG12	1.84	0.59
5:F:109:VAL:CG1	5:F:110:ASP:N	2.66	0.59
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.02	0.59
2:B:168:GLY:H	2:B:450:ALA:HB1	1.68	0.59
2:B:416:LEU:O	2:B:420:LEU:HG	2.02	0.59
1:A:249:SER:HB2	1:A:258:GLY:O	2.02	0.59
1:A:2:VAL:HG21	2:B:1157:ALA:O	2.02	0.59
1:A:332:LYS:HD3	2:B:1206:GLU:OE2	2.02	0.59
1:A:92:HIS:CD2	1:A:94:GLY:H	2.21	0.59
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.17	0.59
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.83	0.59
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.42	0.59
7:I:115:LYS:O	7:I:117:LYS:HG3	2.03	0.59
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.38	0.59
1:A:324:SER:O	1:A:328:ARG:HG3	2.03	0.59
2:B:63:ILE:CG1	2:B:95:ILE:HD11	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:HG22	1:A:597:LEU:N	2.18	0.58
1:A:774:ARG:HG3	1:A:774:ARG:HH11	1.67	0.58
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.33	0.58
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.02	0.58
1:A:58:LEU:HD22	1:A:80:HIS:O	2.03	0.58
3:C:17:ASN:HD22	3:C:17:ASN:N	2.01	0.58
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.51	0.58
6:H:110:ASP:O	6:H:128:ASN:ND2	2.36	0.58
1:A:503:GLN:HE21	5:F:90:ARG:HH22	1.47	0.58
2:B:324:ILE:HD11	2:B:333:PHE:CD1	2.38	0.58
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.67	0.58
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.33	0.58
2:B:882:THR:HB	2:B:934:LYS:O	2.02	0.58
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.39	0.58
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.03	0.58
1:A:494:SER:OG	1:A:497:THR:HB	2.04	0.58
1:A:525:GLN:NE2	1:A:752:LYS:HE3	2.17	0.58
2:B:365:THR:HG22	2:B:367:LEU:N	2.17	0.58
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.86	0.58
2:B:98:THR:HG21	2:B:101:MET:CE	2.34	0.58
4:E:4:GLU:O	4:E:6:GLU:N	2.37	0.58
10:L:27:LEU:HD13	10:L:37:LYS:CD	2.32	0.58
4:E:124:VAL:HB	4:E:125:PRO:CD	2.33	0.58
6:H:40:LEU:CD1	6:H:123:MET:HB2	2.34	0.58
1:A:264:PHE:HB2	1:A:315:LEU:HD13	1.85	0.58
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.67	0.58
1:A:1124:HIS:CB	1:A:1130:GLN:OE1	2.52	0.58
2:B:193:LYS:CD	2:B:787:VAL:HG11	2.34	0.58
4:E:5:ASN:HA	4:E:8:ASN:HB3	1.84	0.58
1:A:1111:MET:HE3	1:A:1114:PRO:HG3	1.85	0.58
1:A:283:GLY:O	1:A:284:ALA:HB2	2.04	0.58
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.69	0.58
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.33	0.58
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.85	0.58
2:B:477:ALA:HB1	2:B:479:VAL:HG23	1.85	0.58
2:B:640:VAL:HG12	2:B:640:VAL:O	2.02	0.58
2:B:120:ARG:HD2	2:B:955:THR:CG2	2.33	0.58
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.33	0.58
1:A:724:GLU:O	1:A:728:LYS:HG2	2.04	0.58
1:A:774:ARG:HB2	1:A:797:LYS:HG2	1.85	0.58
1:A:901:LEU:HA	1:A:907:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:59:VAL:HG12	7:I:61:ASP:H	1.68	0.58
10:L:33:GLU:HB2	10:L:53:HIS:CD2	2.38	0.58
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.03	0.57
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.43	0.57
2:B:979:LYS:CE	2:B:987:LYS:HD2	2.32	0.57
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.85	0.57
6:H:26:ILE:HD13	6:H:49:VAL:HG11	1.86	0.57
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.86	0.57
1:A:65:LEU:HD22	1:A:72:GLU:O	2.04	0.57
1:A:848:ILE:HD13	1:A:864:ILE:HD13	1.87	0.57
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.19	0.57
1:A:144:THR:O	1:A:146:MET:HG3	2.04	0.57
2:B:754:SER:O	2:B:806:THR:HG21	2.04	0.57
2:B:760:ASP:OD1	2:B:761:HIS:HD2	1.87	0.57
7:I:51:ASN:O	7:I:54:GLU:HG3	2.04	0.57
10:L:34:CYS:HB3	10:L:51:CYS:SG	2.44	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.85	0.57
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.19	0.57
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.39	0.57
6:H:89:LEU:C	6:H:91:ASP:H	2.07	0.57
1:A:187:LYS:O	1:A:188:ASP:HB2	2.04	0.57
1:A:70:CYS:O	1:A:72:GLU:HG3	2.04	0.57
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.69	0.57
5:F:109:VAL:CG1	5:F:110:ASP:H	2.17	0.57
1:A:1446:ASP:OD2	1:A:1448:GLU:HB2	2.04	0.57
1:A:112:LYS:NZ	1:A:165:GLY:H	2.02	0.57
1:A:486:GLU:OE2	2:B:1102:LYS:HB3	2.05	0.57
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.86	0.57
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.87	0.57
2:B:876:LYS:HE2	2:B:893:LEU:O	2.05	0.57
1:A:567:LYS:NZ	6:H:95:TYR:HE1	2.02	0.57
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.35	0.57
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.40	0.57
1:A:33:ALA:HB2	1:A:56:PRO:HB2	1.87	0.57
1:A:629:LEU:O	1:A:633:VAL:HG23	2.04	0.57
1:A:903:ASN:C	1:A:903:ASN:ND2	2.57	0.57
2:B:863:GLU:O	2:B:864:LYS:O	2.23	0.57
6:H:87:ARG:O	6:H:89:LEU:N	2.37	0.57
2:B:1022:THR:HG23	2:B:1022:THR:O	2.05	0.56
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.35	0.56
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.05	0.56
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.87	0.56
1:A:33:ALA:CB	1:A:56:PRO:HB2	2.35	0.56
1:A:34:LYS:HE3	1:A:85:ASP:OD2	2.05	0.56
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.20	0.56
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.40	0.56
4:E:120:ALA:O	4:E:123:LEU:HB2	2.05	0.56
1:A:537:ARG:NH1	6:H:120:GLY:O	2.37	0.56
6:H:138:GLU:HG2	6:H:139:ASN:N	2.20	0.56
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.20	0.56
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.38	0.56
2:B:1165:ILE:HD12	2:B:1187:ASN:HD21	1.69	0.56
2:B:642:ASP:CB	2:B:649:LYS:HG2	2.23	0.56
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.87	0.56
6:H:7:ASP:O	6:H:8:ASP:HB2	2.04	0.56
1:A:1064:VAL:HG12	1:A:1370:LEU:CD2	2.36	0.56
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.87	0.56
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.35	0.56
1:A:69:THR:O	1:A:71:GLN:HG3	2.05	0.56
3:C:22:LEU:HD12	3:C:230:MET:HE3	1.87	0.56
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	1.86	0.56
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.87	0.56
1:A:49:LYS:HD3	1:A:55:ASP:CB	2.30	0.56
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.88	0.56
2:B:46:GLN:HG3	2:B:47:GLN:N	2.21	0.56
1:A:1395:GLY:O	1:A:1397:LEU:N	2.37	0.56
2:B:120:ARG:NH1	10:L:54:ARG:NH1	2.53	0.56
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.21	0.56
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.71	0.56
7:I:2:THR:O	7:I:3:THR:C	2.44	0.56
10:L:27:LEU:HD13	10:L:37:LYS:HD3	1.88	0.56
1:A:1394:THR:CG2	1:A:1398:MET:HB2	2.35	0.56
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.40	0.56
1:A:313:GLN:HE21	1:A:322:VAL:N	2.04	0.56
1:A:595:THR:HG23	1:A:599:SER:HB3	1.86	0.56
2:B:915:THR:HG21	2:B:934:LYS:HG2	1.87	0.56
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.06	0.56
4:E:88:VAL:HG13	4:E:92:THR:HB	1.88	0.56
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.87	0.56
2:B:1165:ILE:HD12	2:B:1187:ASN:ND2	2.20	0.56
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:N	2:B:231:PRO:HD2	2.20	0.56
2:B:705:MET:CE	2:B:745:PRO:HB3	2.36	0.56
1:A:1265:ASN:HD21	2:B:263:GLY:C	2.09	0.56
1:A:100:LYS:HE3	1:A:174:ILE:O	2.06	0.56
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.88	0.56
3:C:175:ALA:O	3:C:176:ILE:HG12	2.06	0.56
5:F:111:LEU:H	5:F:111:LEU:CD1	2.13	0.56
10:L:30:ILE:HG22	10:L:31:CYS:H	1.71	0.56
2:B:1103:ILE:O	2:B:1103:ILE:HG22	2.05	0.55
2:B:1165:ILE:CG1	2:B:1187:ASN:HD21	2.20	0.55
2:B:864:LYS:CG	2:B:871:THR:HG23	2.36	0.55
3:C:167:HIS:HD2	3:C:169:LYS:H	1.54	0.55
1:A:1394:THR:HA	1:A:1398:MET:HE1	1.88	0.55
5:F:75:PRO:O	5:F:77:ASP:O	2.24	0.55
1:A:469:ARG:NH2	2:B:991:GLY:O	2.38	0.55
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.88	0.55
2:B:542:MET:HG3	2:B:747:MET:CE	2.27	0.55
2:B:953:LEU:HD21	2:B:955:THR:OG1	2.06	0.55
6:H:103:LYS:HZ2	6:H:114:VAL:C	2.08	0.55
10:L:68:GLU:CD	10:L:68:GLU:H	2.10	0.55
1:A:269:ILE:HD11	1:A:303:TYR:HB2	1.87	0.55
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.69	0.55
2:B:602:THR:O	2:B:606:LYS:HG3	2.07	0.55
2:B:884:ARG:O	2:B:885:MET:HG2	2.07	0.55
10:L:51:CYS:C	10:L:53:HIS:H	2.10	0.55
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.27	0.55
1:A:337:ARG:HH22	1:A:1403:GLU:HA	1.72	0.55
1:A:305:ASP:HB3	1:A:326:ARG:CZ	2.37	0.55
1:A:699:ALA:HB1	7:I:114:GLN:NE2	2.21	0.55
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.34	0.55
1:A:317:LYS:HD3	1:A:321:PRO:CG	2.37	0.55
2:B:561:TRP:O	2:B:590:HIS:HE1	1.90	0.55
2:B:707:PRO:O	2:B:708:GLU:C	2.45	0.55
2:B:809:MET:HG2	2:B:814:PHE:HB3	1.88	0.55
5:F:72:LYS:N	5:F:142:SER:HA	2.21	0.55
10:L:53:HIS:C	10:L:55:ILE:H	2.10	0.55
1:A:805:LEU:HD11	2:B:1052:VAL:HG21	1.87	0.55
6:H:85:GLY:O	6:H:89:LEU:HD21	2.06	0.55
2:B:120:ARG:HH22	10:L:54:ARG:HH11	1.55	0.55
1:A:308:ILE:CG2	1:A:309:ALA:H	1.99	0.55
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.22	0.55
2:B:25:ILE:HD12	2:B:653:VAL:CB	2.35	0.55
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.06	0.55
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.22	0.55
1:A:345:VAL:HG12	1:A:348:SER:OG	2.06	0.55
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.55
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.75	0.55
9:K:18:LYS:HZ2	9:K:38:GLU:CG	2.19	0.55
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.18	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.89	0.54
2:B:707:PRO:O	2:B:709:ASP:N	2.39	0.54
9:K:38:GLU:OE1	9:K:42:LEU:HD22	2.07	0.54
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.47	0.54
1:A:601:LYS:HD2	1:A:603:ASN:HD22	1.71	0.54
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.08	0.54
2:B:105:SER:O	2:B:106:ASP:HB2	2.07	0.54
2:B:229:ALA:C	2:B:231:PRO:HD2	2.28	0.54
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.07	0.54
2:B:311:LEU:HB3	7:I:4:PHE:HZ	1.69	0.54
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.21	0.54
2:B:230:ALA:HA	2:B:261:ARG:NH1	2.22	0.54
2:B:884:ARG:O	2:B:936:ASP:HB2	2.06	0.54
3:C:56:THR:HG23	3:C:57:VAL:N	2.23	0.54
6:H:100:THR:HG23	6:H:138:GLU:CA	2.36	0.54
10:L:38:LEU:O	10:L:39:SER:CB	2.55	0.54
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.90	0.54
2:B:1135:ARG:HG3	2:B:1147:LEU:HD22	1.89	0.54
2:B:604:ARG:NH2	2:B:697:GLU:OE1	2.41	0.54
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.89	0.54
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.34	0.54
3:C:258:ILE:HD13	9:K:35:PHE:CE2	2.40	0.54
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.89	0.54
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.88	0.54
1:A:49:LYS:CD	1:A:55:ASP:HB2	2.30	0.54
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.40	0.54
2:B:515:HIS:HD2	2:B:517:THR:H	1.54	0.54
4:E:116:ILE:HG22	4:E:117:THR:N	2.21	0.54
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.90	0.54
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.73	0.54
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.43	0.54
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:96:VAL:HG13	6:H:143:LEU:CD2	2.37	0.54
7:I:84:VAL:HG12	7:I:102:VAL:HB	1.88	0.54
4:E:9:ILE:HD11	4:E:51:GLY:O	2.07	0.54
1:A:47:ARG:O	1:A:48:ALA:CB	2.56	0.54
2:B:1165:ILE:HG13	2:B:1187:ASN:HD21	1.73	0.54
10:L:27:LEU:O	10:L:27:LEU:HG	2.07	0.54
1:A:562:THR:HB	6:H:98:TYR:HE2	1.72	0.54
1:A:608:ILE:HD12	1:A:613:ILE:HD12	1.90	0.54
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.73	0.54
2:B:1162:ILE:HD13	2:B:1216:LEU:HB2	1.90	0.54
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.43	0.54
3:C:265:MET:CE	9:K:19:LEU:HB2	2.38	0.54
1:A:871:ASP:CB	4:E:204:THR:HG23	2.36	0.54
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.88	0.53
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.72	0.53
1:A:343:LYS:O	1:A:345:VAL:HG23	2.07	0.53
2:B:766:ARG:NH1	2:B:985:GLY:O	2.40	0.53
3:C:165:LYS:O	9:K:6:ARG:NH1	2.41	0.53
1:A:1111:MET:HE3	1:A:1114:PRO:CA	2.38	0.53
1:A:1341:ILE:CD1	1:A:1376:THR:HG23	2.37	0.53
2:B:461:LEU:HD12	2:B:466:TRP:HH2	1.72	0.53
2:B:549:THR:O	2:B:628:THR:CG2	2.56	0.53
3:C:16:ASP:C	3:C:17:ASN:HD22	2.11	0.53
4:E:5:ASN:O	4:E:9:ILE:HG13	2.09	0.53
6:H:103:LYS:HE2	6:H:116:TYR:CE2	2.44	0.53
1:A:243:PRO:C	1:A:245:PRO:HD2	2.29	0.53
1:A:765:VAL:HG23	1:A:802:ASN:O	2.09	0.53
2:B:332:ASP:OD2	2:B:345:LYS:HG3	2.08	0.53
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.43	0.53
1:A:264:PHE:HB3	1:A:315:LEU:CD2	2.27	0.53
1:A:32:VAL:HG23	1:A:33:ALA:H	1.73	0.53
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.44	0.53
2:B:515:HIS:H	2:B:518:HIS:CD2	2.27	0.53
1:A:417:TYR:O	1:A:418:SER:HB2	2.08	0.53
1:A:535:THR:O	1:A:575:LYS:HE3	2.09	0.53
1:A:32:VAL:HB	1:A:57:ARG:CB	2.39	0.53
1:A:626:ASN:O	1:A:631:HIS:CD2	2.62	0.53
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.90	0.53
1:A:423:ASP:CG	1:A:423:ASP:O	2.46	0.53
2:B:199:MET:CE	2:B:491:THR:HG22	2.38	0.53
2:B:542:MET:HE2	2:B:747:MET:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HD13	2:B:95:ILE:HD11	1.91	0.53
6:H:62:SER:O	6:H:63:LEU:C	2.46	0.53
1:A:1390:ASN:O	1:A:1391:ARG:CB	2.56	0.53
1:A:1394:THR:HG22	1:A:1398:MET:HB2	1.91	0.53
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.44	0.53
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.91	0.53
3:C:183:TRP:O	3:C:185:LYS:N	2.39	0.53
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.40	0.53
10:L:38:LEU:HG	10:L:39:SER:N	2.19	0.53
1:A:853:ASP:OD1	1:A:855:THR:HB	2.09	0.53
2:B:680:THR:HG22	2:B:682:SER:N	2.22	0.53
3:C:148:ARG:HD2	8:J:61:LEU:O	2.08	0.53
8:J:43:ARG:O	8:J:47:ARG:HG3	2.09	0.53
10:L:38:LEU:HD22	10:L:56:LEU:HD21	1.91	0.53
1:A:760:GLN:HB2	2:B:1021:MET:HE1	1.91	0.53
2:B:463:THR:HG21	2:B:465:ASN:OD1	2.09	0.53
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.44	0.53
10:L:26:THR:HG22	10:L:27:LEU:N	2.23	0.53
1:A:305:ASP:OD1	1:A:326:ARG:HB2	2.09	0.53
2:B:1081:LEU:CD1	2:B:1085:ILE:HD11	2.39	0.53
10:L:43:THR:O	10:L:43:THR:HG22	2.09	0.53
1:A:1166:ASP:HA	1:A:1169:ILE:HG22	1.91	0.52
1:A:438:ASP:O	1:A:439:ASN:HB2	2.09	0.52
1:A:1438:THR:HG22	2:B:1144:ALA:CB	2.40	0.52
2:B:365:THR:HG22	2:B:366:GLN:N	2.24	0.52
4:E:159:ASP:HA	4:E:162:ARG:NH1	2.23	0.52
4:E:200:ARG:HD2	13:E:221:HOH:O	2.10	0.52
7:I:2:THR:HG22	7:I:2:THR:O	2.09	0.52
1:A:1199:ARG:HA	1:A:1202:MET:HB2	1.91	0.52
1:A:694:THR:O	1:A:698:GLN:HG3	2.08	0.52
1:A:525:GLN:HE21	1:A:752:LYS:HE3	1.73	0.52
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.40	0.52
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.21	0.52
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.39	0.52
1:A:551:TYR:CE2	9:K:62:LYS:HE2	2.45	0.52
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.09	0.52
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.44	0.52
6:H:31:THR:O	6:H:32:THR:HB	2.08	0.52
7:I:31:THR:HG22	7:I:32:CYS:N	2.23	0.52
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.91	0.52
1:A:500:GLU:O	1:A:504:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.44	0.52
1:A:65:LEU:O	1:A:71:GLN:HA	2.08	0.52
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.44	0.52
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.39	0.52
6:H:103:LYS:HZ2	6:H:115:TYR:N	2.07	0.52
1:A:1147:THR:HB	7:I:48:LEU:HD12	1.91	0.52
9:K:47:ARG:HD3	9:K:59:ALA:O	2.10	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.52
2:B:98:THR:HG21	2:B:101:MET:HE1	1.90	0.52
2:B:1153:GLU:CG	2:B:1154:ALA:H	2.21	0.52
2:B:545:ILE:HG12	2:B:633:VAL:HG22	1.90	0.52
1:A:982:THR:HG22	1:A:983:ILE:N	2.24	0.52
1:A:984:LYS:O	1:A:988:LEU:HB2	2.09	0.52
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.09	0.52
2:B:18:PHE:N	2:B:18:PHE:CD2	2.76	0.52
2:B:653:VAL:HG22	13:B:3026:HOH:O	2.10	0.52
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.09	0.52
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.13	0.52
1:A:1277:GLU:CD	1:A:1277:GLU:H	2.13	0.52
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.91	0.52
2:B:731:VAL:CG1	2:B:732:SER:H	2.19	0.52
3:C:73:GLN:HE21	3:C:75:MET:N	2.07	0.52
1:A:32:VAL:HG23	1:A:33:ALA:N	2.24	0.52
2:B:313:MET:HE2	2:B:386:LEU:HD22	1.91	0.52
6:H:96:VAL:HG22	6:H:143:LEU:HD22	1.92	0.52
1:A:262:LEU:O	1:A:266:LEU:HG	2.10	0.52
1:A:443:LEU:HG	1:A:455:MET:HE2	1.91	0.52
2:B:680:THR:HG23	2:B:681:TRP:H	1.75	0.52
2:B:35:SER:HA	2:B:811:TYR:CE2	2.42	0.52
2:B:862:GLN:O	2:B:914:LYS:HE3	2.10	0.52
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.45	0.52
7:I:29:CYS:SG	7:I:31:THR:HB	2.50	0.52
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.45	0.52
2:B:299:GLU:HG2	2:B:571:PRO:CG	2.40	0.52
2:B:351:TYR:O	2:B:355:ILE:HG13	2.11	0.52
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.92	0.51
6:H:76:THR:HG22	6:H:76:THR:O	2.10	0.51
1:A:834:THR:HG21	1:A:1077:THR:HA	1.93	0.51
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.42	0.51
6:H:130:ARG:HA	6:H:133:ASN:HB2	1.93	0.51
6:H:59:ILE:O	6:H:60:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.41	0.51
1:A:753:GLY:O	1:A:754:SER:HB3	2.11	0.51
5:F:93:ILE:HD13	5:F:148:VAL:HG22	1.92	0.51
2:B:120:ARG:NH2	10:L:54:ARG:HH11	2.09	0.51
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.39	0.51
1:A:260:ASP:OD1	1:A:261:ASP:N	2.44	0.51
1:A:317:LYS:HD3	1:A:321:PRO:HG2	1.93	0.51
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.93	0.51
1:A:666:ILE:CD1	2:B:1030:LEU:HB2	2.39	0.51
2:B:101:MET:HB2	2:B:110:HIS:O	2.10	0.51
2:B:199:MET:HE3	2:B:492:LEU:CD2	2.39	0.51
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.45	0.51
1:A:998:LEU:HD12	1:A:1001:ARG:NH1	2.26	0.51
1:A:1402:PHE:C	1:A:1404:GLU:H	2.13	0.51
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.45	0.51
1:A:903:ASN:ND2	1:A:905:ASP:N	2.51	0.51
2:B:1065:GLN:HE22	2:B:1067:ARG:CB	2.23	0.51
2:B:874:PHE:O	2:B:875:GLU:HG3	2.11	0.51
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.40	0.51
2:B:852:ARG:NH2	10:L:70:ARG:O	2.40	0.51
1:A:642:CYS:O	1:A:645:LEU:HB3	2.11	0.51
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.10	0.51
2:B:118:ARG:NH1	2:B:204:ILE:HD11	2.26	0.51
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.91	0.51
1:A:337:ARG:O	1:A:341:MET:HG3	2.11	0.51
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.59	0.51
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.75	0.51
2:B:894:ASP:OD2	10:L:58:LYS:NZ	2.44	0.51
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.91	0.51
1:A:1447:GLU:OE1	1:A:1447:GLU:HA	2.11	0.51
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.93	0.51
2:B:199:MET:HG2	2:B:200:GLY:N	2.25	0.51
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.92	0.51
1:A:535:THR:O	1:A:535:THR:HG22	2.10	0.51
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.40	0.51
6:H:103:LYS:HZ3	6:H:115:TYR:C	2.14	0.51
1:A:710:LEU:HD23	7:I:96:SER:HA	1.93	0.51
9:K:82:ASP:OD1	9:K:84:LYS:N	2.41	0.51
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.24	0.51
1:A:328:ARG:HD3	1:A:332:LYS:NZ	2.26	0.51
2:B:515:HIS:CD2	2:B:517:THR:H	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:48:CYS:SG	10:L:49:LYS:N	2.84	0.51
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.76	0.50
2:B:429:PHE:HA	2:B:432:MET:HE3	1.92	0.50
2:B:43:LEU:HD11	2:B:811:TYR:O	2.11	0.50
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.93	0.50
4:E:90:VAL:HG13	4:E:91:LYS:N	2.25	0.50
1:A:597:LEU:HD23	6:H:104:PHE:CG	2.46	0.50
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.39	0.50
1:A:302:THR:HG23	1:A:306:ASN:OD1	2.12	0.50
1:A:489:LEU:HD23	1:A:489:LEU:C	2.30	0.50
1:A:37:PHE:HD1	1:A:50:ILE:HG21	1.77	0.50
2:B:1099:VAL:O	2:B:1101:ASP:N	2.44	0.50
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.46	0.50
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.50
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.46	0.50
1:A:146:MET:O	1:A:147:VAL:HG23	2.10	0.50
1:A:524:VAL:CG1	1:A:525:GLN:N	2.52	0.50
1:A:672:ASP:OD1	1:A:674:PRO:HD2	2.11	0.50
3:C:43:THR:HG22	3:C:44:LEU:N	2.26	0.50
4:E:71:LYS:O	4:E:73:PRO:HD3	2.11	0.50
6:H:103:LYS:HZ2	6:H:114:VAL:CB	2.24	0.50
1:A:1402:PHE:O	1:A:1404:GLU:N	2.44	0.50
2:B:172:ILE:HD11	2:B:178:ASN:HD22	1.75	0.50
2:B:259:TYR:O	2:B:267:ARG:HG2	2.11	0.50
2:B:557:PHE:HZ	2:B:599:THR:HG21	1.77	0.50
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.41	0.50
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.77	0.50
4:E:93:MET:O	4:E:97:VAL:HG23	2.11	0.50
9:K:103:THR:HG22	9:K:104:ASN:N	2.26	0.50
1:A:709:THR:HB	1:A:712:GLU:HG3	1.93	0.50
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.11	0.50
9:K:113:THR:O	9:K:114:LEU:CB	2.58	0.50
1:A:265:LYS:NZ	1:A:302:THR:HB	2.27	0.50
1:A:823:GLY:O	1:A:827:THR:HB	2.12	0.50
5:F:77:ASP:O	5:F:78:GLN:CB	2.60	0.50
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.41	0.50
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.47	0.50
1:A:225:ASN:ND2	1:A:228:PHE:CD1	2.75	0.50
1:A:345:VAL:HG13	2:B:1150:ARG:HH12	1.76	0.50
1:A:385:ILE:HG13	1:A:428:TYR:HE2	1.77	0.50
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:111:LEU:C	5:F:113:GLY:H	2.15	0.50
1:A:244:PRO:N	1:A:245:PRO:HD2	2.26	0.50
1:A:313:GLN:HB3	1:A:320:ARG:C	2.33	0.50
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.93	0.50
2:B:164:LYS:O	2:B:165:VAL:CB	2.60	0.50
2:B:241:ARG:CG	2:B:251:ILE:HG23	2.42	0.50
2:B:98:THR:HG22	2:B:99:LYS:H	1.77	0.50
1:A:503:GLN:NE2	5:F:90:ARG:HH22	2.10	0.50
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	1.94	0.49
1:A:1187:GLN:CG	1:A:1188:GLN:H	2.25	0.49
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.76	0.49
1:A:282:ASN:O	1:A:283:GLY:O	2.30	0.49
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.94	0.49
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.47	0.49
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.45	0.49
3:C:186:LEU:CD1	3:C:186:LEU:N	2.75	0.49
6:H:101:ALA:C	6:H:103:LYS:H	2.15	0.49
6:H:103:LYS:CG	6:H:115:TYR:O	2.58	0.49
1:A:1391:ARG:NH2	1:A:1417:GLU:HG3	2.27	0.49
1:A:357:PRO:HA	13:A:3038:HOH:O	2.12	0.49
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.45	0.49
1:A:540:PHE:C	1:A:541:ILE:HD12	2.32	0.49
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.92	0.49
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.94	0.49
1:A:327:ALA:HA	1:A:330:LYS:HD2	1.93	0.49
2:B:315:LYS:N	2:B:316:PRO:HD2	2.26	0.49
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.47	0.49
3:C:51:VAL:O	10:L:64:LEU:HD22	2.11	0.49
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.46	0.49
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.47	0.49
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.94	0.49
10:L:46:VAL:O	10:L:54:ARG:HA	2.12	0.49
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.27	0.49
1:A:756:ILE:O	1:A:760:GLN:HG3	2.13	0.49
1:A:831:THR:HG22	1:A:832:ALA:N	2.26	0.49
2:B:60:GLN:O	2:B:63:ILE:HG22	2.13	0.49
3:C:93:ASP:O	3:C:127:ARG:NH2	2.46	0.49
7:I:15:TYR:N	7:I:15:TYR:CD1	2.81	0.49
8:J:48:ARG:O	8:J:52:THR:HB	2.13	0.49
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.43	0.49
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:THR:O	1:A:1386:ARG:HG2	2.12	0.49
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.43	0.49
1:A:614:PHE:C	1:A:614:PHE:CD1	2.86	0.49
1:A:806:ARG:HH12	2:B:729:ILE:HD11	1.77	0.49
2:B:223:VAL:O	2:B:224:GLN:HG3	2.12	0.49
2:B:492:LEU:O	2:B:496:ARG:HG3	2.12	0.49
2:B:680:THR:CG2	2:B:681:TRP:H	2.25	0.49
2:B:884:ARG:O	2:B:936:ASP:HB3	2.12	0.49
2:B:906:SER:HA	2:B:946:ASN:HB2	1.94	0.49
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.42	0.49
7:I:59:VAL:CG1	7:I:60:GLN:N	2.75	0.49
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.28	0.49
1:A:31:SER:OG	1:A:83:HIS:HB2	2.11	0.49
1:A:381:THR:HG21	1:A:383:TYR:HD1	1.77	0.49
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.95	0.49
1:A:704:ALA:HB2	1:A:710:LEU:CD1	2.33	0.49
1:A:90:VAL:HG13	1:A:297:GLN:NE2	2.28	0.49
2:B:1135:ARG:HG3	2:B:1147:LEU:CD2	2.42	0.49
2:B:174:LEU:O	2:B:200:GLY:O	2.29	0.49
3:C:57:VAL:CG1	3:C:57:VAL:O	2.61	0.49
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.11	0.49
3:C:265:MET:HE1	9:K:19:LEU:HB2	1.95	0.49
1:A:362:ASP:N	1:A:362:ASP:OD2	2.46	0.49
1:A:673:GLY:N	1:A:674:PRO:HD2	2.28	0.49
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.95	0.49
2:B:645:SER:O	2:B:647:GLY:N	2.45	0.49
2:B:756:ILE:O	2:B:759:PRO:HD3	2.13	0.49
2:B:906:SER:CB	2:B:946:ASN:HB2	2.43	0.49
2:B:99:LYS:HB3	2:B:180:TYR:CZ	2.47	0.49
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.78	0.49
7:I:50:THR:HG22	7:I:51:ASN:N	2.27	0.49
10:L:39:SER:O	10:L:40:LEU:HD23	2.13	0.49
1:A:57:ARG:HB3	1:A:68:GLN:NE2	2.28	0.49
1:A:878:ILE:HG21	1:A:955:PRO:HB2	1.93	0.49
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.23	0.49
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.48	0.49
2:B:862:GLN:NE2	2:B:963:PHE:CE1	2.81	0.49
3:C:260:LEU:O	3:C:260:LEU:HD12	2.12	0.49
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.47	0.49
4:E:93:MET:HG3	4:E:97:VAL:HG23	1.95	0.49
5:F:107:VAL:HG12	5:F:109:VAL:H	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:154:ASP:O	5:F:155:LEU:HD23	2.12	0.49
10:L:60:ARG:HG2	10:L:61:THR:N	2.25	0.49
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.95	0.49
1:A:849:MET:HE3	1:A:1436:ILE:HA	1.93	0.49
2:B:296:GLU:O	2:B:300:HIS:HD2	1.95	0.49
2:B:733:HIS:O	2:B:735:ALA:N	2.46	0.49
1:A:32:VAL:HG22	1:A:81:PHE:O	2.12	0.49
1:A:32:VAL:CB	1:A:57:ARG:HD2	2.39	0.49
3:C:239:PRO:O	3:C:242:GLN:HB2	2.12	0.49
3:C:89:GLU:O	3:C:90:ASP:CB	2.60	0.49
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.28	0.48
1:A:1107:VAL:O	1:A:1107:VAL:HG12	2.13	0.48
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.13	0.48
2:B:792:MET:SD	2:B:857:ARG:NH2	2.86	0.48
2:B:877:PRO:O	2:B:878:GLN:HG3	2.12	0.48
10:L:61:THR:HG21	10:L:63:ARG:CD	2.40	0.48
1:A:264:PHE:CD1	1:A:315:LEU:HB3	2.48	0.48
1:A:56:PRO:O	1:A:57:ARG:CG	2.61	0.48
4:E:31:THR:C	4:E:33:GLU:N	2.65	0.48
6:H:103:LYS:HZ2	6:H:114:VAL:HB	1.78	0.48
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.48	0.48
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.48	0.48
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.95	0.48
1:A:1147:THR:HB	7:I:48:LEU:CD1	2.43	0.48
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.93	0.48
1:A:326:ARG:O	1:A:330:LYS:HG3	2.13	0.48
1:A:559:VAL:HA	6:H:78:SER:HB3	1.96	0.48
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.15	0.48
2:B:69:LEU:CD2	2:B:425:THR:HG23	2.42	0.48
2:B:816:GLU:O	8:J:56:LEU:HD21	2.14	0.48
3:C:20:PHE:CE1	3:C:22:LEU:HG	2.43	0.48
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.94	0.48
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.01	0.48
1:A:1169:ILE:O	1:A:1173:HIS:CD2	2.67	0.48
1:A:264:PHE:CB	1:A:315:LEU:HD13	2.43	0.48
2:B:648:HIS:N	2:B:648:HIS:CD2	2.79	0.48
10:L:32:ALA:HB2	10:L:55:ILE:CG2	2.43	0.48
1:A:535:THR:HG22	1:A:575:LYS:HE2	1.95	0.48
1:A:602:ASP:O	1:A:615:GLY:HA2	2.13	0.48
1:A:5:GLN:CG	1:A:6:TYR:H	2.26	0.48
2:B:864:LYS:HD3	2:B:871:THR:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:THR:O	3:C:55:THR:HG22	2.14	0.48
6:H:103:LYS:NZ	6:H:114:VAL:CG2	2.76	0.48
6:H:4:THR:O	6:H:5:LEU:HD23	2.13	0.48
1:A:345:VAL:HA	2:B:1150:ARG:NH1	2.23	0.48
1:A:41:MET:O	1:A:42:ASP:HB2	2.13	0.48
1:A:763:ALA:O	1:A:803:SER:HB3	2.13	0.48
2:B:199:MET:HG2	2:B:200:GLY:H	1.78	0.48
2:B:957:ASN:OD1	2:B:958:GLN:N	2.33	0.48
2:B:98:THR:HG22	2:B:99:LYS:N	2.28	0.48
3:C:209:TYR:N	3:C:209:TYR:CD1	2.82	0.48
5:F:81:THR:HG21	5:F:136:ARG:CD	2.43	0.48
1:A:1386:ARG:HG3	1:A:1386:ARG:O	2.13	0.48
1:A:13:THR:CB	1:A:1432:GLN:NE2	2.77	0.48
1:A:313:GLN:HG2	1:A:322:VAL:CG1	2.43	0.48
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.44	0.48
1:A:849:MET:HE1	1:A:1437:GLY:H	1.77	0.48
2:B:806:THR:HG22	2:B:809:MET:N	2.14	0.48
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.43	0.48
4:E:54:GLN:HG3	4:E:57:MET:HE1	1.94	0.48
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.96	0.48
1:A:672:ASP:H	1:A:736:ASN:ND2	2.11	0.48
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.96	0.48
2:B:755:ILE:CG2	2:B:755:ILE:O	2.62	0.48
3:C:5:GLY:O	3:C:24:ASN:ND2	2.40	0.48
4:E:114:ASN:O	4:E:115:ASN:HB3	2.14	0.48
6:H:31:THR:O	6:H:32:THR:CB	2.61	0.48
1:A:1398:MET:O	1:A:1399:ARG:C	2.52	0.48
1:A:857:ARG:HD3	1:A:861:GLY:O	2.13	0.48
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.14	0.48
2:B:880:THR:O	2:B:882:THR:N	2.38	0.48
4:E:4:GLU:O	4:E:5:ASN:C	2.52	0.48
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.49	0.48
8:J:2:ILE:CG2	8:J:3:VAL:N	2.77	0.48
10:L:34:CYS:C	10:L:36:SER:H	2.17	0.48
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.49	0.47
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.61	0.47
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.61	0.47
1:A:84:ILE:CG2	1:A:239:LEU:O	2.62	0.47
1:A:338:GLY:HA2	1:A:341:MET:HE3	1.96	0.47
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.49	0.47
1:A:476:SER:N	1:A:477:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:ASN:HD21	1:A:862:ASN:H	1.62	0.47
2:B:1162:ILE:HD12	2:B:1194:ILE:HD13	1.95	0.47
2:B:953:LEU:C	2:B:953:LEU:HD23	2.34	0.47
8:J:12:LYS:NZ	8:J:17:LYS:NZ	2.63	0.47
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.14	0.47
1:A:329:LEU:HD23	1:A:332:LYS:HB2	1.96	0.47
2:B:879:ARG:HB3	2:B:883:LEU:HD22	1.93	0.47
3:C:53:THR:O	3:C:153:LEU:HA	2.13	0.47
4:E:88:VAL:HG21	4:E:110:PHE:HZ	1.79	0.47
4:E:94:LYS:CG	4:E:123:LEU:HD11	2.41	0.47
4:E:38:PRO:HG2	4:E:41:ASP:OD2	2.14	0.47
1:A:35:ILE:HG23	1:A:52:GLY:O	2.15	0.47
1:A:84:ILE:HG22	1:A:241:VAL:HG23	1.96	0.47
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.45	0.47
2:B:579:ARG:HG3	2:B:581:PHE:HE1	1.79	0.47
4:E:204:THR:CG2	4:E:205:SER:N	2.76	0.47
1:A:446:ARG:HB2	1:A:487:MET:SD	2.54	0.47
2:B:454:THR:O	2:B:458:LYS:HB2	2.15	0.47
2:B:710:LEU:HD23	2:B:738:PHE:CE1	2.49	0.47
3:C:120:ILE:HD13	3:C:124:LEU:HD11	1.96	0.47
3:C:185:LYS:HD2	3:C:213:PRO:HD3	1.96	0.47
1:A:1067:LEU:HD13	13:B:3028:HOH:O	2.13	0.47
1:A:760:GLN:HB2	2:B:1021:MET:CE	2.44	0.47
1:A:982:THR:HG22	1:A:984:LYS:N	2.23	0.47
2:B:268:THR:CG2	2:B:270:LYS:HE3	2.43	0.47
2:B:650:GLU:HG2	2:B:654:ARG:NH1	2.29	0.47
2:B:616:ILE:CD1	2:B:696:GLU:HG3	2.44	0.47
3:C:43:THR:CG2	3:C:44:LEU:N	2.78	0.47
6:H:81:PRO:CB	6:H:82:PRO:CD	2.92	0.47
8:J:36:LEU:HB2	8:J:47:ARG:HH21	1.80	0.47
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.96	0.47
1:A:696:GLU:OE2	1:A:702:LEU:HD23	2.15	0.47
6:H:125:LEU:HB3	6:H:130:ARG:CZ	2.44	0.47
7:I:111:THR:CG2	7:I:112:SER:N	2.77	0.47
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.96	0.47
2:B:100:PRO:HA	2:B:125:SER:O	2.15	0.47
2:B:915:THR:HG22	2:B:916:THR:N	2.30	0.47
4:E:93:MET:HG3	4:E:97:VAL:CG2	2.43	0.47
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.94	0.47
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.95	0.47
2:B:175:ARG:HB3	2:B:175:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.96	0.47
4:E:88:VAL:HG21	4:E:110:PHE:CZ	2.50	0.47
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.15	0.47
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.96	0.47
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.96	0.47
1:A:329:LEU:HD21	2:B:1203:LEU:HD13	1.97	0.47
2:B:221:ASN:OD1	2:B:242:SER:HA	2.15	0.47
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.96	0.47
1:A:264:PHE:O	1:A:267:ALA:HB3	2.15	0.47
1:A:329:LEU:HD21	2:B:1203:LEU:CD1	2.45	0.47
2:B:126:SER:OG	2:B:172:ILE:HD12	2.15	0.47
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.50	0.47
7:I:69:PRO:HG2	7:I:85:PHE:O	2.15	0.47
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.35	0.46
1:A:761:MET:O	1:A:803:SER:HB2	2.15	0.46
2:B:172:ILE:HD11	2:B:178:ASN:ND2	2.31	0.46
1:A:114:LEU:HD13	1:A:171:GLN:OE1	2.15	0.46
1:A:130:ASP:CB	1:A:133:LYS:HB2	2.40	0.46
1:A:1391:ARG:HB3	1:A:1392:SER:H	1.59	0.46
2:B:1004:GLU:HA	3:C:177:GLU:HG2	1.98	0.46
2:B:130:VAL:CG1	2:B:131:ASP:H	2.22	0.46
2:B:357:GLN:OE1	2:B:358:LYS:HE3	2.16	0.46
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.97	0.46
1:A:328:ARG:HD3	1:A:332:LYS:HZ1	1.81	0.46
1:A:17:VAL:HA	2:B:1215:ARG:O	2.15	0.46
2:B:906:SER:O	2:B:907:GLY:C	2.53	0.46
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.80	0.46
1:A:1171:GLN:O	1:A:1173:HIS:N	2.48	0.46
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.78	0.46
1:A:569:LYS:HE3	3:C:221:TYR:O	2.15	0.46
2:B:98:THR:O	2:B:126:SER:HB3	2.16	0.46
2:B:130:VAL:CG1	2:B:131:ASP:N	2.79	0.46
2:B:879:ARG:HE	2:B:885:MET:CE	2.28	0.46
3:C:125:MET:HE2	3:C:127:ARG:NH2	2.29	0.46
3:C:174:ALA:O	8:J:10:CYS:O	2.33	0.46
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.49	0.46
1:A:1336:MET:HE1	1:A:1381:LEU:H	1.76	0.46
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.56	0.46
1:A:318:SER:O	1:A:320:ARG:HG3	2.15	0.46
1:A:329:LEU:C	1:A:331:GLY:H	2.18	0.46
1:A:982:THR:O	1:A:985:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.96	0.46
1:A:562:THR:HB	6:H:98:TYR:CE2	2.50	0.46
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.98	0.46
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.97	0.46
1:A:1015:VAL:O	1:A:1015:VAL:CG1	2.63	0.46
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.15	0.46
1:A:326:ARG:CG	1:A:1406:VAL:HG21	2.42	0.46
1:A:322:VAL:CG2	1:A:323:LYS:N	2.78	0.46
1:A:47:ARG:HH12	1:A:255:SER:CA	2.07	0.46
1:A:57:ARG:C	1:A:68:GLN:HE21	2.19	0.46
2:B:731:VAL:CG1	2:B:732:SER:N	2.78	0.46
2:B:806:THR:HG22	2:B:809:MET:HB2	1.97	0.46
2:B:859:TYR:CD1	2:B:859:TYR:N	2.84	0.46
7:I:55:THR:O	7:I:58:VAL:HG23	2.15	0.46
7:I:90:GLN:O	7:I:91:ARG:HD3	2.15	0.46
10:L:48:CYS:HB3	10:L:51:CYS:O	2.16	0.46
1:A:1113:THR:N	1:A:1114:PRO:HD3	2.31	0.46
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.98	0.46
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.46	0.46
1:A:817:ALA:HA	2:B:764:SER:OG	2.15	0.46
2:B:1185:CYS:O	2:B:1186:ASP:HB2	2.15	0.46
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.45	0.46
5:F:82:THR:HG22	5:F:83:PRO:HD2	1.97	0.46
6:H:139:ASN:O	6:H:140:ALA:HB2	2.15	0.46
2:B:309:GLN:HE22	7:I:50:THR:HG21	1.81	0.46
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.97	0.46
1:A:1169:ILE:O	1:A:1173:HIS:HD2	1.99	0.46
1:A:1161:THR:HG21	1:A:1239:ARG:NH2	2.31	0.46
1:A:1256:GLU:O	1:A:1258:HIS:N	2.49	0.46
1:A:112:LYS:HZ1	1:A:165:GLY:H	1.63	0.46
2:B:18:PHE:O	2:B:19:GLU:HB2	2.16	0.46
3:C:57:VAL:O	3:C:57:VAL:HG12	2.16	0.46
10:L:34:CYS:O	10:L:36:SER:N	2.49	0.46
1:A:246:VAL:O	1:A:328:ARG:NH1	2.45	0.46
1:A:445:ASN:HD21	1:A:449:SER:HB3	1.79	0.46
1:A:5:GLN:HG2	1:A:6:TYR:H	1.80	0.46
1:A:93:VAL:HG13	1:A:301:ALA:CB	2.43	0.46
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.98	0.46
2:B:1065:GLN:O	2:B:1065:GLN:HG3	2.15	0.46
2:B:1183:LYS:C	2:B:1185:CYS:H	2.20	0.46
2:B:365:THR:CG2	2:B:367:LEU:H	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:112:ILE:HD12	6:H:131:ASN:HD21	1.81	0.46
1:A:1111:MET:CE	1:A:1331:SER:HB2	2.45	0.45
1:A:381:THR:HG23	1:A:383:TYR:N	2.20	0.45
1:A:567:LYS:HZ1	6:H:46:LEU:HD12	1.82	0.45
2:B:108:VAL:HG12	2:B:109:THR:N	2.30	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.45
3:C:263:THR:C	3:C:265:MET:H	2.19	0.45
3:C:52:GLU:HA	10:L:64:LEU:HD21	1.97	0.45
5:F:81:THR:CG2	5:F:82:THR:N	2.79	0.45
9:K:61:TYR:HA	9:K:72:LYS:O	2.16	0.45
1:A:108:MET:HA	1:A:210:ILE:HD13	1.98	0.45
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.17	0.45
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.45	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
2:B:241:ARG:HG2	2:B:251:ILE:HG23	1.97	0.45
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.52	0.45
4:E:14:ARG:O	4:E:17:ARG:HB3	2.15	0.45
4:E:64:PRO:HG2	4:E:75:MET:O	2.16	0.45
5:F:134:ILE:HD12	5:F:151:LEU:CD1	2.46	0.45
2:B:104:GLU:CG	10:L:54:ARG:NH1	2.79	0.45
1:A:315:LEU:C	1:A:317:LYS:H	2.19	0.45
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.97	0.45
2:B:424:LEU:O	2:B:428:ILE:HG13	2.16	0.45
2:B:914:LYS:O	2:B:937:ALA:O	2.33	0.45
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.81	0.45
6:H:103:LYS:HE2	6:H:116:TYR:CZ	2.51	0.45
6:H:32:THR:HG22	6:H:33:GLN:N	2.31	0.45
9:K:111:LEU:N	9:K:111:LEU:HD23	2.31	0.45
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.97	0.45
1:A:345:VAL:HG13	2:B:1150:ARG:NH1	2.31	0.45
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.51	0.45
1:A:45:GLN:O	1:A:47:ARG:N	2.49	0.45
1:A:715:GLU:OE1	1:A:774:ARG:NH1	2.49	0.45
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.16	0.45
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.33	0.45
2:B:451:LYS:HE2	2:B:455:SER:OG	2.16	0.45
4:E:202:SER:O	4:E:205:SER:O	2.33	0.45
4:E:5:ASN:O	4:E:9:ILE:N	2.48	0.45
7:I:51:ASN:HB2	7:I:118:ARG:NH1	2.31	0.45
1:A:106:VAL:HG22	1:A:111:GLY:HA2	1.99	0.45
1:A:32:VAL:CG2	1:A:58:LEU:HD23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	1:A:79:GLY:C	2.55	0.45
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.47	0.45
3:C:17:ASN:HA	3:C:232:VAL:O	2.16	0.45
4:E:19:VAL:HG11	4:E:80:VAL:HG11	1.96	0.45
1:A:1146:VAL:O	1:A:1146:VAL:HG12	2.16	0.45
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.64	0.45
1:A:167:CYS:SG	1:A:167:CYS:O	2.75	0.45
1:A:736:ASN:O	1:A:737:LEU:C	2.55	0.45
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.56	0.45
2:B:254:LEU:HD23	2:B:361:LEU:HD21	1.99	0.45
1:A:382:PRO:HD2	5:F:104:ASN:OD1	2.16	0.45
6:H:62:SER:O	6:H:63:LEU:O	2.34	0.45
10:L:25:ALA:O	10:L:26:THR:HB	2.16	0.45
1:A:806:ARG:NH1	2:B:729:ILE:HD11	2.31	0.45
2:B:169:ARG:N	2:B:454:THR:OG1	2.49	0.45
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.47	0.45
4:E:114:ASN:OD1	4:E:115:ASN:N	2.50	0.45
6:H:12:VAL:HA	6:H:28:ALA:CB	2.46	0.45
6:H:26:ILE:CD1	6:H:42:ILE:HD12	2.31	0.45
6:H:89:LEU:O	6:H:91:ASP:N	2.49	0.45
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.32	0.45
1:A:220:THR:O	1:A:222:LEU:O	2.35	0.45
2:B:794:ASN:C	2:B:795:ILE:HD12	2.36	0.45
1:A:1395:GLY:C	1:A:1397:LEU:N	2.69	0.45
1:A:92:HIS:HE1	2:B:1210:MET:O	2.00	0.45
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.98	0.45
1:A:1277:GLU:CD	1:A:1277:GLU:N	2.71	0.45
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.75	0.45
1:A:35:ILE:CD1	1:A:241:VAL:HG21	2.46	0.45
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.31	0.45
2:B:999:MET:CE	2:B:1011:ILE:HD11	2.46	0.45
2:B:227:LYS:HD3	2:B:236:HIS:CE1	2.51	0.45
6:H:100:THR:HG22	6:H:101:ALA:N	2.32	0.45
7:I:45:ARG:NH1	7:I:45:ARG:CG	2.77	0.45
3:C:8:VAL:HG21	9:K:105:PHE:CB	2.45	0.45
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.48	0.44
1:A:185:TRP:O	1:A:186:LYS:HB2	2.17	0.44
1:A:278:THR:O	1:A:278:THR:HG22	2.17	0.44
1:A:535:THR:CG2	1:A:575:LYS:HE2	2.47	0.44
1:A:95:PHE:O	1:A:99:ILE:HG13	2.17	0.44
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:147:HIS:CD2	4:E:149:LEU:H	2.35	0.44
6:H:130:ARG:CA	6:H:133:ASN:HD22	2.12	0.44
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.18	0.44
1:A:44:THR:O	1:A:45:GLN:CB	2.65	0.44
1:A:511:ILE:O	1:A:519:PRO:HA	2.17	0.44
2:B:235:SER:OG	2:B:236:HIS:HD2	2.00	0.44
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.51	0.44
2:B:860:MET:O	2:B:861:ASP:HB2	2.17	0.44
7:I:111:THR:CG2	7:I:113:ASP:H	2.06	0.44
8:J:2:ILE:HG22	8:J:3:VAL:H	1.82	0.44
1:A:466:SER:C	1:A:467:THR:HG23	2.38	0.44
1:A:684:ALA:O	1:A:688:LYS:HG3	2.17	0.44
2:B:102:VAL:HG22	2:B:112:LEU:HD13	2.00	0.44
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.18	0.44
2:B:1162:ILE:CD1	2:B:1216:LEU:HD12	2.46	0.44
2:B:502:ILE:O	2:B:502:ILE:HG22	2.16	0.44
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.51	0.44
2:B:899:ILE:HG22	2:B:900:ALA:H	1.81	0.44
1:A:67:CYS:O	1:A:70:CYS:SG	2.76	0.44
2:B:280:ILE:HA	2:B:281:PRO:HD2	1.89	0.44
3:C:148:ARG:HG2	3:C:149:LYS:N	2.33	0.44
3:C:99:LEU:HD12	3:C:99:LEU:N	2.32	0.44
5:F:79:ARG:HB3	5:F:144:GLU:OE1	2.18	0.44
9:K:68:PHE:N	9:K:68:PHE:CD1	2.86	0.44
1:A:5:GLN:HG2	1:A:6:TYR:N	2.33	0.44
1:A:73:GLY:C	1:A:75:ASN:H	2.20	0.44
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.17	0.44
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.99	0.44
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.32	0.44
3:C:97:VAL:HB	3:C:159:ALA:HB3	1.99	0.44
1:A:1260:LEU:HA	1:A:1260:LEU:HD12	1.85	0.44
1:A:1422:ARG:HA	1:A:1435:PRO:CG	2.48	0.44
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.99	0.44
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.35	0.44
2:B:916:THR:O	2:B:935:ARG:HB2	2.17	0.44
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.98	0.44
6:H:79:TRP:HA	6:H:80:ARG:N	2.15	0.44
7:I:4:PHE:N	7:I:4:PHE:CD2	2.81	0.44
1:A:672:ASP:H	1:A:736:ASN:HD21	1.63	0.44
1:A:829:VAL:O	1:A:830:LYS:C	2.56	0.44
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:CG2	2:B:550:ASP:N	2.80	0.44
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.21	0.44
1:A:1328:TYR:CG	1:A:1329:THR:N	2.85	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.00	0.44
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.50	0.44
1:A:775:ILE:O	1:A:797:LYS:HE3	2.17	0.44
1:A:34:LYS:HG3	1:A:83:HIS:CD2	2.53	0.44
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.98	0.44
3:C:22:LEU:HA	3:C:22:LEU:HD23	1.87	0.44
4:E:159:ASP:HA	4:E:162:ARG:HH11	1.82	0.44
9:K:108:GLU:O	9:K:112:GLN:HG2	2.18	0.44
1:A:709:THR:HG22	1:A:710:LEU:N	2.33	0.44
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.99	0.44
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.51	0.44
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.33	0.44
1:A:1138:ILE:CG2	1:A:1279:ILE:HG21	2.47	0.43
1:A:179:LEU:HD21	1:A:308:ILE:CD1	2.43	0.43
1:A:41:MET:HG2	1:A:48:ALA:O	2.18	0.43
1:A:5:GLN:CG	1:A:6:TYR:N	2.81	0.43
1:A:971:PHE:O	1:A:972:HIS:C	2.55	0.43
2:B:357:GLN:O	2:B:357:GLN:HG2	2.17	0.43
4:E:156:LEU:HD21	4:E:197:LYS:HB2	2.00	0.43
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.17	0.43
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.33	0.43
1:A:282:ASN:C	1:A:283:GLY:O	2.57	0.43
1:A:789:LYS:O	1:A:790:ASP:HB2	2.18	0.43
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.53	0.43
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.18	0.43
2:B:420:LEU:HD11	2:B:456:GLY:HA3	1.98	0.43
2:B:526:GLU:O	2:B:526:GLU:HG2	2.18	0.43
2:B:796:LEU:HD12	2:B:796:LEU:HA	1.87	0.43
3:C:134:ILE:CG2	3:C:139:GLY:HA2	2.48	0.43
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.82	0.43
7:I:50:THR:CB	7:I:92:ARG:HH22	2.31	0.43
1:A:1171:GLN:C	1:A:1173:HIS:H	2.21	0.43
1:A:1217:LYS:C	1:A:1219:THR:H	2.22	0.43
1:A:1394:THR:CG2	1:A:1395:GLY:N	2.65	0.43
1:A:43:GLU:O	1:A:44:THR:HB	2.17	0.43
1:A:854:ASN:HD22	1:A:1000:LEU:HD23	1.82	0.43
1:A:90:VAL:HG12	1:A:91:PHE:O	2.19	0.43
2:B:487:THR:HG22	2:B:489:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.18	0.43
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.01	0.43
5:F:93:ILE:CD1	5:F:148:VAL:HG22	2.49	0.43
6:H:103:LYS:CE	6:H:116:TYR:CZ	3.02	0.43
7:I:55:THR:CG2	7:I:55:THR:O	2.65	0.43
1:A:1100:ARG:O	1:A:1100:ARG:HD2	2.18	0.43
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.43
3:C:100:THR:HG22	3:C:101:LEU:N	2.34	0.43
4:E:86:PRO:HA	4:E:113:GLN:HB2	2.00	0.43
6:H:123:MET:HE3	6:H:142:LEU:CD2	2.48	0.43
6:H:27:GLU:HA	6:H:38:LEU:O	2.17	0.43
7:I:103:CYS:HB3	7:I:108:HIS:H	1.83	0.43
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.53	0.43
1:A:1295:THR:O	1:A:1295:THR:HG22	2.17	0.43
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.43
1:A:246:VAL:O	1:A:248:PRO:HD3	2.19	0.43
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.54	0.43
2:B:339:THR:HG23	2:B:343:ILE:HB	2.01	0.43
2:B:623:GLU:OE1	2:B:625:LYS:HE3	2.18	0.43
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.38	0.43
9:K:90:ALA:O	9:K:94:ILE:HG13	2.19	0.43
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.54	0.43
1:A:596:THR:C	1:A:598:LEU:H	2.22	0.43
1:A:598:LEU:HG	6:H:115:TYR:CE2	2.52	0.43
1:A:914:GLU:HB2	1:A:979:SER:O	2.19	0.43
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.49	0.43
2:B:1098:MET:O	2:B:1099:VAL:C	2.57	0.43
2:B:636:PRO:HA	2:B:691:GLU:O	2.19	0.43
2:B:63:ILE:CD1	2:B:95:ILE:HD11	2.49	0.43
4:E:129:PRO:O	4:E:130:ALA:C	2.56	0.43
6:H:138:GLU:O	6:H:139:ASN:C	2.56	0.43
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.18	0.43
1:A:1421:CYS:HA	1:A:1426:GLU:OE1	2.19	0.43
1:A:626:ASN:O	1:A:631:HIS:HD2	2.00	0.43
2:B:248:SER:HG	2:B:250:PHE:HE1	1.66	0.43
2:B:29:ASP:HB3	2:B:658:ILE:HD12	1.91	0.43
2:B:952:VAL:HB	10:L:58:LYS:CB	2.46	0.43
9:K:1:MET:HG3	9:K:2:ASN:N	2.33	0.43
10:L:61:THR:HB	10:L:63:ARG:HG2	2.00	0.43
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.32	0.43
1:A:1402:PHE:C	1:A:1404:GLU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:C	1:A:52:GLY:H	2.21	0.43
1:A:535:THR:HG22	1:A:616:VAL:HA	2.01	0.43
1:A:858:ASN:HD22	1:A:858:ASN:C	2.21	0.43
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.17	0.43
2:B:638:PHE:CE2	2:B:653:VAL:HG21	2.54	0.43
4:E:45:LYS:HG2	4:E:45:LYS:O	2.18	0.43
6:H:99:GLY:N	6:H:118:PHE:CD2	2.87	0.43
6:H:89:LEU:C	6:H:91:ASP:N	2.72	0.43
7:I:95:THR:CG2	7:I:96:SER:N	2.79	0.43
8:J:48:ARG:HG3	8:J:49:MET:N	2.33	0.43
9:K:30:ALA:HB2	9:K:76:GLN:HG3	2.01	0.43
1:A:444:PHE:CE2	1:A:487:MET:HE1	2.53	0.43
1:A:49:LYS:HB3	1:A:55:ASP:HB2	2.00	0.43
1:A:557:ASP:N	1:A:557:ASP:OD1	2.51	0.43
1:A:786:HIS:HE1	2:B:742:GLU:OE2	2.02	0.43
1:A:84:ILE:CG2	1:A:241:VAL:HG23	2.48	0.43
2:B:397:ASP:OD2	2:B:515:HIS:HE1	2.01	0.43
4:E:45:LYS:HE2	4:E:46:TYR:CZ	2.54	0.43
4:E:28:TYR:CE2	4:E:78:LEU:HG	2.54	0.43
6:H:47:PHE:CD2	6:H:47:PHE:O	2.71	0.43
6:H:11:GLN:HE22	6:H:52:GLN:HA	1.80	0.43
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.18	0.43
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.19	0.43
1:A:261:ASP:O	1:A:264:PHE:HB2	2.19	0.43
1:A:347:PHE:H	2:B:1107:ALA:HA	1.84	0.43
1:A:565:ILE:HG23	1:A:567:LYS:HE2	2.00	0.43
1:A:69:THR:HB	2:B:1174:LYS:HE2	2.01	0.43
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.19	0.43
2:B:487:THR:CG2	2:B:488:TYR:N	2.82	0.43
3:C:179:GLU:HG3	3:C:180:TYR:H	1.82	0.43
5:F:140:ASP:OD1	5:F:141:GLY:N	2.51	0.43
6:H:111:LEU:HB3	6:H:127:GLY:O	2.18	0.43
9:K:63:VAL:O	9:K:63:VAL:HG22	2.19	0.43
10:L:46:VAL:HG13	10:L:56:LEU:CD1	2.40	0.43
10:L:49:LYS:HD3	10:L:49:LYS:HA	1.77	0.43
1:A:907:THR:CG2	1:A:908:LEU:N	2.81	0.42
2:B:1127:GLY:O	2:B:1128:LEU:CB	2.65	0.42
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.19	0.42
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.54	0.42
1:A:946:VAL:CG2	4:E:201:LYS:HD2	2.48	0.42
5:F:81:THR:HG21	5:F:136:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:59:VAL:HG12	7:I:60:GLN:N	2.33	0.42
8:J:12:LYS:HZ1	8:J:17:LYS:NZ	2.16	0.42
1:A:313:GLN:HB3	1:A:321:PRO:N	2.34	0.42
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.52	0.42
1:A:54:ASN:O	1:A:55:ASP:HB2	2.18	0.42
1:A:557:ASP:O	1:A:559:VAL:N	2.53	0.42
2:B:108:VAL:CG1	2:B:109:THR:N	2.82	0.42
2:B:1148:LYS:HG3	2:B:1152:MET:HE3	1.99	0.42
2:B:858:SER:HA	2:B:966:VAL:O	2.20	0.42
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.54	0.42
10:L:30:ILE:O	10:L:56:LEU:HA	2.19	0.42
1:A:311:GLN:O	1:A:313:GLN:HG3	2.20	0.42
1:A:834:THR:HG21	1:A:1077:THR:CA	2.49	0.42
2:B:276:ILE:HG23	2:B:337:ARG:HB2	2.01	0.42
2:B:872:GLU:HA	2:B:915:THR:O	2.18	0.42
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.85	0.42
4:E:55:ARG:HB2	4:E:84:ASP:OD2	2.20	0.42
6:H:142:LEU:O	6:H:143:LEU:HD23	2.18	0.42
6:H:63:LEU:C	6:H:90:ALA:CB	2.87	0.42
9:K:28:PRO:O	9:K:29:ASN:HB2	2.20	0.42
9:K:56:VAL:HA	9:K:77:THR:HG22	2.00	0.42
1:A:740:LEU:CD1	1:A:740:LEU:N	2.82	0.42
1:A:31:SER:HB2	1:A:83:HIS:HB2	2.00	0.42
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.84	0.42
1:A:879:GLU:O	1:A:955:PRO:HA	2.20	0.42
2:B:969:ARG:NH1	2:B:969:ARG:HB3	2.33	0.42
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.60	0.42
8:J:48:ARG:CG	8:J:48:ARG:HH11	2.31	0.42
10:L:61:THR:CG2	10:L:63:ARG:HG2	2.50	0.42
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.20	0.42
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	2.02	0.42
1:A:1434:ALA:O	1:A:1436:ILE:N	2.46	0.42
1:A:324:SER:H	1:A:327:ALA:HB3	1.84	0.42
2:B:899:ILE:CG2	2:B:900:ALA:N	2.81	0.42
6:H:93:TYR:CD1	6:H:93:TYR:N	2.87	0.42
8:J:32:GLU:CD	8:J:32:GLU:H	2.22	0.42
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.60	0.42
1:A:1111:MET:HE3	1:A:1114:PRO:CG	2.48	0.42
1:A:1215:ARG:CA	1:A:1218:GLN:HG2	2.50	0.42
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.19	0.42
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:C	1:A:159:THR:N	2.71	0.42
1:A:44:THR:O	1:A:44:THR:HG22	2.19	0.42
1:A:367:PRO:HB3	1:A:465:TYR:O	2.19	0.42
1:A:699:ALA:O	1:A:700:ASN:HB3	2.20	0.42
2:B:1072:MET:HE2	2:B:1087:PHE:CG	2.55	0.42
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.59	0.42
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.83	0.42
2:B:63:ILE:O	2:B:63:ILE:HG23	2.19	0.42
2:B:978:ASP:O	2:B:989:THR:HA	2.20	0.42
3:C:44:LEU:CG	3:C:159:ALA:HB1	2.49	0.42
3:C:51:VAL:HG12	10:L:60:ARG:HH12	1.84	0.42
4:E:98:ILE:O	4:E:102:GLU:HG3	2.20	0.42
7:I:111:THR:HG22	7:I:112:SER:N	2.34	0.42
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.01	0.42
1:A:353:ILE:HD13	1:A:487:MET:CE	2.48	0.42
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.02	0.42
1:A:486:GLU:OE1	2:B:1102:LYS:HD3	2.20	0.42
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.84	0.42
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.34	0.42
5:F:138:LEU:HD12	5:F:142:SER:OG	2.19	0.42
6:H:55:LEU:HD22	6:H:144:ILE:CG2	2.50	0.42
7:I:15:TYR:CZ	7:I:30:ARG:HD2	2.54	0.42
10:L:30:ILE:CG2	10:L:31:CYS:N	2.82	0.42
1:A:1145:SER:HB2	1:A:1205:LYS:NZ	2.34	0.42
1:A:535:THR:CG2	1:A:616:VAL:HA	2.49	0.42
1:A:68:GLN:O	1:A:69:THR:HB	2.20	0.42
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.50	0.42
2:B:446:LEU:O	2:B:447:ALA:HB3	2.20	0.42
2:B:496:ARG:NH2	2:B:541:LEU:HA	2.34	0.42
2:B:881:ASN:HB2	2:B:933:SER:OG	2.20	0.42
3:C:114:TYR:HB3	3:C:140:ASN:O	2.20	0.42
3:C:179:GLU:CG	3:C:180:TYR:N	2.82	0.42
2:B:847:ASP:O	3:C:65:HIS:HE1	2.02	0.42
4:E:58:MET:O	4:E:59:SER:O	2.38	0.42
6:H:97:MET:CE	6:H:142:LEU:HD23	2.50	0.42
1:A:1342:GLU:CG	4:E:198:ILE:HD13	2.49	0.42
1:A:368:LYS:HB2	1:A:368:LYS:HE3	1.66	0.42
1:A:856:THR:HB	1:A:865:GLN:HB2	2.01	0.42
2:B:125:SER:HA	2:B:171:PRO:HA	2.01	0.42
2:B:89:GLU:N	2:B:135:ARG:O	2.53	0.42
2:B:512:ARG:HB2	2:B:534:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:THR:HA	1:A:1398:MET:CE	2.50	0.42
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.33	0.42
1:A:475:THR:HG22	1:A:476:SER:N	2.34	0.42
1:A:49:LYS:HB3	1:A:55:ASP:CB	2.49	0.42
1:A:63:ARG:HA	1:A:74:MET:CE	2.48	0.42
1:A:836:TYR:O	1:A:840:ARG:HG2	2.20	0.42
1:A:946:VAL:HG22	4:E:201:LYS:CD	2.49	0.42
2:B:310:MET:O	2:B:313:MET:HB2	2.20	0.42
2:B:882:THR:C	2:B:884:ARG:H	2.23	0.42
3:C:64:ALA:HA	3:C:67:LEU:HD12	2.01	0.42
3:C:71:PRO:O	3:C:72:LEU:HD23	2.19	0.42
7:I:75:CYS:O	7:I:77:LYS:N	2.53	0.42
1:A:125:ALA:O	1:A:134:ARG:HG3	2.20	0.41
1:A:40:THR:O	1:A:41:MET:HB2	2.20	0.41
1:A:879:GLU:CD	1:A:962:ARG:HH22	2.23	0.41
2:B:563:MET:HE3	2:B:580:VAL:HB	2.00	0.41
2:B:863:GLU:OE1	2:B:962:LYS:HD2	2.20	0.41
5:F:74:ILE:HG23	5:F:75:PRO:HD2	2.01	0.41
6:H:18:GLY:O	6:H:20:TYR:N	2.52	0.41
7:I:17:ARG:HG3	7:I:28:GLU:OE1	2.20	0.41
1:A:329:LEU:O	1:A:333:GLU:HG2	2.20	0.41
1:A:48:ALA:C	1:A:49:LYS:HG3	2.40	0.41
2:B:181:LEU:HD22	2:B:189:LEU:HD23	2.01	0.41
2:B:239:GLU:HG2	2:B:255:GLN:HG2	2.02	0.41
2:B:335:GLY:O	2:B:339:THR:HB	2.20	0.41
2:B:274:PRO:HG3	2:B:359:GLU:HB3	2.01	0.41
2:B:787:VAL:O	2:B:787:VAL:HG12	2.19	0.41
3:C:263:THR:HG22	3:C:264:GLN:N	2.34	0.41
4:E:144:ILE:HG13	4:E:145:THR:N	2.34	0.41
8:J:5:VAL:HG12	8:J:6:ARG:HG2	2.02	0.41
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	2.02	0.41
1:A:1163:ILE:HA	1:A:1164:PRO:HD2	1.90	0.41
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.20	0.41
1:A:1199:ARG:CG	1:A:1236:LEU:HD11	2.50	0.41
1:A:450:LEU:CB	1:A:838:GLN:NE2	2.83	0.41
2:B:92:PHE:CD2	2:B:132:VAL:HG22	2.56	0.41
2:B:314:LEU:O	2:B:317:CYS:HB2	2.20	0.41
2:B:324:ILE:HD11	2:B:333:PHE:CG	2.55	0.41
7:I:113:ASP:O	7:I:116:ASN:CG	2.59	0.41
2:B:104:GLU:CD	10:L:54:ARG:CZ	2.89	0.41
1:A:451:HIS:CG	1:A:1074:GLU:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:HG22	1:A:336:ILE:O	2.20	0.41
1:A:340:LEU:HD13	1:A:1399:ARG:HA	2.02	0.41
1:A:531:ILE:HG23	1:A:617:VAL:O	2.21	0.41
3:C:112:ASN:CB	3:C:114:TYR:CE1	3.04	0.41
3:C:186:LEU:HD12	3:C:186:LEU:N	2.36	0.41
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.50	0.41
3:C:237:SER:O	3:C:238:ILE:HG13	2.19	0.41
4:E:62:ALA:O	4:E:77:SER:HB2	2.20	0.41
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.51	0.41
9:K:18:LYS:NZ	9:K:38:GLU:CG	2.82	0.41
1:A:465:TYR:CE2	9:K:4:PRO:HD2	2.54	0.41
9:K:76:GLN:HE21	9:K:76:GLN:HB3	1.69	0.41
3:C:166:GLU:HG2	10:L:70:ARG:NH1	2.35	0.41
1:A:112:LYS:NZ	1:A:164:ARG:HB2	2.35	0.41
1:A:164:ARG:O	1:A:165:GLY:C	2.59	0.41
1:A:82:GLY:HA3	1:A:241:VAL:HB	2.02	0.41
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	2.02	0.41
2:B:344:LYS:H	2:B:347:LYS:HE3	1.85	0.41
2:B:549:THR:HG22	2:B:628:THR:CG2	2.51	0.41
2:B:879:ARG:HG3	2:B:885:MET:HE1	2.03	0.41
4:E:98:ILE:HG22	4:E:102:GLU:OE1	2.20	0.41
1:A:1391:ARG:O	1:A:1392:SER:HB3	2.21	0.41
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.01	0.41
2:B:274:PRO:O	2:B:275:TYR:HB2	2.21	0.41
6:H:100:THR:HG23	6:H:138:GLU:CB	2.50	0.41
9:K:18:LYS:O	9:K:19:LEU:HD23	2.20	0.41
1:A:267:ALA:O	1:A:271:LYS:HG3	2.20	0.41
2:B:1103:ILE:O	2:B:1104:HIS:C	2.59	0.41
2:B:365:THR:CG2	2:B:366:GLN:N	2.84	0.41
2:B:564:GLU:OE2	2:B:591:ARG:NE	2.47	0.41
4:E:40:GLU:OE1	4:E:43:LYS:HD2	2.21	0.41
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.61	0.41
7:I:43:VAL:HG12	7:I:43:VAL:O	2.20	0.41
3:C:265:MET:HE3	9:K:19:LEU:HB2	2.03	0.41
1:A:548:ASN:ND2	9:K:47:ARG:HH21	2.19	0.41
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.34	0.41
1:A:1422:ARG:HA	1:A:1435:PRO:HG3	2.03	0.41
1:A:262:LEU:HD11	1:A:328:ARG:HD2	2.03	0.41
1:A:901:LEU:HG	1:A:929:LEU:HD12	2.03	0.41
2:B:174:LEU:HD22	2:B:202:TYR:CZ	2.56	0.41
5:F:140:ASP:OD1	5:F:140:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HB	1:A:57:ARG:HB3	2.03	0.41
1:A:774:ARG:CB	1:A:797:LYS:HG2	2.51	0.41
2:B:1148:LYS:HG3	2:B:1152:MET:CE	2.51	0.41
1:A:16:GLU:HG3	2:B:1220:ARG:HA	2.03	0.41
2:B:708:GLU:O	2:B:711:GLU:CD	2.59	0.41
2:B:744:HIS:CD2	2:B:746:SER:H	2.38	0.41
2:B:806:THR:HG23	2:B:808:ALA:H	1.86	0.41
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.02	0.41
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.34	0.41
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.86	0.41
1:A:1384:VAL:O	1:A:1386:ARG:N	2.48	0.41
2:B:1084:GLN:HE22	3:C:192:TRP:N	2.16	0.41
2:B:1109:GLY:H	2:B:1110:PRO:HD2	1.85	0.41
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.56	0.41
3:C:248:ILE:HD13	9:K:101:LEU:HD13	2.03	0.41
4:E:116:ILE:CG2	4:E:117:THR:N	2.84	0.41
4:E:40:GLU:OE1	4:E:40:GLU:HA	2.21	0.41
5:F:111:LEU:C	5:F:113:GLY:N	2.73	0.41
1:A:1446:ASP:CG	1:A:1448:GLU:HB2	2.41	0.41
1:A:834:THR:CG2	1:A:1077:THR:OG1	2.69	0.41
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.49	0.41
2:B:784:ASN:O	2:B:788:ARG:HG3	2.21	0.41
3:C:8:VAL:HG11	9:K:105:PHE:CD1	2.56	0.41
5:F:109:VAL:HG22	5:F:129:LYS:HD2	2.03	0.41
5:F:85:MET:HB2	5:F:151:LEU:HB3	2.03	0.41
1:A:1221:LYS:HD2	1:A:1223:ASP:OD2	2.21	0.40
1:A:269:ILE:HD11	1:A:303:TYR:CB	2.50	0.40
2:B:1222:ARG:H	2:B:1222:ARG:HG3	1.63	0.40
2:B:326:ASP:C	2:B:326:ASP:OD2	2.59	0.40
2:B:549:THR:HG22	2:B:628:THR:HG23	2.03	0.40
2:B:589:VAL:CG1	2:B:590:HIS:N	2.83	0.40
2:B:862:GLN:HB3	2:B:863:GLU:H	1.59	0.40
2:B:872:GLU:OE2	2:B:914:LYS:HE2	2.21	0.40
2:B:914:LYS:CB	2:B:937:ALA:O	2.63	0.40
3:C:114:TYR:CD1	3:C:114:TYR:N	2.90	0.40
4:E:31:THR:C	4:E:33:GLU:H	2.24	0.40
9:K:103:THR:O	9:K:104:ASN:C	2.59	0.40
10:L:26:THR:CG2	10:L:27:LEU:N	2.84	0.40
10:L:51:CYS:C	10:L:53:HIS:N	2.74	0.40
1:A:872:GLY:O	1:A:1058:VAL:HG12	2.21	0.40
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.43	0.40
1:A:858:ASN:ND2	1:A:858:ASN:C	2.74	0.40
2:B:1153:GLU:CG	2:B:1154:ALA:N	2.78	0.40
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.55	0.40
2:B:89:GLU:HB2	2:B:137:TYR:CD1	2.57	0.40
2:B:911:ILE:HD11	2:B:941:LEU:HD12	2.02	0.40
3:C:78:GLU:C	3:C:80:LEU:H	2.24	0.40
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.56	0.40
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	2.04	0.40
1:A:219:PHE:O	1:A:224:PHE:HB2	2.22	0.40
1:A:337:ARG:HG2	1:A:341:MET:HE2	2.03	0.40
1:A:342:GLY:HA3	2:B:1130:PHE:O	2.22	0.40
1:A:685:GLU:HA	1:A:688:LYS:HD2	2.04	0.40
1:A:92:HIS:C	1:A:92:HIS:CD2	2.94	0.40
3:C:106:GLU:O	3:C:149:LYS:HE3	2.22	0.40
4:E:100:ILE:CD1	4:E:108:GLY:HA3	2.45	0.40
6:H:105:GLU:H	6:H:105:GLU:CD	2.24	0.40
6:H:26:ILE:HD11	6:H:49:VAL:HG11	2.03	0.40
8:J:52:THR:O	8:J:52:THR:HG22	2.21	0.40
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.55	0.40
1:A:247:ARG:HD2	1:A:263:THR:OG1	2.21	0.40
1:A:577:ILE:H	1:A:577:ILE:HG12	1.49	0.40
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.51	0.40
2:B:53:GLN:HG2	2:B:547:VAL:HG13	2.03	0.40
1:A:782:ARG:NH2	2:B:699:GLU:O	2.54	0.40
2:B:889:THR:HG21	2:B:891:ASP:OD2	2.21	0.40
3:C:70:ILE:HD11	3:C:144:ILE:HG12	2.03	0.40
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.57	0.40
6:H:111:LEU:HD22	6:H:127:GLY:O	2.21	0.40
7:I:78:CYS:SG	7:I:103:CYS:SG	3.19	0.40
1:A:1216:ILE:O	1:A:1219:THR:HB	2.21	0.40
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.62	0.40
2:B:1154:ALA:O	2:B:1155:SER:C	2.60	0.40
2:B:305:VAL:HG12	2:B:305:VAL:O	2.21	0.40
2:B:429:PHE:HA	2:B:432:MET:CE	2.52	0.40
1:A:825:ILE:CD1	2:B:512:ARG:HG3	2.49	0.40
3:C:221:TYR:HD1	3:C:222:LYS:HG3	1.85	0.40
9:K:7:PHE:CD1	9:K:7:PHE:C	2.95	0.40
10:L:34:CYS:SG	10:L:51:CYS:SG	3.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1411/1733 (81%)	1203 (85%)	149 (11%)	59 (4%)	3	9
2	B	1074/1224 (88%)	953 (89%)	100 (9%)	21 (2%)	7	24
3	C	264/318 (83%)	228 (86%)	30 (11%)	6 (2%)	6	21
4	E	213/215 (99%)	184 (86%)	24 (11%)	5 (2%)	6	21
5	F	82/155 (53%)	74 (90%)	6 (7%)	2 (2%)	6	20
6	H	129/146 (88%)	83 (64%)	28 (22%)	18 (14%)	0	0
7	I	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	5	19
8	J	63/70 (90%)	58 (92%)	4 (6%)	1 (2%)	9	31
9	K	112/120 (93%)	101 (90%)	11 (10%)	0	100	100
10	L	44/70 (63%)	21 (48%)	13 (30%)	10 (23%)	0	0
All	All	3512/4173 (84%)	3008 (86%)	379 (11%)	125 (4%)	3	11

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	46	THR
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	79	GLY
1	A	84	ILE
1	A	464	PRO
1	A	465	TYR
1	A	567	LYS
1	A	626	ASN
1	A	752	LYS
1	A	1391	ARG
1	A	1393	ASN

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Mol	Chain	Res	Type
2	B	646	LEU
2	B	864	LYS
2	B	879	ARG
2	B	881	ASN
2	B	1099	VAL
3	C	4	GLU
3	C	90	ASP
3	C	184	ASN
4	E	4	GLU
4	E	5	ASN
6	H	19	ARG
6	H	79	TRP
6	H	81	PRO
6	H	83	GLN
6	H	88	SER
6	H	138	GLU
10	L	39	SER
1	A	57	ARG
1	A	67	CYS
1	A	74	MET
1	A	418	SER
1	A	558	GLY
1	A	1172	LEU
1	A	1257	ASP
1	A	1392	SER
1	A	1396	ALA
1	A	1399	ARG
1	A	1403	GLU
2	B	165	VAL
2	B	734	HIS
2	B	907	GLY
2	B	1066	SER
2	B	1100	ASP
2	B	1155	SER
2	B	1222	ARG
3	C	263	THR
4	E	3	GLN
4	E	50	MET
4	E	59	SER
5	F	73	ALA
6	H	18	GLY
6	H	78	SER

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Mol	Chain	Res	Type
6	H	82	PRO
6	H	90	ALA
6	H	105	GLU
6	H	128	ASN
6	H	140	ALA
10	L	52	GLY
10	L	59	ALA
1	A	45	GLN
1	A	72	GLU
1	A	148	CYS
1	A	885	THR
1	A	1221	LYS
1	A	1386	ARG
1	A	1402	PHE
2	B	883	LEU
3	C	206	ASN
6	H	32	THR
6	H	139	ASN
7	I	3	THR
10	L	35	SER
10	L	64	LEU
1	A	58	LEU
1	A	188	ASP
1	A	253	ASN
1	A	283	GLY
1	A	307	ASP
1	A	342	GLY
1	A	599	SER
1	A	737	LEU
1	A	958	VAL
1	A	1278	ASN
1	A	1385	THR
2	B	266	ALA
5	F	112	GLU
6	H	8	ASP
6	H	77	ARG
7	I	76	PRO
7	I	79	HIS
10	L	37	LYS
10	L	54	ARG
1	A	35	ILE
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	197	PRO
1	A	525	GLN
1	A	593	GLU
1	A	628	GLY
1	A	736	ASN
1	A	1097	GLY
1	A	1122	PRO
2	B	21	GLU
2	B	90	ILE
2	B	262	GLU
2	B	369	GLY
2	B	906	SER
3	C	264	GLN
6	H	61	SER
8	J	26	GLN
10	L	27	LEU
10	L	50	ASP
10	L	56	LEU
1	A	308	ILE
1	A	409	SER
1	A	419	LYS
1	A	1094	VAL
1	A	147	VAL
1	A	1437	GLY
2	B	231	PRO
2	B	1017	ILE
1	A	1114	PRO

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	1239/1520 (82%)	1172 (95%)	67 (5%)	22	53
2	B	950/1061 (90%)	908 (96%)	42 (4%)	28	61
3	C	234/274 (85%)	222 (95%)	12 (5%)	24	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	197/197 (100%)	191 (97%)	6 (3%)	41	75
5	F	74/137 (54%)	72 (97%)	2 (3%)	44	78
6	H	117/128 (91%)	116 (99%)	1 (1%)	78	94
7	I	116/116 (100%)	109 (94%)	7 (6%)	19	48
8	J	60/65 (92%)	56 (93%)	4 (7%)	16	43
9	K	99/102 (97%)	93 (94%)	6 (6%)	18	48
10	L	40/57 (70%)	36 (90%)	4 (10%)	7	22
All	All	3126/3657 (86%)	2975 (95%)	151 (5%)	25	58

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	22	PHE
1	A	92	HIS
1	A	93	VAL
1	A	156	ASP
1	A	197	PRO
1	A	208	LEU
1	A	219	PHE
1	A	291	GLU
1	A	351	THR
1	A	381	THR
1	A	385	ILE
1	A	434	ARG
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	479	ASN
1	A	493	GLN
1	A	497	THR
1	A	503	GLN
1	A	504	LEU
1	A	571	LEU
1	A	577	ILE
1	A	597	LEU
1	A	603	ASN

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Mol	Chain	Res	Type
1	A	612	ILE
1	A	614	PHE
1	A	618	GLU
1	A	622	VAL
1	A	672	ASP
1	A	710	LEU
1	A	740	LEU
1	A	756	ILE
1	A	774	ARG
1	A	788	SER
1	A	821	ARG
1	A	822	GLU
1	A	827	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	920	LEU
1	A	1015	VAL
1	A	1030	ARG
1	A	1043	ASP
1	A	1122	PRO
1	A	1165	GLU
1	A	1255	GLU
1	A	1258	HIS
1	A	1264	GLU
1	A	1297	GLU
1	A	1309	ASP
1	A	1318	THR
1	A	1364	ASN
1	A	1366	ARG
1	A	1385	THR
1	A	1415	SER
1	A	1419	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1438	THR
2	B	18	PHE
2	B	20	ASP
2	B	102	VAL

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Mol	Chain	Res	Type
2	B	120	ARG
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	194	GLU
2	B	199	MET
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	391	ASP
2	B	466	TRP
2	B	485	ARG
2	B	513	GLN
2	B	531	GLN
2	B	541	LEU
2	B	547	VAL
2	B	549	THR
2	B	589	VAL
2	B	644	GLU
2	B	648	HIS
2	B	653	VAL
2	B	806	THR
2	B	951	GLN
2	B	963	PHE
2	B	974	PRO
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1060	ARG
2	B	1065	GLN
2	B	1150	ARG
2	B	1159	ARG
2	B	1193	GLN
2	B	1211	ASN
2	B	1219	ASP
3	C	17	ASN
3	C	26	ASP
3	C	56	THR

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Mol	Chain	Res	Type
3	C	77	ILE
3	C	129	ILE
3	C	163	ILE
3	C	189	THR
3	C	209	TYR
3	C	226	ASP
3	C	233	GLU
3	C	240	VAL
3	C	252	GLN
4	E	81	GLU
4	E	104	ASN
4	E	123	LEU
4	E	146	HIS
4	E	149	LEU
4	E	204	THR
5	F	82	THR
5	F	111	LEU
6	H	91	ASP
7	I	4	PHE
7	I	30	ARG
7	I	45	ARG
7	I	50	THR
7	I	52	ILE
7	I	87	GLN
7	I	98	VAL
8	J	1	MET
8	J	22	LEU
8	J	28	ASP
8	J	48	ARG
9	K	11	LEU
9	K	47	ARG
9	K	68	PHE
9	K	73	LEU
9	K	74	ARG
9	K	101	LEU
10	L	42	ARG
10	L	50	ASP
10	L	61	THR
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	68	GLN
1	A	92	HIS
1	A	118	HIS
1	A	171	GLN
1	A	299	HIS
1	A	313	GLN
1	A	390	GLN
1	A	394	ASN
1	A	397	ASN
1	A	445	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	603	ASN
1	A	626	ASN
1	A	631	HIS
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
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	994	GLN
1	A	1173	HIS
1	A	1218	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	366	GLN
2	B	465	ASN
2	B	513	GLN
2	B	515	HIS

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Mol	Chain	Res	Type
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	590	HIS
2	B	648	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	761	HIS
2	B	786	ASN
2	B	1015	HIS
2	B	1025	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1176	ASN
2	B	1179	GLN
2	B	1187	ASN
2	B	1193	GLN
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	167	HIS
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	12	ASN
7	I	89	GLN
7	I	114	GLN
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
10	L	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
6	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	710:LEU	C	711:GLU	N	1.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	707:PRO	C	708:GLU	N	1.08
1	H	79:TRP	C	80:ARG	N	0.72

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.