



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:54 PM UTC

PDB ID : 8U9R / pdb_00008u9r
Title : STRUCTURAL BASIS OF TRANSCRIPTION: RNA POLYMERASE II
SUBSTRATE BINDING AND METAL COORDINATION USING A FREE-
ELECTRON LASER
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Deposited on : 2023-09-20
Resolution : 3.34 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

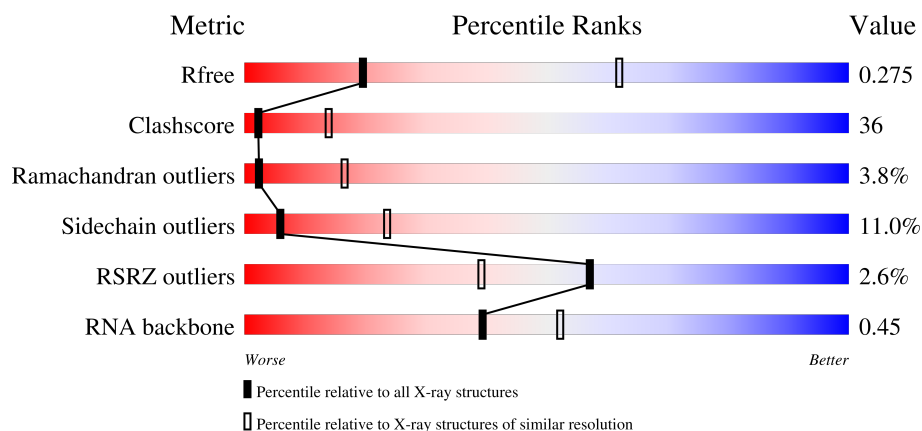
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)
RNA backbone	3983	1083 (3.68-3.00)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	30% 44% 6% 19%
2	B	1224	3% 32% 48% 7% 13%
3	C	318	40% 37% 6% 17%

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	10	
14	T	14	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	MG	B	1302	-	-	-	X
18	ATP	A	1806	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 30677 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 subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1396	Total	C	N	O	S	0	0	0
			10967	6917	1917	2072	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1060	Total	C	N	O	S	0	0	0
			8420	5341	1476	1548	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2083	1310	346	414	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	161	Total	C	N	O	S	0	0	0
			1274	790	223	259	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	206	Total	C	N	O	S	0	0	0
			1693	1078	298	310	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	85	Total	C	N	O	S	0	0	0
			684	437	116	128	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	117	Total	C	N	O	S	0	0	0
			951	605	158	184	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	113	Total	C	N	O	S	0	0	0
			910	557	166	177	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	43	Total	C	N	O	S	0	0	0
			343	211	69	59	4			

- Molecule 13 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

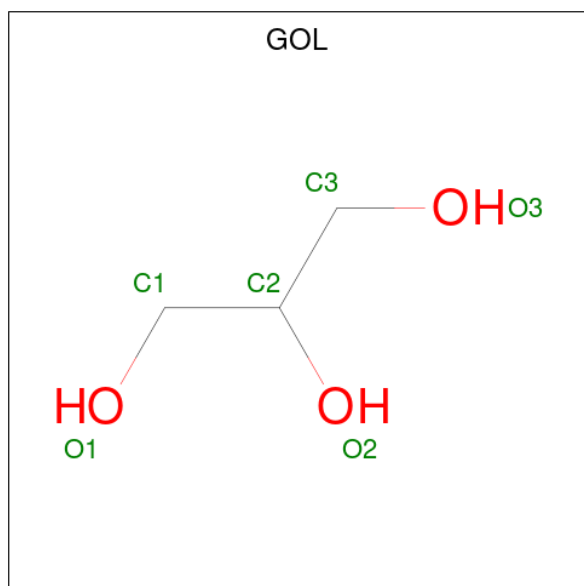
- Molecule 14 is a DNA chain called DNA (5'-D(P*CP*AP*CP*GP*TP*CP*CP*CP*TP*CP*TP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	14	Total	C	N	O	P	0	0	0
			279	133	47	85	14			

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

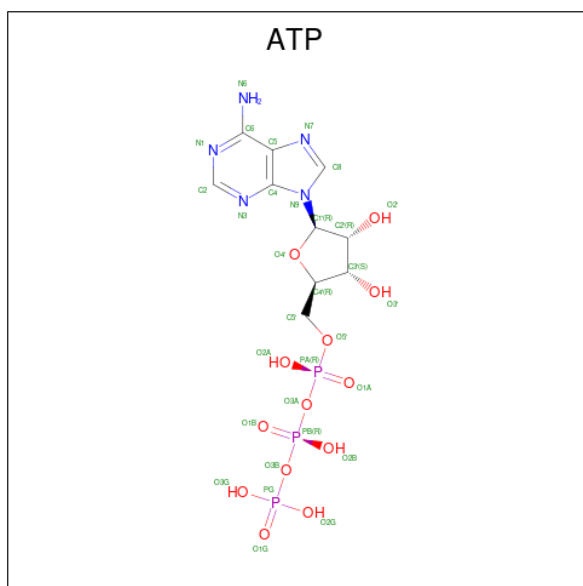


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Mg	0	0
			2	2		
17	B	1	Total	Mg	0	0
			1	1		

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

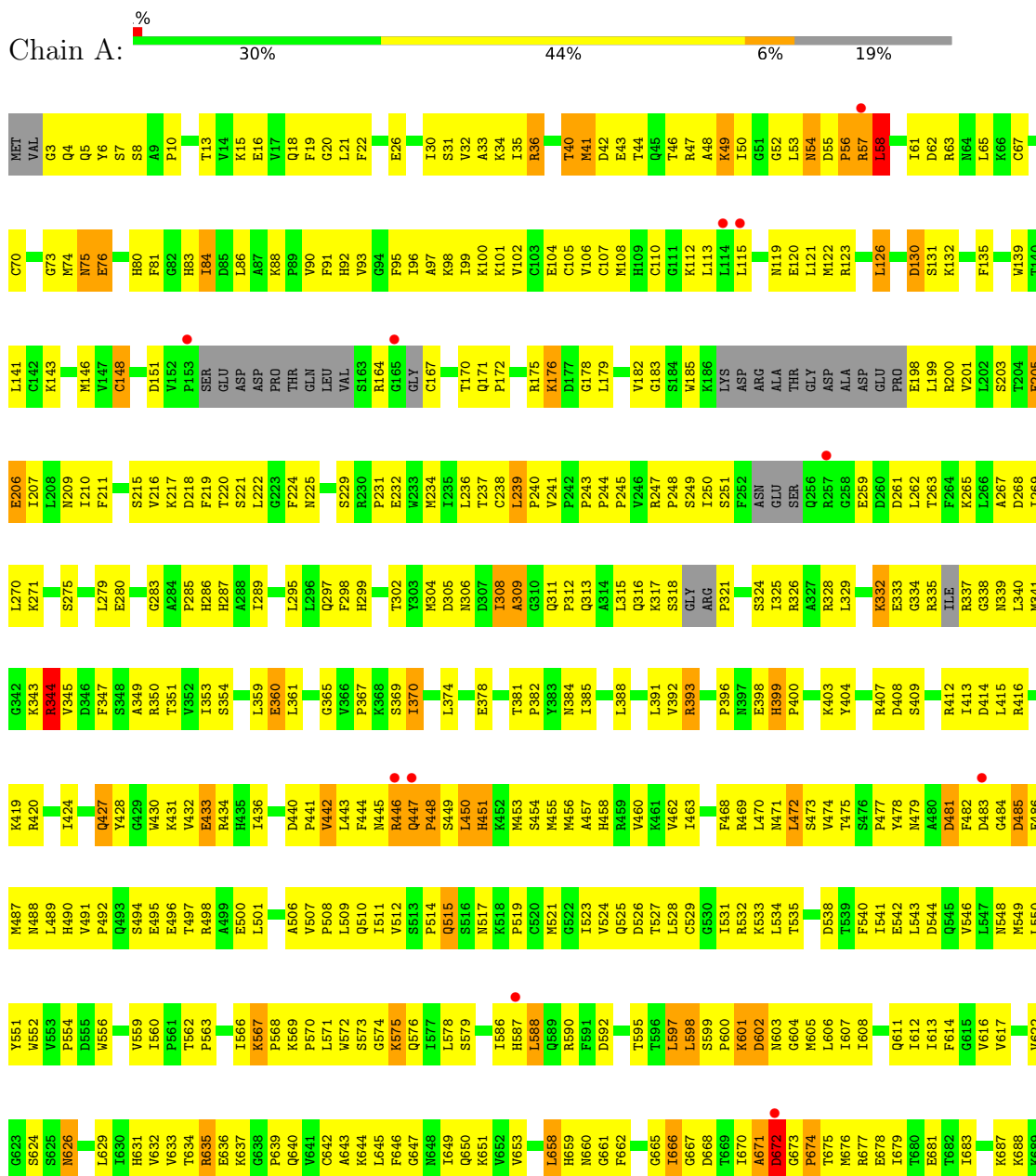
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	11	Total	O	0	0
			11	11		
19	B	3	Total	O	0	0
			3	3		
19	D	1	Total	O	0	0
			1	1		
19	G	1	Total	O	0	0
			1	1		
19	K	1	Total	O	0	0
			1	1		

3 Residue-property plots

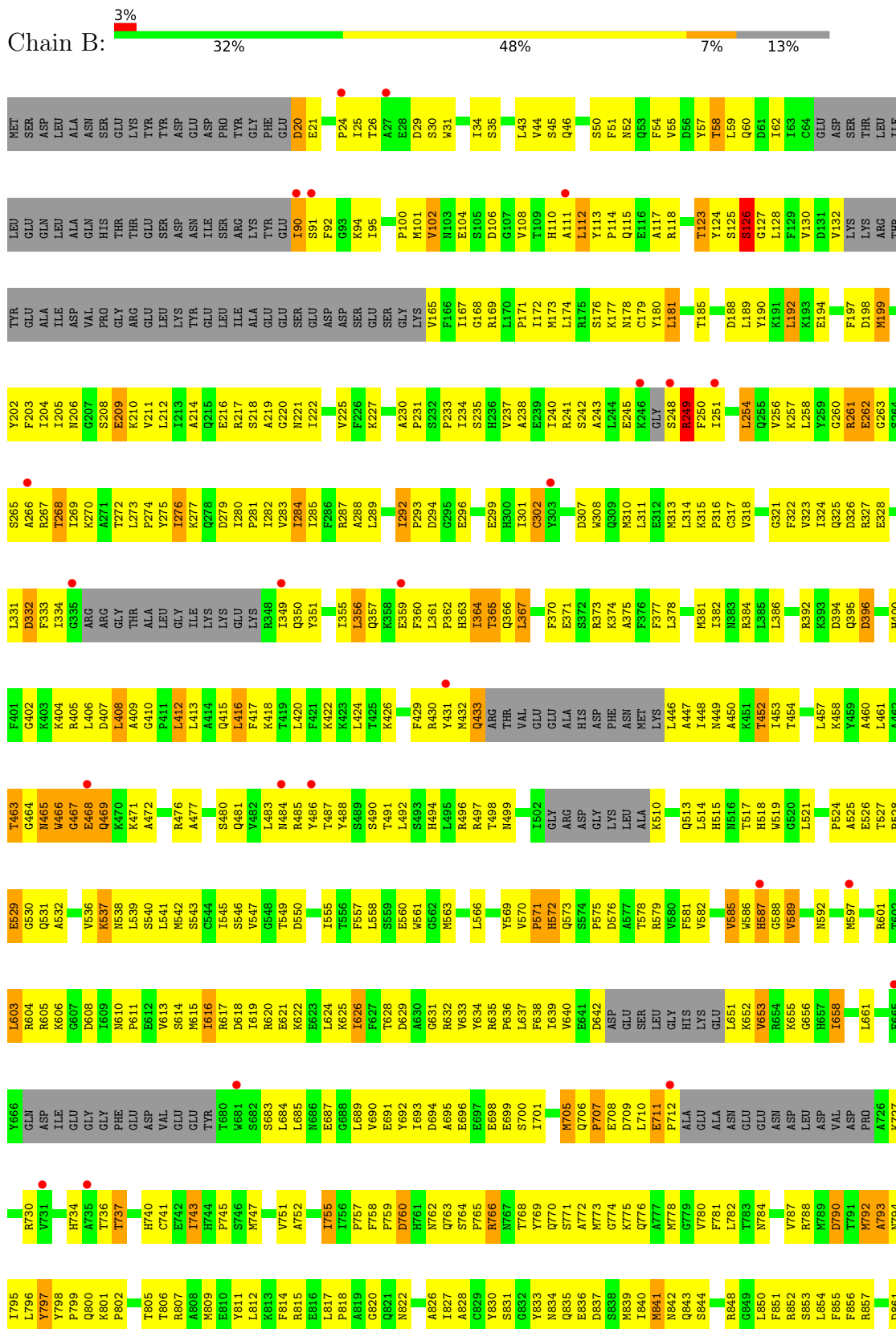
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

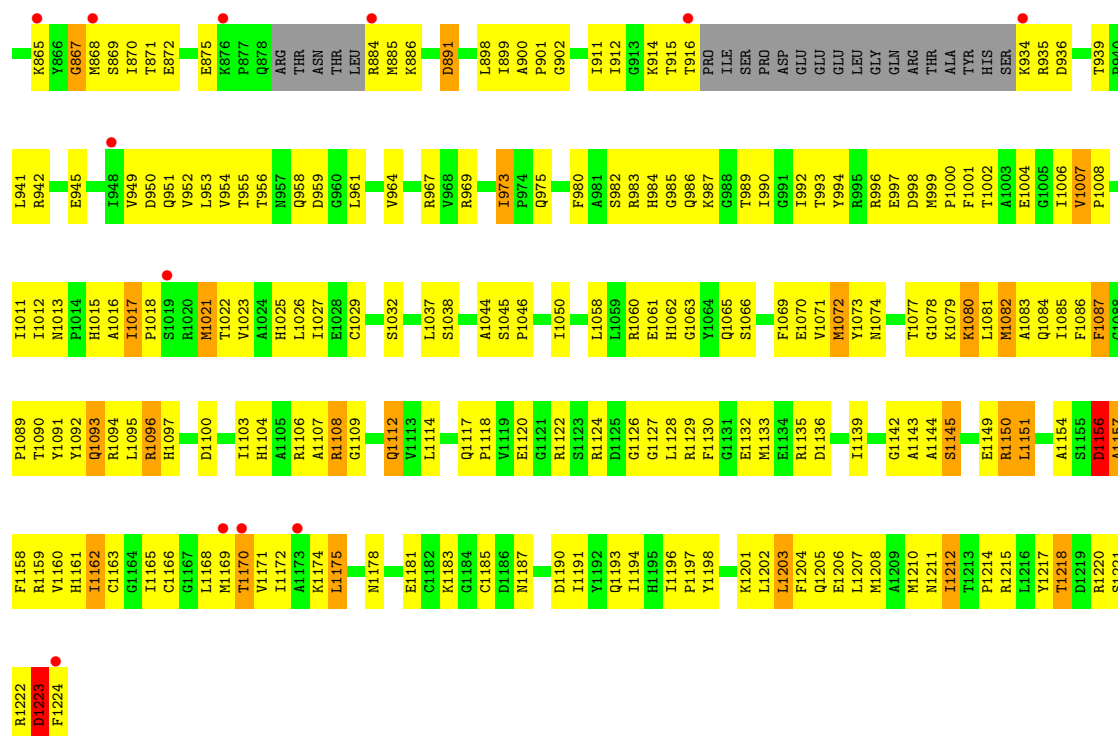
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1



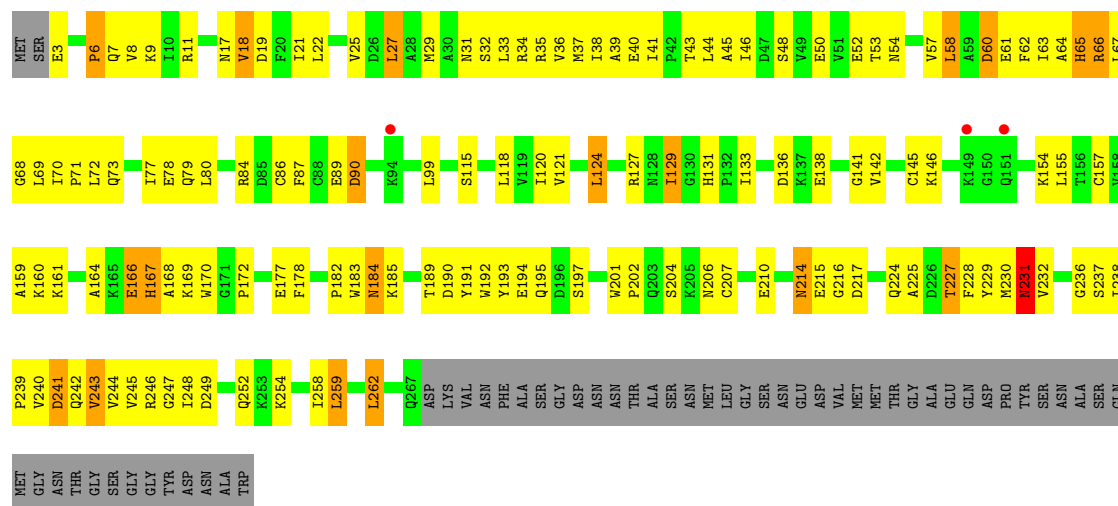


- Molecule 2: DNA-directed RNA polymerase subunit beta

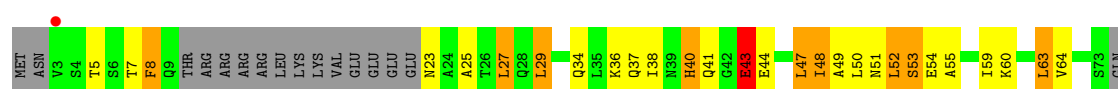


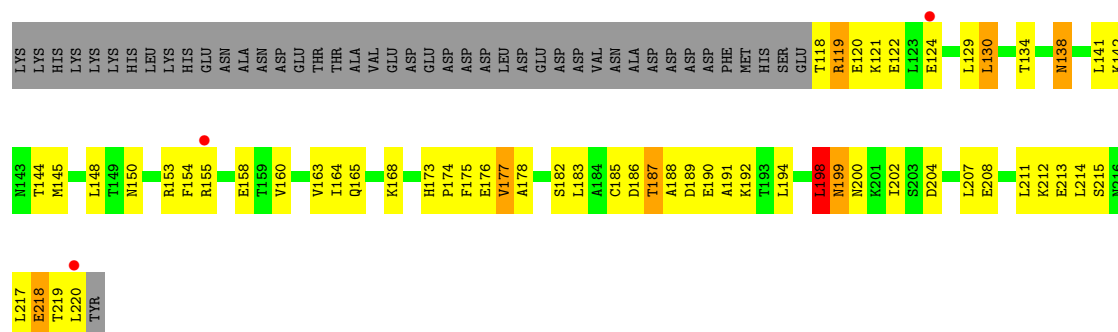


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

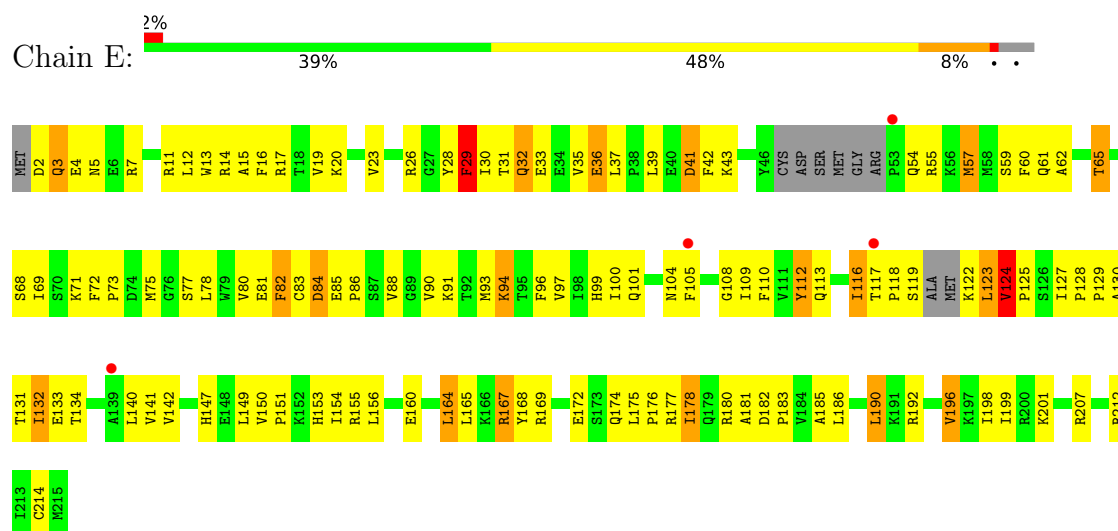


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

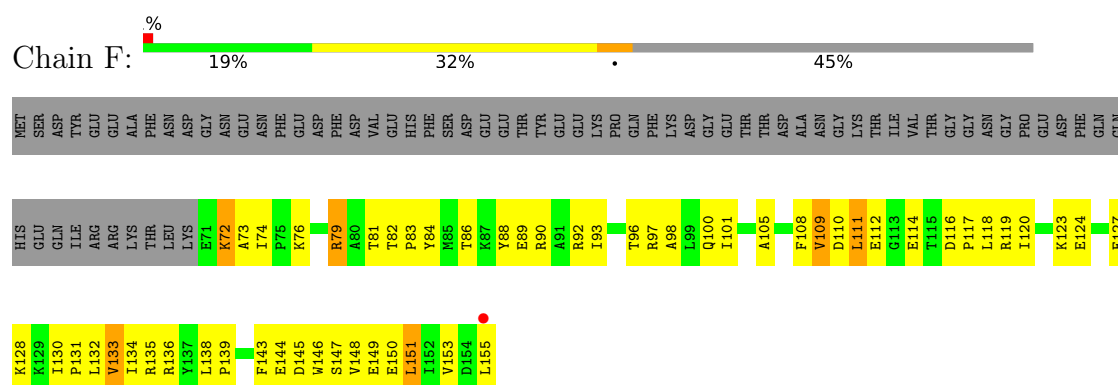




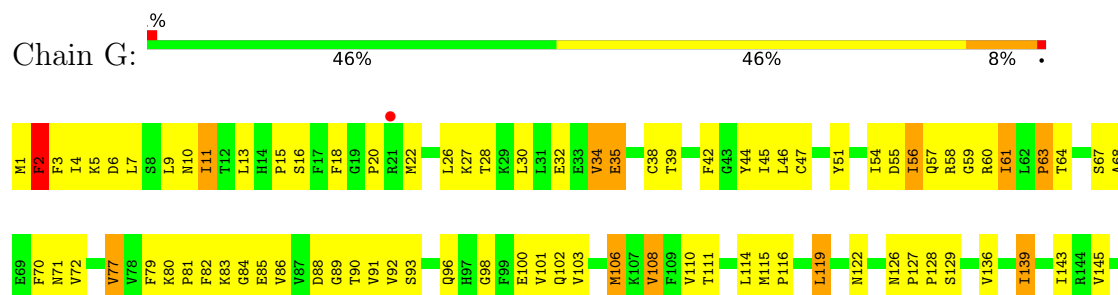
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

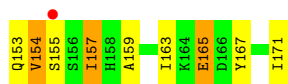


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

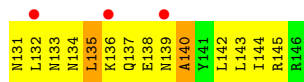
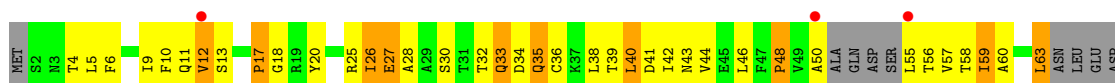
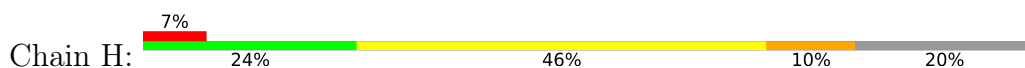


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

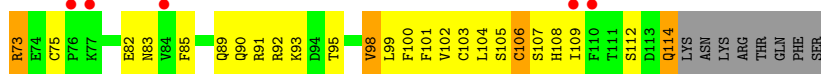




- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



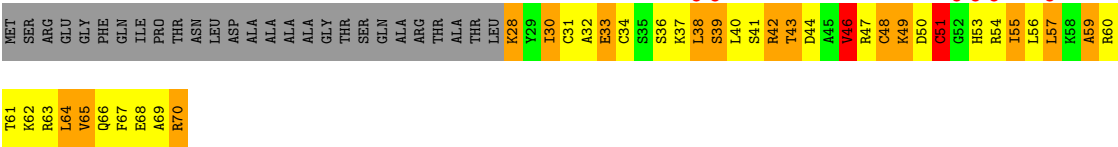
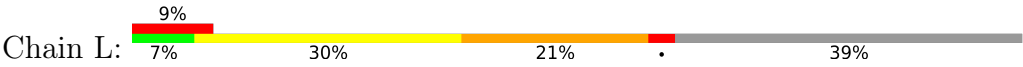
- Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



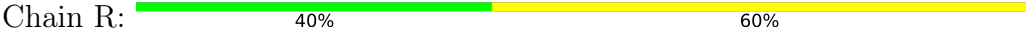
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



• Molecule 13: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*G)-3')



• Molecule 14: DNA (5'-D(P*CP*AP*CP*GP*TP*CP*CP*CP*TP*CP*TP*CP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	217.19Å 387.44Å 276.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.34 19.97 – 3.34	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.97-3.34) 99.4 (19.97-3.34)	Depositor EDS
R_{merge}	0.60	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.261 0.267 , 0.275	Depositor DCC
R_{free} test set	8305 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.146 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.160 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	30677	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.19	0/11158	0.43	5/15080 (0.0%)
2	B	0.21	0/8583	0.41	2/11570 (0.0%)
3	C	0.23	0/2121	0.41	0/2876
4	D	0.13	0/1282	0.32	0/1723
5	E	0.16	0/1727	0.33	0/2323
6	F	0.18	0/696	0.38	0/940
7	G	0.11	0/1368	0.30	0/1844
8	H	0.10	0/965	0.31	0/1302
9	I	0.09	0/927	0.30	0/1250
10	J	0.11	0/541	0.35	0/727
11	K	0.12	0/937	0.28	0/1265
12	L	0.18	0/345	0.48	0/457
13	R	0.13	0/244	0.29	0/380
14	T	0.34	0/310	0.45	0/474
All	All	0.19	0/31204	0.40	7/42211 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	N-CA-C	-10.62	101.45	114.20
1	A	446	ARG	N-CA-C	-6.98	101.54	110.19
1	A	1378	GLN	N-CA-C	-6.88	106.77	114.62
1	A	671	ALA	N-CA-C	-6.34	103.44	112.13
1	A	344	ARG	N-CA-C	-5.77	101.14	110.32
2	B	364	ILE	N-CA-C	-5.30	107.44	111.62
2	B	249	ARG	N-CA-C	-5.25	106.94	113.55

There are no chirality outliers.

There are no planarity outliers.

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	10967	0	11024	950	0
2	B	8420	0	8456	673	0
3	C	2083	0	2036	154	0
4	D	1274	0	1287	83	0
5	E	1693	0	1715	118	0
6	F	684	0	703	60	0
7	G	1340	0	1357	104	0
8	H	951	0	926	96	0
9	I	910	0	857	56	0
10	J	532	0	542	48	0
11	K	919	0	929	50	0
12	L	343	0	363	47	0
13	R	217	0	109	4	0
14	T	279	0	158	11	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	6	0	8	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
18	A	31	0	12	9	0
19	A	11	0	0	0	0
19	B	3	0	0	0	0
19	D	1	0	0	0	0
19	G	1	0	0	2	0
19	K	1	0	0	0	0
All	All	30677	0	30482	2196	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 36.

All (2196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1160:VAL:HG11	2:B:1169:MET:SD	1.66	1.34
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.14	1.08
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	1.96	1.04
1:A:393:ARG:HH11	1:A:393:ARG:CG	1.72	1.02
2:B:510:LYS:HB2	2:B:513:GLN:HG2	1.42	1.02
1:A:315:LEU:HD23	1:A:318:SER:HB2	1.44	0.96
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.45	0.94
1:A:203:SER:HB3	1:A:206:GLU:HB3	1.52	0.91
2:B:1160:VAL:CG1	2:B:1169:MET:SD	2.57	0.89
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.55	0.87
1:A:445:ASN:OD1	1:A:488:ASN:HB2	1.74	0.87
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.59	0.85
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.58	0.85
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.58	0.84
2:B:307:ASP:OD2	2:B:310:MET:HB3	1.76	0.84
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.59	0.84
2:B:429:PHE:HA	2:B:432:MET:HE2	1.60	0.83
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.43	0.83
1:A:262:LEU:HD13	1:A:328:ARG:HH21	1.44	0.82
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.61	0.82
5:E:59:SER:HB3	5:E:81:GLU:HA	1.61	0.82
2:B:20:ASP:OD1	2:B:20:ASP:N	2.12	0.82
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.61	0.82
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.10	0.82
9:I:19:ASP:HB2	9:I:24:ARG:HG2	1.60	0.82
2:B:125:SER:HB3	2:B:169:ARG:HB3	1.61	0.81
1:A:579:SER:HB3	1:A:611:GLN:HA	1.60	0.81
1:A:701:LEU:HD21	9:I:114:GLN:HB3	1.60	0.81
4:D:27:LEU:HD11	4:D:173:HIS:HB2	1.61	0.81
1:A:396:PRO:HG2	1:A:416:ARG:HG2	1.62	0.81
1:A:835:GLY:HA3	14:T:18:DT:H1'	1.62	0.81
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.63	0.81
1:A:442:VAL:HG12	1:A:491:VAL:HG22	1.61	0.81
1:A:43:GLU:HG3	1:A:44:THR:H	1.43	0.81
1:A:515:GLN:HE21	1:A:1071:SER:HA	1.45	0.81
10:J:54:VAL:HG23	10:J:56:LEU:HD11	1.63	0.81
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.62	0.80
1:A:1207:LEU:HD23	1:A:1274:ARG:HH21	1.45	0.80
4:D:134:THR:HG21	4:D:141:LEU:HD23	1.63	0.80
1:A:315:LEU:HD23	1:A:318:SER:CB	2.11	0.80
2:B:1163:CYS:CB	2:B:1166:CYS:SG	2.62	0.80
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:VAL:HG22	1:A:525:GLN:HG2	1.64	0.80
1:A:67:CYS:SG	1:A:70:CYS:O	2.40	0.79
2:B:114:PRO:HB2	2:B:118:ARG:HH21	1.45	0.79
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.64	0.79
1:A:697:ALA:HB2	1:A:702:LEU:HD13	1.64	0.79
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.64	0.79
1:A:514:PRO:HB3	1:A:875:ALA:HB3	1.64	0.79
3:C:58:LEU:HB3	3:C:62:PHE:HD2	1.47	0.79
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.64	0.79
3:C:11:ARG:HH11	3:C:19:ASP:HB3	1.48	0.79
1:A:886:ILE:HG23	1:A:887:GLY:H	1.48	0.79
2:B:901:PRO:HA	2:B:949:VAL:HG12	1.65	0.79
2:B:465:ASN:HA	2:B:477:ALA:HA	1.64	0.78
3:C:77:ILE:HD12	3:C:129:ILE:HD11	1.64	0.78
1:A:526:ASP:HB2	2:B:835:GLN:NE2	1.98	0.78
10:J:48:ARG:HE	10:J:49:MET:HE2	1.49	0.78
1:A:1163:ILE:HB	1:A:1166:ASP:HB2	1.66	0.78
4:D:220:LEU:H	4:D:220:LEU:HD12	1.47	0.78
1:A:777:PHE:CE1	1:A:797:LYS:NZ	2.50	0.78
1:A:412:ARG:HH22	2:B:1108:ARG:HD2	1.49	0.77
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.48	0.77
1:A:738:LYS:H	1:A:738:LYS:HD2	1.49	0.77
12:L:28:LYS:N	12:L:39:SER:HB3	2.00	0.77
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.66	0.77
2:B:639:ILE:O	2:B:652:LYS:HB2	1.85	0.77
1:A:446:ARG:NH1	1:A:448:PRO:HG2	2.00	0.76
1:A:838:GLN:HG3	1:A:1073:GLY:HA3	1.65	0.76
1:A:848:ILE:HD13	1:A:1370:LEU:HD21	1.67	0.76
5:E:12:LEU:HD11	5:E:55:ARG:HE	1.49	0.76
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.46	0.76
7:G:1:MET:SD	7:G:2:PHE:N	2.56	0.76
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.66	0.76
2:B:934:LYS:HD3	2:B:935:ARG:H	1.49	0.76
4:D:52:LEU:H	4:D:182:SER:HB3	1.50	0.76
10:J:8:PHE:H	10:J:49:MET:HE3	1.51	0.76
1:A:838:GLN:O	1:A:842:VAL:HG23	1.84	0.76
10:J:1:MET:O	10:J:2:ILE:HG22	1.85	0.76
1:A:683:ILE:HG21	1:A:801:GLU:CG	2.16	0.76
1:A:1120:LEU:HD23	1:A:1125:ALA:HA	1.68	0.76
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	1.86	0.76
2:B:1082:MET:HA	3:C:189:THR:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ASP:HA	2:B:349:ILE:HG21	1.67	0.75
1:A:1120:LEU:HD22	1:A:1304:TRP:HB2	1.67	0.75
3:C:210:GLU:HG3	3:C:229:TYR:OH	1.85	0.75
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.66	0.75
1:A:40:THR:HG22	1:A:41:MET:HG3	1.68	0.75
1:A:775:ILE:HG21	1:A:815:PHE:CD1	2.22	0.75
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.69	0.75
1:A:441:PRO:HG2	1:A:498:ARG:HG3	1.69	0.75
2:B:652:LYS:HD2	2:B:689:LEU:HD23	1.68	0.75
1:A:471:ASN:O	1:A:474:VAL:HG12	1.87	0.75
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.68	0.75
2:B:363:HIS:HD2	2:B:585:VAL:HG12	1.51	0.75
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.69	0.75
1:A:1376:THR:O	1:A:1378:GLN:N	2.20	0.74
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.68	0.74
1:A:519:PRO:O	1:A:624:SER:HB2	1.86	0.74
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.68	0.74
1:A:1113:THR:HG23	1:A:1113:THR:O	1.85	0.74
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.68	0.74
1:A:1235:LYS:HB3	1:A:1237:ILE:HD13	1.68	0.74
2:B:237:VAL:HG22	2:B:257:LYS:HG2	1.68	0.74
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.69	0.74
4:D:208:GLU:O	4:D:212:LYS:HG3	1.86	0.74
1:A:588:LEU:HD12	1:A:632:VAL:HG21	1.69	0.74
8:H:63:LEU:C	8:H:90:ALA:HB3	2.11	0.74
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.70	0.73
1:A:1433:MET:HE2	2:B:1145:SER:HB3	1.68	0.73
1:A:1445:ILE:HD12	7:G:22:MET:HE1	1.68	0.73
2:B:546:SER:OG	2:B:631:GLY:N	2.21	0.73
2:B:772:ALA:HA	2:B:775:LYS:HE2	1.70	0.73
5:E:169:ARG:HH22	6:F:74:ILE:HD11	1.51	0.73
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.34	0.73
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.69	0.73
5:E:31:THR:HG22	5:E:33:GLU:H	1.52	0.73
2:B:619:ILE:H	2:B:619:ILE:HD12	1.54	0.73
1:A:46:THR:HG22	1:A:48:ALA:H	1.51	0.73
4:D:168:LYS:HE2	4:D:177:VAL:HG11	1.69	0.73
5:E:71:LYS:HE3	5:E:160:GLU:OE2	1.89	0.73
1:A:470:LEU:HD13	1:A:474:VAL:HG13	1.70	0.73
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.69	0.73
1:A:590:ARG:NH1	1:A:592:ASP:OD1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ASP:OD2	2:B:310:MET:HE2	1.88	0.73
3:C:115:SER:HB2	3:C:142:VAL:H	1.54	0.73
1:A:98:LYS:NZ	1:A:1411:GLU:OE2	2.20	0.72
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.24	0.72
2:B:30:SER:O	2:B:34:ILE:HD12	1.89	0.72
2:B:307:ASP:OD2	2:B:310:MET:CB	2.36	0.72
1:A:393:ARG:HG2	1:A:393:ARG:NH1	1.93	0.72
1:A:1445:ILE:HG23	6:F:132:LEU:HD23	1.71	0.72
2:B:463:THR:HB	2:B:465:ASN:ND2	2.05	0.72
1:A:484:GLY:H	2:B:989:THR:HG23	1.53	0.72
1:A:1066:VAL:HG11	2:B:1139:ILE:HG22	1.71	0.72
2:B:90:ILE:HD12	2:B:91:SER:H	1.55	0.72
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.04	0.72
1:A:262:LEU:HD13	1:A:328:ARG:NH2	2.04	0.72
1:A:919:ILE:HD11	1:A:925:LEU:HD13	1.70	0.72
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.71	0.72
1:A:337:ARG:NE	1:A:839:ARG:HH21	1.88	0.72
1:A:775:ILE:HG23	1:A:818:MET:HE1	1.72	0.72
3:C:238:ILE:HG13	3:C:243:VAL:HG23	1.71	0.72
1:A:1348:LEU:HD21	1:A:1375:MET:HE3	1.71	0.72
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.72	0.72
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.72	0.71
2:B:848:ARG:HH21	3:C:168:ALA:HB1	1.54	0.71
1:A:343:LYS:NZ	2:B:1151:LEU:HB3	2.04	0.71
2:B:282:ILE:HD11	2:B:317:CYS:HB3	1.70	0.71
4:D:41:GLN:OE1	4:D:41:GLN:N	2.23	0.71
10:J:12:LYS:HD3	10:J:13:VAL:N	2.05	0.71
1:A:599:SER:OG	1:A:603:ASN:N	2.23	0.71
2:B:1023:VAL:O	2:B:1027:ILE:HG13	1.91	0.71
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.73	0.71
1:A:30:ILE:HD12	1:A:31:SER:N	2.05	0.71
2:B:776:GLN:NE2	13:R:9:G:OP1	2.23	0.71
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.72	0.71
1:A:532:ARG:HG2	1:A:749:ALA:HB2	1.72	0.71
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.26	0.71
1:A:868:TYR:CE1	1:A:1064:VAL:HB	2.26	0.71
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.71	0.71
4:D:130:LEU:HD22	4:D:142:LYS:HG2	1.73	0.71
12:L:33:GLU:OE2	12:L:53:HIS:HB2	1.90	0.71
1:A:76:GLU:OE2	2:B:1159:ARG:NH2	2.23	0.70
2:B:582:VAL:O	2:B:585:VAL:HG22	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:130:ARG:O	8:H:130:ARG:HD2	1.90	0.70
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.72	0.70
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	1.73	0.70
2:B:1156:ASP:HB2	2:B:1198:TYR:H	1.57	0.70
2:B:221:ASN:ND2	2:B:243:ALA:O	2.24	0.70
1:A:472:LEU:HD22	2:B:835:GLN:NE2	2.06	0.70
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	1.92	0.70
2:B:792:MET:HA	2:B:856:PHE:O	1.92	0.70
1:A:53:LEU:HD23	1:A:54:ASN:N	2.07	0.70
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.73	0.70
1:A:1370:LEU:O	1:A:1374:VAL:HG23	1.90	0.70
2:B:546:SER:HG	2:B:631:GLY:H	1.39	0.70
3:C:248:ILE:CD1	11:K:101:LEU:HD12	2.21	0.70
1:A:95:PHE:O	1:A:99:ILE:HG13	1.91	0.70
1:A:344:ARG:HB2	2:B:1118:PRO:HB2	1.74	0.70
1:A:488:ASN:ND2	2:B:1128:LEU:HD23	2.05	0.70
1:A:1059:HIS:HB3	6:F:86:THR:HG23	1.74	0.70
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.22	0.70
1:A:1295:THR:HB	1:A:1297:GLU:OE1	1.90	0.70
1:A:908:LEU:HD23	1:A:1029:ARG:HH21	1.54	0.70
1:A:960:ILE:CG2	1:A:1025:ARG:HD2	2.22	0.70
2:B:581:PHE:O	2:B:626:ILE:HD12	1.92	0.70
2:B:848:ARG:HH12	2:B:996:ARG:HD3	1.57	0.70
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.74	0.70
3:C:177:GLU:HB3	3:C:231:ASN:HB3	1.74	0.70
2:B:288:ALA:HB1	2:B:331:LEU:HD23	1.74	0.70
3:C:99:LEU:HD11	3:C:120:ILE:HG12	1.73	0.70
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.74	0.69
1:A:1396:ALA:HA	1:A:1399:ARG:HH21	1.57	0.69
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.73	0.69
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.74	0.69
3:C:50:GLU:HB3	12:L:64:LEU:HD23	1.73	0.69
4:D:47:LEU:HD23	4:D:48:ILE:H	1.57	0.69
6:F:86:THR:HB	6:F:89:GLU:HG3	1.73	0.69
7:G:143:ILE:HG23	7:G:145:VAL:HG13	1.74	0.69
9:I:58:VAL:HG13	9:I:62:ILE:HG13	1.75	0.69
1:A:407:ARG:HG3	1:A:413:ILE:HD11	1.74	0.69
2:B:242:SER:HB2	2:B:362:PRO:HD2	1.74	0.69
11:K:90:ALA:O	11:K:94:ILE:HG13	1.93	0.69
1:A:809:THR:H	1:A:812:GLU:HB2	1.57	0.69
1:A:172:PRO:HB2	1:A:183:GLY:HA3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HG3	1:A:339:ASN:HB2	1.75	0.69
1:A:456:MET:HB2	1:A:478:TYR:OH	1.93	0.69
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.73	0.69
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.27	0.69
4:D:213:GLU:O	4:D:217:LEU:HD13	1.93	0.69
12:L:30:ILE:O	12:L:56:LEU:HA	1.91	0.69
1:A:285:PRO:O	1:A:287:HIS:N	2.25	0.69
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.73	0.69
3:C:183:TRP:O	3:C:185:LYS:N	2.25	0.69
5:E:54:GLN:O	5:E:57:MET:HG3	1.92	0.69
1:A:693:VAL:HG12	1:A:714:PHE:HD1	1.56	0.69
2:B:315:LYS:HB2	2:B:316:PRO:HD3	1.75	0.69
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.74	0.69
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.28	0.69
1:A:1146:VAL:HG21	1:A:1202:MET:HE1	1.74	0.69
1:A:315:LEU:HG	1:A:321:PRO:HA	1.74	0.68
1:A:1264:GLU:OE2	9:I:46:HIS:ND1	2.23	0.68
2:B:318:VAL:O	2:B:322:PHE:N	2.26	0.68
12:L:30:ILE:HG22	12:L:31:CYS:H	1.59	0.68
3:C:242:GLN:HB3	3:C:246:ARG:HD2	1.74	0.68
4:D:8:PHE:CE2	7:G:6:ASP:HB2	2.28	0.68
2:B:43:LEU:HD13	2:B:492:LEU:HD13	1.75	0.68
2:B:173:MET:HG3	2:B:176:SER:HB3	1.75	0.68
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.75	0.68
5:E:83:CYS:HB2	5:E:110:PHE:CZ	2.28	0.68
7:G:106:MET:CE	7:G:108:VAL:HG23	2.24	0.68
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.75	0.68
1:A:262:LEU:HD21	1:A:325:ILE:HG12	1.74	0.68
2:B:302:CYS:SG	2:B:311:LEU:HD21	2.33	0.68
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.75	0.68
1:A:599:SER:HB2	1:A:614:PHE:CD1	2.29	0.68
3:C:262:LEU:HD13	11:K:88:LYS:HG2	1.73	0.68
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.29	0.68
11:K:53:ASP:HB3	11:K:56:VAL:HB	1.75	0.68
1:A:33:ALA:HB2	1:A:57:ARG:HB2	1.76	0.68
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.74	0.68
1:A:446:ARG:HG2	1:A:448:PRO:HD2	1.76	0.67
1:A:107:CYS:SG	1:A:110:CYS:CB	2.82	0.67
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.74	0.67
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.24	0.67
3:C:37:MET:HE1	3:C:232:VAL:HG11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD13	1:A:487:MET:HG3	1.76	0.67
1:A:393:ARG:CG	1:A:393:ARG:NH1	2.42	0.67
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.77	0.67
2:B:307:ASP:OD2	2:B:392:ARG:NH2	2.24	0.67
1:A:451:HIS:HB3	1:A:454:SER:H	1.60	0.67
7:G:81:PRO:HD2	7:G:157:ILE:HD11	1.76	0.67
1:A:575:LYS:HD2	8:H:120:GLY:HA2	1.77	0.67
1:A:833:GLU:O	1:A:837:ILE:HG23	1.93	0.67
8:H:118:PHE:N	8:H:121:LEU:O	2.24	0.67
8:H:143:LEU:C	8:H:144:ILE:HD12	2.20	0.67
10:J:54:VAL:HG23	10:J:56:LEU:CD1	2.25	0.67
1:A:672:ASP:H	1:A:676:MET:HG3	1.59	0.67
1:A:1004:ASN:CG	5:E:167:ARG:HG3	2.20	0.67
7:G:106:MET:HE1	7:G:108:VAL:HG23	1.75	0.67
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.75	0.67
3:C:248:ILE:HD11	11:K:101:LEU:HD12	1.75	0.67
9:I:73:ARG:HB3	9:I:73:ARG:HH11	1.60	0.67
1:A:658:LEU:HD22	2:B:1074:ASN:HD21	1.59	0.67
1:A:1428:VAL:HG13	2:B:1151:LEU:HD13	1.76	0.67
6:F:128:LYS:HE2	6:F:151:LEU:O	1.94	0.67
7:G:126:ASN:HB3	7:G:127:PRO:HD3	1.77	0.67
1:A:178:GLY:O	1:A:179:LEU:HB2	1.95	0.67
2:B:622:LYS:HD2	9:I:59:VAL:HG11	1.75	0.67
1:A:283:GLY:O	1:A:285:PRO:HD3	1.95	0.66
1:A:391:LEU:HD23	1:A:400:PRO:O	1.95	0.66
2:B:102:VAL:HB	2:B:112:LEU:HD13	1.76	0.66
2:B:1222:ARG:HG2	2:B:1223:ASP:H	1.59	0.66
5:E:68:SER:HB3	5:E:75:MET:HE1	1.78	0.66
6:F:134:ILE:HD12	6:F:151:LEU:CD1	2.25	0.66
1:A:1004:ASN:ND2	5:E:167:ARG:HG3	2.10	0.66
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.78	0.66
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.31	0.66
1:A:1121:GLU:CG	1:A:1122:PRO:CD	2.74	0.66
3:C:73:GLN:HB2	3:C:131:HIS:HB2	1.77	0.66
1:A:1163:ILE:O	1:A:1167:GLU:HG3	1.95	0.66
1:A:206:GLU:O	1:A:210:ILE:HG13	1.96	0.66
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.77	0.66
2:B:287:ARG:HG3	2:B:292:ILE:HG13	1.77	0.66
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.77	0.66
5:E:176:PRO:O	5:E:212:ARG:HA	1.96	0.66
1:A:1039:LYS:HE2	1:A:1043:ASP:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:134:ILE:HD12	6:F:151:LEU:HD13	1.77	0.66
1:A:440:ASP:O	1:A:460:VAL:HG23	1.96	0.66
1:A:901:LEU:HG	1:A:929:LEU:HD12	1.77	0.66
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.77	0.66
3:C:22:LEU:HB3	3:C:25:VAL:HG21	1.78	0.66
1:A:445:ASN:OD1	1:A:445:ASN:O	2.14	0.66
5:E:127:ILE:HB	5:E:130:ALA:HB3	1.78	0.66
8:H:44:VAL:HG23	8:H:48:PRO:HA	1.78	0.66
1:A:231:PRO:HA	1:A:234:MET:HE2	1.78	0.65
1:A:1054:LEU:HD13	6:F:84:TYR:OH	1.96	0.65
1:A:15:LYS:HD3	2:B:1218:THR:O	1.95	0.65
1:A:562:THR:HG22	8:H:79:TRP:HD1	1.61	0.65
2:B:851:PHE:CD1	2:B:1094:ARG:HB2	2.31	0.65
12:L:38:LEU:HD21	12:L:49:LYS:H	1.61	0.65
1:A:43:GLU:HG3	1:A:44:THR:N	2.12	0.65
1:A:782:ARG:HB3	1:A:789:LYS:HA	1.78	0.65
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.78	0.65
2:B:302:CYS:HB2	2:B:310:MET:HE3	1.79	0.65
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.60	0.65
1:A:1229:SER:HB3	1:A:1233:ASP:CG	2.21	0.65
2:B:578:THR:HG22	2:B:622:LYS:CA	2.26	0.65
5:E:55:ARG:HB2	5:E:84:ASP:HA	1.77	0.65
1:A:1004:ASN:OD1	1:A:1007:ILE:HG13	1.97	0.65
1:A:817:ALA:HA	2:B:764:SER:OG	1.97	0.65
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.44	0.65
1:A:1445:ILE:CD1	7:G:22:MET:HE1	2.27	0.65
3:C:11:ARG:NH1	3:C:19:ASP:HB3	2.11	0.65
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.31	0.65
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.30	0.65
2:B:171:PRO:HG2	2:B:461:LEU:HD12	1.77	0.65
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.27	0.65
6:F:116:ASP:O	6:F:120:ILE:HG13	1.97	0.65
1:A:850:VAL:HG23	1:A:1064:VAL:HG11	1.79	0.65
2:B:573:GLN:C	2:B:575:PRO:HD3	2.22	0.65
5:E:178:ILE:HG23	5:E:214:CYS:HA	1.79	0.65
1:A:20:GLY:O	1:A:21:LEU:HD23	1.96	0.65
1:A:540:PHE:HE2	8:H:43:ASN:HD22	1.44	0.65
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.78	0.64
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.31	0.64
2:B:954:VAL:O	12:L:56:LEU:HB2	1.96	0.64
1:A:642:CYS:O	1:A:645:LEU:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:LEU:HD23	2:B:954:VAL:N	2.12	0.64
1:A:626:ASN:O	1:A:631:HIS:ND1	2.28	0.64
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.79	0.64
3:C:53:THR:HG22	3:C:154:LYS:HB2	1.79	0.64
3:C:78:GLU:HG2	3:C:246:ARG:HH21	1.62	0.64
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.25	0.64
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.31	0.64
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.80	0.64
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.32	0.64
5:E:7:ARG:O	5:E:11:ARG:HG3	1.97	0.64
1:A:275:SER:O	1:A:279:LEU:HB2	1.98	0.64
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.31	0.64
5:E:32:GLN:OE1	5:E:32:GLN:HA	1.97	0.64
1:A:100:LYS:NZ	1:A:104:GLU:OE2	2.30	0.64
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.78	0.64
5:E:15:ALA:O	5:E:19:VAL:HG23	1.98	0.64
1:A:500:GLU:OE1	1:A:1438:THR:HG21	1.97	0.64
1:A:883:LEU:O	1:A:886:ILE:HG22	1.97	0.64
1:A:1424:VAL:HG21	2:B:1139:ILE:HD13	1.79	0.64
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.79	0.64
1:A:738:LYS:HE2	3:C:194:GLU:HA	1.79	0.64
1:A:843:LYS:HD3	1:A:846:GLU:OE2	1.97	0.64
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.80	0.64
1:A:447:GLN:OE1	1:A:447:GLN:HA	1.95	0.64
1:A:1445:ILE:HG23	6:F:132:LEU:CD2	2.28	0.64
2:B:60:GLN:HG3	2:B:95:ILE:HG22	1.79	0.64
2:B:1150:ARG:NE	2:B:1150:ARG:HA	2.13	0.64
5:E:12:LEU:HD21	5:E:55:ARG:HH21	1.62	0.64
6:F:128:LYS:HD3	6:F:149:GLU:HA	1.79	0.64
8:H:58:THR:HG22	8:H:59:ILE:H	1.63	0.64
1:A:640:GLN:CD	1:A:640:GLN:H	2.06	0.63
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.80	0.63
1:A:1424:VAL:HG21	2:B:1139:ILE:CD1	2.28	0.63
2:B:100:PRO:HD3	2:B:178:ASN:O	1.98	0.63
2:B:834:ASN:O	2:B:1013:ASN:HB2	1.98	0.63
5:E:3:GLN:HG3	5:E:5:ASN:H	1.62	0.63
2:B:557:PHE:CE2	2:B:603:LEU:HD11	2.32	0.63
2:B:613:VAL:HG12	2:B:628:THR:HA	1.79	0.63
2:B:1007:VAL:HG13	2:B:1008:PRO:HD2	1.80	0.63
12:L:61:THR:HB	12:L:63:ARG:HG3	1.80	0.63
7:G:145:VAL:HG12	7:G:163:ILE:CG2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:C	1:A:337:ARG:N	2.56	0.63
1:A:341:MET:HE3	1:A:1429:ILE:HG13	1.81	0.63
1:A:414:ASP:OD1	1:A:416:ARG:HG3	1.99	0.63
4:D:37:GLN:OE1	7:G:5:LYS:HE3	1.99	0.63
1:A:757:ASN:ND2	2:B:1021:MET:HE2	2.13	0.63
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.81	0.63
4:D:7:THR:HG22	7:G:7:LEU:HA	1.81	0.63
4:D:168:LYS:CE	4:D:177:VAL:HG11	2.28	0.63
5:E:132:ILE:HD12	5:E:132:ILE:H	1.62	0.63
1:A:783:THR:HG21	1:A:796:SER:O	1.98	0.63
2:B:57:TYR:O	2:B:59:LEU:N	2.32	0.63
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.34	0.63
3:C:57:VAL:HG23	3:C:58:LEU:HD23	1.81	0.63
5:E:29:PHE:C	5:E:30:ILE:HD12	2.24	0.63
1:A:306:ASN:H	1:A:324:SER:HB3	1.64	0.62
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.26	0.62
7:G:10:ASN:OD1	7:G:71:ASN:ND2	2.29	0.62
12:L:28:LYS:NZ	12:L:41:SER:HA	2.14	0.62
12:L:68:GLU:HB2	12:L:70:ARG:HH21	1.64	0.62
1:A:690:VAL:CG1	1:A:718:VAL:HG13	2.29	0.62
9:I:50:THR:O	9:I:90:GLN:NE2	2.28	0.62
1:A:86:LEU:HD12	1:A:236:LEU:O	1.99	0.62
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.34	0.62
1:A:1197:LEU:HD22	1:A:1202:MET:HE1	1.80	0.62
1:A:1435:PRO:C	1:A:1436:ILE:HD12	2.24	0.62
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.34	0.62
2:B:26:THR:HG23	2:B:29:ASP:H	1.64	0.62
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.82	0.62
2:B:570:VAL:HG23	2:B:570:VAL:O	1.98	0.62
1:A:40:THR:HG23	1:A:259:GLU:HG3	1.80	0.62
1:A:112:LYS:HE3	1:A:215:SER:HB2	1.81	0.62
1:A:446:ARG:HH12	18:A:1806:ATP:H1'	1.64	0.62
1:A:447:GLN:O	1:A:449:SER:N	2.32	0.62
1:A:508:PRO:HA	1:A:511:ILE:HG13	1.80	0.62
1:A:541:ILE:HG21	1:A:549:MET:HE2	1.80	0.62
2:B:709:ASP:O	2:B:730:ARG:NH2	2.33	0.62
3:C:167:HIS:CD2	12:L:70:ARG:HG2	2.34	0.62
1:A:335:ARG:H	1:A:339:ASN:HB2	1.63	0.62
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.25	0.62
2:B:62:ILE:HD12	2:B:417:PHE:CD2	2.35	0.62
1:A:495:GLU:HG2	6:F:98:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ILE:HG21	1:A:1025:ARG:HD2	1.80	0.62
1:A:960:ILE:HG22	1:A:1025:ARG:HD3	1.82	0.62
1:A:1197:LEU:HD13	1:A:1202:MET:HE3	1.82	0.62
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.82	0.62
2:B:377:PHE:HE1	2:B:381:MET:HE2	1.65	0.62
2:B:848:ARG:HH22	2:B:996:ARG:HH11	1.47	0.62
1:A:199:LEU:HD23	1:A:199:LEU:O	2.00	0.62
1:A:730:GLY:HA3	1:A:759:ALA:HB2	1.81	0.62
4:D:40:HIS:CD2	7:G:6:ASP:HB3	2.35	0.62
9:I:85:PHE:HD2	9:I:99:LEU:HD22	1.65	0.62
11:K:40:HIS:H	11:K:40:HIS:CD2	2.18	0.62
2:B:707:PRO:HG2	2:B:708:GLU:OE1	1.99	0.62
2:B:802:PRO:HG3	2:B:1091:TYR:CZ	2.35	0.62
7:G:111:THR:HB	7:G:114:LEU:HD23	1.81	0.62
1:A:443:LEU:HB3	1:A:490:HIS:HB2	1.82	0.61
2:B:308:TRP:HH2	9:I:47:GLU:HG3	1.65	0.61
2:B:851:PHE:HD1	2:B:1094:ARG:HB2	1.64	0.61
8:H:135:LEU:HD12	8:H:137:GLN:HG3	1.80	0.61
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.15	0.61
1:A:474:VAL:HG22	1:A:478:TYR:HE2	1.66	0.61
1:A:1165:GLU:OE2	1:A:1235:LYS:HE3	2.00	0.61
12:L:32:ALA:HB2	12:L:55:ILE:HG21	1.80	0.61
12:L:32:ALA:CB	12:L:55:ILE:HG21	2.29	0.61
1:A:113:LEU:HB3	1:A:115:LEU:O	2.00	0.61
2:B:332:ASP:C	2:B:334:ILE:H	2.09	0.61
6:F:110:ASP:O	6:F:123:LYS:HE2	1.99	0.61
1:A:412:ARG:NH2	2:B:1108:ARG:HD2	2.14	0.61
1:A:1377:THR:HA	5:E:212:ARG:NH2	2.14	0.61
1:A:1444:MET:HA	7:G:59:GLY:O	2.01	0.61
2:B:1069:PHE:O	2:B:1070:GLU:HG3	2.00	0.61
6:F:74:ILE:HB	6:F:143:PHE:O	2.00	0.61
1:A:312:PRO:O	1:A:313:GLN:HB3	1.99	0.61
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.35	0.61
3:C:33:LEU:HD21	3:C:247:GLY:C	2.25	0.61
3:C:242:GLN:HA	3:C:245:VAL:HB	1.82	0.61
4:D:8:PHE:CZ	7:G:6:ASP:HB2	2.35	0.61
1:A:1260:LEU:HA	1:A:1263:ILE:HD12	1.82	0.61
2:B:235:SER:HB2	2:B:258:LEU:HD22	1.83	0.61
3:C:58:LEU:HB3	3:C:62:PHE:CD2	2.32	0.61
1:A:215:SER:HB3	1:A:218:ASP:CB	2.29	0.61
1:A:446:ARG:NH2	1:A:448:PRO:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASN:O	1:A:517:ASN:ND2	2.34	0.61
1:A:1410:PHE:CZ	2:B:1210:MET:HE2	2.35	0.61
2:B:560:GLU:HG2	2:B:560:GLU:O	2.00	0.61
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.65	0.61
3:C:70:ILE:HG23	3:C:71:PRO:HD2	1.82	0.61
9:I:82:GLU:HG3	9:I:82:GLU:O	1.99	0.61
1:A:1146:VAL:CG2	1:A:1197:LEU:HD22	2.31	0.61
2:B:579:ARG:HG2	2:B:586:TRP:CZ2	2.35	0.61
8:H:25:ARG:HD3	8:H:41:ASP:OD2	2.01	0.61
1:A:49:LYS:H	1:A:49:LYS:HD2	1.66	0.61
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.25	0.61
1:A:334:GLY:O	1:A:335:ARG:C	2.44	0.61
1:A:443:LEU:HD11	1:A:455:MET:HB3	1.83	0.61
2:B:760:ASP:OD1	2:B:760:ASP:N	2.26	0.61
2:B:770:GLN:CD	2:B:983:ARG:HA	2.25	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.35	0.61
9:I:19:ASP:CB	9:I:24:ARG:HG2	2.30	0.61
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.60
1:A:1140:HIS:H	1:A:1275:GLY:HA3	1.65	0.60
2:B:60:GLN:HE21	2:B:94:LYS:HG3	1.65	0.60
5:E:68:SER:HB3	5:E:75:MET:CE	2.31	0.60
8:H:118:PHE:O	8:H:120:GLY:N	2.33	0.60
1:A:49:LYS:HE2	1:A:61:ILE:HB	1.83	0.60
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.83	0.60
2:B:705:MET:HA	2:B:705:MET:HE3	1.83	0.60
2:B:1081:LEU:C	2:B:1083:ALA:H	2.09	0.60
5:E:61:GLN:HG2	5:E:78:LEU:O	2.01	0.60
1:A:107:CYS:CB	1:A:148:CYS:SG	2.90	0.60
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.84	0.60
2:B:308:TRP:CD1	2:B:308:TRP:H	2.18	0.60
7:G:18:PHE:HZ	7:G:68:ALA:H	1.47	0.60
8:H:124:ARG:NH2	8:H:126:GLU:OE2	2.34	0.60
9:I:15:TYR:HB2	9:I:30:ARG:NH1	2.16	0.60
1:A:693:VAL:HG12	1:A:714:PHE:CD1	2.35	0.60
1:A:1260:LEU:HD12	1:A:1263:ILE:HD12	1.83	0.60
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.41	0.60
2:B:351:TYR:O	2:B:355:ILE:HG13	2.01	0.60
3:C:80:LEU:O	3:C:161:LYS:HD2	2.02	0.60
7:G:35:GLU:OE1	7:G:35:GLU:HA	2.00	0.60
8:H:33:GLN:O	8:H:35:GLN:N	2.34	0.60
12:L:38:LEU:CD2	12:L:48:CYS:HA	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:NZ	1:A:205:GLU:OE2	2.30	0.60
1:A:481:ASP:OD1	1:A:481:ASP:N	2.30	0.60
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.31	0.60
5:E:127:ILE:HG22	5:E:129:PRO:HD2	1.83	0.60
8:H:13:SER:HB2	8:H:27:GLU:O	2.01	0.60
12:L:68:GLU:HB2	12:L:70:ARG:HE	1.67	0.60
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.83	0.60
2:B:622:LYS:HD2	9:I:59:VAL:CG1	2.30	0.60
1:A:757:ASN:HD22	2:B:1021:MET:HE2	1.65	0.60
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.67	0.60
1:A:780:VAL:HG22	2:B:699:GLU:OE1	2.01	0.60
1:A:1172:LEU:HD12	1:A:1172:LEU:N	2.16	0.60
2:B:1161:HIS:HB3	2:B:1171:VAL:HB	1.83	0.60
2:B:1201:LYS:O	2:B:1205:GLN:HG3	2.02	0.60
7:G:80:LYS:NZ	19:G:201:HOH:O	2.35	0.60
8:H:9:ILE:HG23	8:H:56:THR:HA	1.83	0.60
1:A:848:ILE:HG21	1:A:1370:LEU:HD21	1.83	0.59
1:A:960:ILE:CG2	1:A:1025:ARG:CD	2.80	0.59
1:A:1135:ARG:HG2	1:A:1282:VAL:HG11	1.83	0.59
2:B:466:TRP:O	2:B:468:GLU:N	2.35	0.59
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.82	0.59
1:A:42:ASP:OD1	1:A:42:ASP:N	2.34	0.59
2:B:234:ILE:HG12	2:B:257:LYS:HD3	1.84	0.59
2:B:382:ILE:O	2:B:386:LEU:HG	2.03	0.59
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.85	0.59
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.84	0.59
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.83	0.59
7:G:18:PHE:CD1	7:G:22:MET:HE3	2.37	0.59
1:A:58:LEU:HB3	1:A:80:HIS:O	2.02	0.59
1:A:981:LEU:HD23	1:A:1039:LYS:HD2	1.84	0.59
1:A:446:ARG:NH1	18:A:1806:ATP:H1'	2.17	0.59
1:A:671:ALA:O	1:A:673:GLY:N	2.29	0.59
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.84	0.59
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.03	0.59
4:D:118:THR:O	4:D:119:ARG:HG3	2.03	0.59
1:A:120:GLU:HG2	1:A:123:ARG:HH21	1.67	0.59
1:A:496:GLU:OE2	7:G:64:THR:HA	2.03	0.59
1:A:1444:MET:HB2	6:F:133:VAL:HG23	1.84	0.59
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.37	0.59
7:G:126:ASN:HB3	7:G:127:PRO:CD	2.32	0.59
1:A:32:VAL:HG11	1:A:80:HIS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:O	1:A:316:GLN:HG3	2.00	0.59
1:A:337:ARG:NE	1:A:839:ARG:NH2	2.50	0.59
1:A:924:LYS:O	1:A:927:VAL:HG12	2.02	0.59
1:A:1146:VAL:HG23	1:A:1197:LEU:CD2	2.32	0.59
1:A:1445:ILE:CG2	6:F:132:LEU:HD23	2.33	0.59
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.84	0.59
2:B:1012:ILE:HG21	2:B:1092:TYR:OH	2.02	0.59
5:E:154:ILE:O	5:E:196:VAL:HA	2.02	0.59
1:A:75:ASN:O	1:A:76:GLU:HB2	2.02	0.59
1:A:329:LEU:HD21	2:B:1206:GLU:OE1	2.03	0.59
1:A:419:LYS:HG3	1:A:420:ARG:N	2.18	0.59
1:A:850:VAL:HG23	1:A:1064:VAL:CG1	2.32	0.59
10:J:25:LEU:HD21	10:J:32:GLU:HG3	1.84	0.59
1:A:98:LYS:O	1:A:102:VAL:HG23	2.03	0.59
1:A:224:PHE:HE2	1:A:231:PRO:HA	1.68	0.59
1:A:474:VAL:HG22	1:A:478:TYR:CE2	2.38	0.59
2:B:579:ARG:HA	2:B:589:VAL:HG12	1.84	0.59
3:C:99:LEU:CD1	3:C:120:ILE:HG12	2.33	0.59
4:D:187:THR:HB	4:D:190:GLU:H	1.68	0.59
5:E:100:ILE:HG23	5:E:105:PHE:CD2	2.38	0.59
1:A:605:MET:HE3	1:A:606:LEU:H	1.67	0.59
1:A:765:VAL:HB	1:A:800:VAL:HB	1.85	0.59
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.02	0.59
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.85	0.59
1:A:62:ASP:HB3	1:A:65:LEU:HB2	1.84	0.58
1:A:496:GLU:HG3	1:A:497:THR:N	2.18	0.58
9:I:13:MET:HG3	9:I:14:LEU:N	2.17	0.58
1:A:110:CYS:SG	1:A:167:CYS:N	2.76	0.58
1:A:672:ASP:HA	1:A:676:MET:HG3	1.86	0.58
2:B:578:THR:HG22	2:B:622:LYS:HA	1.84	0.58
2:B:872:GLU:HG2	2:B:916:THR:HA	1.85	0.58
1:A:1163:ILE:HG21	1:A:1166:ASP:OD2	2.03	0.58
2:B:766:ARG:HG3	2:B:1022:THR:CG2	2.33	0.58
4:D:155:ARG:H	4:D:219:THR:HG21	1.68	0.58
1:A:83:HIS:C	1:A:84:ILE:HG13	2.28	0.58
1:A:315:LEU:CD2	1:A:318:SER:HB2	2.28	0.58
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.39	0.58
8:H:5:LEU:HD13	8:H:135:LEU:HD21	1.84	0.58
1:A:35:ILE:O	1:A:84:ILE:HG23	2.03	0.58
1:A:562:THR:HG22	8:H:79:TRP:CD1	2.38	0.58
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:THR:O	2:B:1044:ALA:N	2.35	0.58
2:B:204:ILE:C	2:B:205:ILE:HD12	2.29	0.58
2:B:743:ILE:HD12	2:B:743:ILE:H	1.67	0.58
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.85	0.58
7:G:89:GLY:HA3	7:G:103:VAL:HG22	1.84	0.58
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.04	0.58
1:A:678:GLU:HG2	1:A:732:LEU:CD2	2.34	0.58
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.84	0.58
1:A:1118:VAL:HB	1:A:1327:ILE:HD11	1.85	0.58
1:A:1220:PHE:C	1:A:1221:LYS:HD2	2.28	0.58
1:A:1371:LEU:O	1:A:1374:VAL:HB	2.04	0.58
6:F:101:ILE:HG22	6:F:117:PRO:HB3	1.84	0.58
1:A:1370:LEU:HD23	1:A:1374:VAL:HG23	1.84	0.58
2:B:983:ARG:CD	2:B:1091:TYR:HB3	2.34	0.58
3:C:182:PRO:HG3	3:C:206:ASN:O	2.04	0.58
1:A:302:THR:HG22	1:A:308:ILE:HD11	1.86	0.58
1:A:456:MET:HB3	1:A:507:VAL:HG22	1.86	0.58
2:B:468:GLU:O	2:B:469:GLN:HB2	2.04	0.58
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.19	0.58
4:D:202:ILE:CG2	4:D:207:LEU:HB2	2.33	0.58
9:I:15:TYR:HD2	9:I:30:ARG:HD3	1.69	0.58
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.86	0.58
1:A:702:LEU:HD23	1:A:710:LEU:HB3	1.86	0.58
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.86	0.58
9:I:17:ARG:HG2	9:I:18:GLU:H	1.68	0.58
1:A:175:ARG:HG3	1:A:182:VAL:HG23	1.85	0.57
1:A:1342:GLU:HG2	5:E:198:ILE:HG21	1.85	0.57
2:B:794:ASN:C	2:B:795:ILE:HD12	2.28	0.57
5:E:16:PHE:CE2	5:E:20:LYS:HD2	2.39	0.57
5:E:97:VAL:O	5:E:101:GLN:HB2	2.04	0.57
8:H:132:LEU:HD23	8:H:132:LEU:H	1.69	0.57
1:A:350:ARG:HB2	2:B:1128:LEU:HD21	1.85	0.57
1:A:1121:GLU:HG2	1:A:1122:PRO:CD	2.33	0.57
2:B:463:THR:HB	2:B:465:ASN:HD22	1.70	0.57
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.68	0.57
11:K:50:LEU:O	11:K:56:VAL:HG11	2.04	0.57
1:A:143:LYS:O	1:A:146:MET:HE3	2.03	0.57
1:A:341:MET:HA	1:A:341:MET:HE2	1.85	0.57
1:A:432:VAL:O	1:A:434:ARG:N	2.37	0.57
5:E:123:LEU:H	5:E:123:LEU:CD2	2.17	0.57
9:I:13:MET:HG2	9:I:15:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:SER:HB3	2:B:1015:HIS:CE1	2.39	0.57
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.04	0.57
2:B:356:LEU:O	2:B:374:LYS:NZ	2.36	0.57
2:B:364:ILE:O	2:B:365:THR:HB	2.03	0.57
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.34	0.57
1:A:1193:LEU:HD13	1:A:1260:LEU:HD21	1.84	0.57
2:B:563:MET:HG3	2:B:588:GLY:HA3	1.87	0.57
3:C:232:VAL:HG21	3:C:244:VAL:CG2	2.35	0.57
5:E:3:GLN:CD	5:E:5:ASN:HB2	2.29	0.57
12:L:34:CYS:SG	12:L:36:SER:OG	2.45	0.57
1:A:540:PHE:HB3	1:A:571:LEU:HD22	1.84	0.57
2:B:1129:ARG:HG2	14:T:20:DC:H5'	1.85	0.57
5:E:26:ARG:HG2	5:E:155:ARG:HH12	1.70	0.57
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.86	0.57
1:A:601:LYS:HE3	1:A:603:ASN:HD21	1.69	0.57
1:A:690:VAL:HG13	1:A:718:VAL:HG13	1.84	0.57
1:A:1188:GLN:HA	1:A:1243:VAL:HA	1.86	0.57
2:B:578:THR:HG22	2:B:622:LYS:HB3	1.87	0.57
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.86	0.57
2:B:951:GLN:HG3	12:L:57:LEU:HD21	1.85	0.57
1:A:447:GLN:HE21	14:T:20:DC:H2''	1.69	0.57
1:A:936:LEU:O	1:A:939:ASP:HB2	2.05	0.57
2:B:597:MET:O	2:B:601:ARG:HB2	2.05	0.57
1:A:361:LEU:HA	1:A:471:ASN:HD22	1.68	0.57
1:A:1015:VAL:O	1:A:1017:LEU:N	2.38	0.57
2:B:546:SER:HG	2:B:631:GLY:N	2.00	0.57
1:A:403:LYS:O	1:A:415:LEU:HB2	2.05	0.57
1:A:541:ILE:HD11	1:A:574:GLY:HA2	1.87	0.57
1:A:668:ASP:CG	1:A:742:ASN:HB2	2.29	0.57
2:B:26:THR:HG22	2:B:29:ASP:OD2	2.04	0.57
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.87	0.57
3:C:37:MET:CE	3:C:232:VAL:HG11	2.35	0.57
1:A:18:GLN:HA	1:A:1418:LEU:HD12	1.86	0.56
1:A:49:LYS:H	1:A:49:LYS:CD	2.17	0.56
1:A:542:GLU:HG2	1:A:543:LEU:H	1.70	0.56
1:A:901:LEU:HG	1:A:929:LEU:CD1	2.35	0.56
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.85	0.56
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.86	0.56
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.33	0.56
9:I:17:ARG:HG2	9:I:18:GLU:N	2.20	0.56
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:CZ	1:A:207:ILE:HD12	2.36	0.56
3:C:11:ARG:NH2	3:C:21:ILE:HD11	2.20	0.56
4:D:130:LEU:HD22	4:D:142:LYS:CG	2.35	0.56
1:A:262:LEU:CD2	1:A:325:ILE:HG12	2.35	0.56
1:A:316:GLN:O	1:A:317:LYS:HG2	2.04	0.56
1:A:332:LYS:O	1:A:333:GLU:HB2	2.05	0.56
1:A:1166:ASP:O	1:A:1170:ILE:HG23	2.05	0.56
1:A:1169:ILE:HG21	1:A:1229:SER:HA	1.87	0.56
1:A:1263:ILE:O	1:A:1267:MET:HB2	2.05	0.56
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.87	0.56
1:A:1377:THR:HB	5:E:176:PRO:HB3	1.88	0.56
2:B:367:LEU:HD11	2:B:370:PHE:HD2	1.70	0.56
2:B:377:PHE:CE1	2:B:381:MET:HE2	2.39	0.56
2:B:467:GLY:O	2:B:472:ALA:HB2	2.05	0.56
2:B:852:ARG:HH12	12:L:70:ARG:C	2.14	0.56
2:B:956:THR:HA	2:B:961:LEU:O	2.05	0.56
2:B:1060:ARG:NE	3:C:202:PRO:HG3	2.19	0.56
2:B:1181:GLU:OE2	2:B:1183:LYS:HB2	2.05	0.56
3:C:32:SER:O	3:C:36:VAL:HG23	2.06	0.56
3:C:99:LEU:HD13	3:C:120:ILE:HA	1.87	0.56
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.87	0.56
11:K:10:PHE:HA	11:K:37:LYS:HB3	1.86	0.56
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.86	0.56
1:A:55:ASP:C	1:A:57:ARG:H	2.13	0.56
1:A:474:VAL:HG22	1:A:474:VAL:O	2.05	0.56
1:A:525:GLN:HG3	2:B:836:GLU:HG2	1.87	0.56
1:A:672:ASP:N	1:A:676:MET:HG3	2.20	0.56
2:B:525:ALA:O	2:B:768:THR:HG23	2.05	0.56
5:E:12:LEU:CD2	5:E:55:ARG:HH21	2.19	0.56
5:E:65:THR:O	5:E:69:ILE:HG12	2.05	0.56
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.38	0.56
1:A:392:VAL:HG13	1:A:415:LEU:HD21	1.86	0.56
2:B:90:ILE:HD12	2:B:91:SER:N	2.19	0.56
2:B:287:ARG:NH1	2:B:324:ILE:O	2.32	0.56
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.87	0.56
4:D:154:PHE:CE2	4:D:163:VAL:HG21	2.40	0.56
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.41	0.56
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.51	0.56
2:B:499:ASN:HA	2:B:536:VAL:HG22	1.87	0.56
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.41	0.56
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:VAL:CB	5:E:125:PRO:HD3	2.35	0.56
7:G:9:LEU:HD23	7:G:11:ILE:HG12	1.87	0.56
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.87	0.56
1:A:633:VAL:O	1:A:637:LYS:HB2	2.05	0.56
1:A:1288:ASP:HB3	1:A:1300:LYS:HE2	1.87	0.56
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.03	0.56
1:A:1434:ALA:O	1:A:1436:ILE:N	2.37	0.56
2:B:208:SER:OG	2:B:210:LYS:NZ	2.34	0.56
2:B:218:SER:HA	2:B:404:LYS:HG2	1.88	0.56
3:C:57:VAL:HG21	10:J:57:ILE:HG13	1.88	0.56
5:E:90:VAL:O	5:E:94:LYS:HB2	2.06	0.56
9:I:15:TYR:CD2	9:I:30:ARG:HD3	2.40	0.56
2:B:578:THR:HG22	2:B:622:LYS:CB	2.36	0.56
1:A:590:ARG:NH1	1:A:592:ASP:CG	2.64	0.56
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.86	0.56
1:A:1445:ILE:HB	1:A:1450:LEU:HD11	1.88	0.56
2:B:287:ARG:HD3	2:B:325:GLN:C	2.30	0.56
2:B:453:ILE:HD12	2:B:453:ILE:H	1.71	0.56
2:B:615:MET:CG	2:B:626:ILE:HG23	2.34	0.56
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.06	0.56
4:D:23:ASN:ND2	19:G:201:HOH:O	2.38	0.56
1:A:84:ILE:HG21	1:A:270:LEU:HD13	1.88	0.56
1:A:337:ARG:NH2	1:A:839:ARG:CZ	2.69	0.56
5:E:83:CYS:HB2	5:E:110:PHE:HZ	1.70	0.56
10:J:54:VAL:O	10:J:56:LEU:HD12	2.06	0.56
5:E:96:PHE:HA	5:E:99:HIS:HB2	1.88	0.55
5:E:119:SER:C	5:E:123:LEU:HB3	2.30	0.55
2:B:318:VAL:O	2:B:321:GLY:N	2.39	0.55
2:B:617:ARG:HD3	2:B:619:ILE:HG13	1.89	0.55
2:B:848:ARG:NH2	3:C:168:ALA:HB1	2.21	0.55
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.72	0.55
3:C:63:ILE:O	3:C:67:LEU:HG	2.06	0.55
4:D:215:SER:HA	4:D:218:GLU:HG3	1.86	0.55
1:A:76:GLU:HG3	2:B:1159:ARG:HH22	1.70	0.55
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.88	0.55
3:C:145:CYS:SG	3:C:146:LYS:N	2.80	0.55
1:A:34:LYS:HG3	1:A:36:ARG:HG3	1.88	0.55
1:A:122:MET:O	1:A:126:LEU:HB2	2.07	0.55
1:A:514:PRO:CB	1:A:875:ALA:HB3	2.36	0.55
1:A:700:ASN:C	1:A:702:LEU:H	2.14	0.55
1:A:1121:GLU:HG3	1:A:1122:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG22	2:B:809:MET:HG3	1.87	0.55
1:A:53:LEU:HD23	1:A:54:ASN:H	1.71	0.55
1:A:335:ARG:HG3	1:A:339:ASN:CB	2.36	0.55
2:B:104:GLU:CD	12:L:54:ARG:HH12	2.13	0.55
2:B:249:ARG:HE	2:B:415:GLN:HG3	1.71	0.55
2:B:299:GLU:HG3	2:B:572:HIS:CD2	2.41	0.55
2:B:528:PRO:HG2	2:B:532:ALA:HB3	1.87	0.55
4:D:119:ARG:HD2	4:D:120:GLU:H	1.72	0.55
1:A:182:VAL:HG12	1:A:201:VAL:HA	1.87	0.55
1:A:675:THR:OG1	1:A:736:ASN:HB2	2.06	0.55
1:A:867:ILE:HG21	1:A:1000:LEU:HD11	1.87	0.55
1:A:980:ASP:OD1	1:A:980:ASP:N	2.40	0.55
1:A:1410:PHE:HZ	2:B:1210:MET:HE2	1.71	0.55
2:B:549:THR:HB	2:B:628:THR:HB	1.89	0.55
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.88	0.55
1:A:678:GLU:HG2	1:A:732:LEU:HD22	1.89	0.55
1:A:1301:GLU:HG3	1:A:1301:GLU:O	2.05	0.55
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.87	0.55
4:D:52:LEU:N	4:D:182:SER:HB3	2.21	0.55
8:H:96:VAL:HA	8:H:142:LEU:O	2.07	0.55
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.89	0.55
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.36	0.55
1:A:714:PHE:CZ	1:A:718:VAL:HG21	2.42	0.55
1:A:827:THR:O	1:A:827:THR:HG22	2.07	0.55
3:C:133:ILE:HD13	3:C:236:GLY:C	2.32	0.55
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.89	0.55
1:A:1420:ASP:CG	1:A:1422:ARG:HG3	2.32	0.55
2:B:416:LEU:HD22	2:B:420:LEU:HD11	1.88	0.55
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.42	0.55
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.89	0.55
1:A:1226:VAL:O	1:A:1227:ILE:HG13	2.07	0.55
2:B:542:MET:HB3	2:B:636:PRO:CD	2.37	0.55
2:B:616:ILE:O	2:B:624:LEU:HD22	2.07	0.55
2:B:620:ARG:NH2	9:I:68:LEU:HD21	2.22	0.55
9:I:83:ASN:HB2	9:I:102:VAL:O	2.07	0.55
13:R:4:G:H2'	13:R:5:A:H8	1.72	0.55
1:A:130:ASP:O	1:A:132:LYS:N	2.40	0.54
1:A:775:ILE:HG21	1:A:815:PHE:CE1	2.42	0.54
1:A:960:ILE:HG22	1:A:1025:ARG:CD	2.37	0.54
4:D:202:ILE:HG23	4:D:207:LEU:HB2	1.88	0.54
7:G:93:SER:HB2	7:G:100:GLU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.72	0.54
1:A:1155:ASP:CG	1:A:1162:VAL:HG12	2.31	0.54
1:A:1276:VAL:HG11	1:A:1315:GLU:HB3	1.90	0.54
4:D:25:ALA:HB3	7:G:84:GLY:C	2.32	0.54
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.72	0.54
1:A:857:ARG:HD3	1:A:861:GLY:O	2.08	0.54
1:A:1036:ARG:HH11	1:A:1036:ARG:HA	1.72	0.54
1:A:1411:GLU:O	1:A:1415:SER:OG	2.23	0.54
2:B:282:ILE:HD11	2:B:317:CYS:CB	2.35	0.54
2:B:378:LEU:HD12	2:B:378:LEU:O	2.07	0.54
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.72	0.54
5:E:108:GLY:C	5:E:109:ILE:HD12	2.33	0.54
7:G:28:THR:O	7:G:32:GLU:HG3	2.08	0.54
8:H:27:GLU:HG3	8:H:39:THR:HG22	1.89	0.54
8:H:38:LEU:HD12	8:H:124:ARG:O	2.07	0.54
8:H:56:THR:HG22	8:H:57:VAL:H	1.73	0.54
1:A:328:ARG:HB3	1:A:335:ARG:NH2	2.23	0.54
1:A:1441:PHE:CE2	6:F:92:ARG:HD3	2.43	0.54
2:B:912:ILE:HB	2:B:939:THR:HB	1.90	0.54
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.08	0.54
4:D:130:LEU:HD21	4:D:141:LEU:HG	1.90	0.54
6:F:105:ALA:HA	7:G:16:SER:HA	1.90	0.54
1:A:470:LEU:HD13	1:A:474:VAL:CG1	2.36	0.54
1:A:495:GLU:CG	6:F:98:ALA:HB1	2.37	0.54
1:A:575:LYS:HD2	8:H:120:GLY:CA	2.36	0.54
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.37	0.54
1:A:1202:MET:O	1:A:1207:LEU:HB2	2.07	0.54
2:B:360:PHE:CZ	2:B:361:LEU:HD13	2.43	0.54
2:B:638:PHE:HB2	2:B:741:CYS:HB3	1.90	0.54
4:D:119:ARG:CG	4:D:120:GLU:H	2.21	0.54
1:A:19:PHE:HZ	1:A:1397:LEU:HD21	1.71	0.54
1:A:451:HIS:NE2	1:A:453:MET:HE2	2.22	0.54
1:A:456:MET:HE2	1:A:510:GLN:HB2	1.90	0.54
1:A:700:ASN:O	1:A:702:LEU:N	2.40	0.54
1:A:841:LEU:O	1:A:845:LEU:HD13	2.08	0.54
1:A:1031:VAL:HG13	1:A:1037:LEU:HD13	1.89	0.54
2:B:367:LEU:HD11	2:B:370:PHE:CD2	2.42	0.54
2:B:581:PHE:HB2	2:B:625:LYS:HA	1.90	0.54
5:E:20:LYS:HE3	5:E:35:VAL:HA	1.90	0.54
1:A:33:ALA:HB1	1:A:56:PRO:HB2	1.90	0.54
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:VAL:CG2	1:A:1292:PRO:HD2	2.38	0.54
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.23	0.54
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.88	0.54
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.75	0.54
1:A:457:ALA:HB2	1:A:501:LEU:HD22	1.89	0.54
1:A:566:ILE:O	1:A:568:PRO:HD2	2.07	0.54
1:A:601:LYS:HG3	1:A:603:ASN:ND2	2.23	0.54
1:A:850:VAL:HG22	1:A:868:TYR:HB2	1.90	0.54
1:A:1008:GLN:O	1:A:1011:GLN:HB3	2.08	0.54
1:A:1444:MET:HB3	7:G:58:ARG:HB3	1.89	0.54
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.90	0.54
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.38	0.54
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.89	0.54
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.90	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.23	0.54
5:E:41:ASP:N	5:E:41:ASP:OD1	2.40	0.54
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.89	0.54
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.43	0.54
1:A:671:ALA:HB1	1:A:736:ASN:HD22	1.73	0.54
2:B:95:ILE:HG13	2:B:130:VAL:HB	1.90	0.54
2:B:185:THR:HG22	2:B:188:ASP:OD2	2.07	0.54
2:B:545:ILE:HG22	2:B:546:SER:O	2.07	0.54
2:B:766:ARG:HG3	2:B:1022:THR:HG23	1.89	0.54
2:B:973:ILE:O	2:B:973:ILE:HG12	2.07	0.54
1:A:93:VAL:HG11	1:A:304:MET:HB2	1.90	0.54
1:A:534:LEU:O	1:A:574:GLY:HA3	2.07	0.54
1:A:1255:GLU:OE1	1:A:1259:MET:HE2	2.08	0.54
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.08	0.54
3:C:142:VAL:CG1	10:J:5:VAL:HG22	2.38	0.54
5:E:11:ARG:NH2	5:E:141:VAL:HG21	2.22	0.54
6:F:135:ARG:NE	6:F:145:ASP:OD2	2.34	0.54
2:B:310:MET:HB2	2:B:392:ARG:NH2	2.23	0.53
4:D:154:PHE:CD2	4:D:163:VAL:HG21	2.43	0.53
10:J:12:LYS:HD3	10:J:13:VAL:H	1.73	0.53
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.22	0.53
2:B:265:SER:HA	2:B:267:ARG:NH1	2.23	0.53
7:G:111:THR:CB	7:G:114:LEU:HD23	2.37	0.53
8:H:13:SER:OG	8:H:28:ALA:HA	2.08	0.53
1:A:219:PHE:O	1:A:224:PHE:HB2	2.07	0.53
1:A:354:SER:HB2	1:A:469:ARG:HH11	1.74	0.53
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:GLY:HA3	14:T:18:DT:C1'	2.35	0.53
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.15	0.53
2:B:1203:LEU:O	2:B:1207:LEU:HG	2.08	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.53
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.41	0.53
1:A:747:VAL:HG22	1:A:753:GLY:HA3	1.90	0.53
1:A:101:LYS:HD3	1:A:139:TRP:NE1	2.23	0.53
1:A:447:GLN:NE2	14:T:20:DC:H4'	2.22	0.53
1:A:960:ILE:HD12	1:A:1021:LEU:HD23	1.89	0.53
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.09	0.53
4:D:25:ALA:N	7:G:83:LYS:O	2.39	0.53
4:D:48:ILE:HD13	7:G:4:ILE:O	2.09	0.53
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.91	0.53
8:H:25:ARG:HD3	8:H:41:ASP:CG	2.33	0.53
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.89	0.53
14:T:24:DT:H3'	14:T:25:DC:H5''	1.91	0.53
2:B:758:PHE:N	2:B:759:PRO:HD3	2.24	0.53
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.43	0.53
2:B:884:ARG:O	2:B:936:ASP:HB3	2.09	0.53
4:D:153:ARG:HH12	4:D:214:LEU:HD23	1.73	0.53
10:J:18:TRP:CZ2	10:J:55:ASP:HB2	2.44	0.53
10:J:64:ASN:HB2	10:J:65:PRO:CD	2.39	0.53
1:A:16:GLU:OE2	2:B:1221:SER:N	2.41	0.53
1:A:447:GLN:HG3	14:T:20:DC:H2''	1.89	0.53
1:A:472:LEU:O	1:A:475:THR:HG23	2.08	0.53
1:A:844:ALA:C	1:A:845:LEU:HD12	2.34	0.53
1:A:879:GLU:OE1	1:A:959:ASN:ND2	2.38	0.53
1:A:1236:LEU:O	1:A:1237:ILE:HD12	2.09	0.53
2:B:487:THR:HG22	2:B:488:TYR:N	2.24	0.53
3:C:167:HIS:CG	12:L:70:ARG:HG2	2.43	0.53
1:A:306:ASN:H	1:A:324:SER:CB	2.21	0.53
1:A:598:LEU:HD22	8:H:25:ARG:NH2	2.23	0.53
1:A:731:ARG:HB3	1:A:755:PHE:HZ	1.73	0.53
1:A:738:LYS:CE	3:C:194:GLU:HA	2.38	0.53
1:A:80:HIS:H	1:A:243:PRO:HB3	1.74	0.53
1:A:599:SER:O	8:H:25:ARG:NH1	2.29	0.53
5:E:125:PRO:HA	5:E:132:ILE:HD13	1.91	0.53
8:H:9:ILE:HG13	8:H:56:THR:HG23	1.91	0.53
1:A:176:LYS:HG2	1:A:178:GLY:H	1.73	0.53
1:A:329:LEU:HD23	1:A:335:ARG:HH21	1.74	0.53
18:A:1806:ATP:H5'2	18:A:1806:ATP:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:PRO:HG2	2:B:461:LEU:CD1	2.39	0.53
2:B:640:VAL:HG13	2:B:651:LEU:HA	1.90	0.53
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.24	0.53
4:D:154:PHE:HA	4:D:219:THR:HG22	1.90	0.53
7:G:154:VAL:HG12	7:G:155:SER:H	1.74	0.53
1:A:248:PRO:HD3	2:B:1114:LEU:HD13	1.91	0.52
1:A:302:THR:HA	1:A:305:ASP:O	2.09	0.52
1:A:763:ALA:O	1:A:803:SER:HB3	2.09	0.52
1:A:775:ILE:HG21	1:A:815:PHE:HD1	1.70	0.52
1:A:919:ILE:CD1	1:A:925:LEU:HD13	2.39	0.52
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.39	0.52
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.74	0.52
2:B:1181:GLU:HG2	2:B:1183:LYS:H	1.75	0.52
6:F:86:THR:HB	6:F:89:GLU:CG	2.37	0.52
10:J:48:ARG:NE	10:J:49:MET:HE2	2.21	0.52
5:E:17:ARG:HA	5:E:20:LYS:HD3	1.90	0.52
1:A:40:THR:HG22	1:A:41:MET:CG	2.37	0.52
3:C:177:GLU:O	3:C:230:MET:HA	2.09	0.52
4:D:190:GLU:HB2	7:G:167:TYR:CE1	2.44	0.52
9:I:10:CYS:SG	9:I:32:CYS:HB2	2.50	0.52
12:L:38:LEU:HD21	12:L:48:CYS:CA	2.36	0.52
1:A:237:THR:HG22	1:A:237:THR:O	2.09	0.52
1:A:412:ARG:HH22	2:B:1108:ARG:CD	2.20	0.52
1:A:1107:VAL:HG23	1:A:1383:SER:HB3	1.91	0.52
2:B:778:MET:HE2	2:B:794:ASN:OD1	2.08	0.52
5:E:26:ARG:CG	5:E:155:ARG:HH12	2.22	0.52
1:A:34:LYS:HB3	1:A:36:ARG:NH2	2.25	0.52
1:A:280:GLU:HG3	1:A:289:ILE:HD13	1.91	0.52
1:A:442:VAL:O	1:A:457:ALA:HA	2.10	0.52
1:A:697:ALA:HB2	1:A:702:LEU:HB2	1.92	0.52
1:A:1084:PHE:O	2:B:763:GLN:NE2	2.42	0.52
2:B:769:TYR:O	2:B:772:ALA:N	2.43	0.52
2:B:792:MET:HG2	2:B:855:PHE:CZ	2.44	0.52
3:C:27:LEU:HB2	3:C:228:PHE:CE2	2.45	0.52
3:C:33:LEU:HD13	3:C:37:MET:HG3	1.91	0.52
4:D:8:PHE:HE2	7:G:6:ASP:HB2	1.75	0.52
4:D:29:LEU:HG	7:G:82:PHE:CZ	2.45	0.52
4:D:48:ILE:HD12	4:D:48:ILE:N	2.25	0.52
10:J:2:ILE:HD12	10:J:57:ILE:HD12	1.90	0.52
10:J:64:ASN:HB2	10:J:65:PRO:HD3	1.91	0.52
1:A:1084:PHE:CE2	2:B:769:TYR:OH	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.49	0.52
1:A:1446:ASP:HB3	7:G:58:ARG:HE	1.74	0.52
2:B:604:ARG:HG3	2:B:611:PRO:HA	1.92	0.52
2:B:1063:GLY:O	3:C:202:PRO:HG2	2.08	0.52
2:B:1181:GLU:HA	2:B:1187:ASN:O	2.09	0.52
4:D:52:LEU:O	4:D:53:SER:HB2	2.10	0.52
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.90	0.52
7:G:108:VAL:CG2	7:G:159:ALA:HB3	2.39	0.52
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.55	0.52
2:B:357:GLN:HB3	2:B:366:GLN:O	2.10	0.52
2:B:573:GLN:O	2:B:575:PRO:HD3	2.10	0.52
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.07	0.52
5:E:169:ARG:NH2	6:F:74:ILE:HD11	2.23	0.52
1:A:55:ASP:C	1:A:57:ARG:N	2.67	0.52
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.45	0.52
1:A:532:ARG:CG	1:A:749:ALA:HB2	2.39	0.52
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.92	0.52
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.91	0.52
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.90	0.52
2:B:912:ILE:HD11	2:B:964:VAL:HG12	1.91	0.52
6:F:93:ILE:HD13	6:F:148:VAL:HG22	1.90	0.52
8:H:39:THR:O	8:H:124:ARG:N	2.41	0.52
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.45	0.52
1:A:532:ARG:HD3	1:A:749:ALA:HB2	1.91	0.52
1:A:542:GLU:O	1:A:546:VAL:HG23	2.10	0.52
2:B:698:GLU:HA	2:B:701:ILE:HG12	1.92	0.52
2:B:794:ASN:O	2:B:795:ILE:HD12	2.09	0.52
5:E:77:SER:O	5:E:105:PHE:HB3	2.10	0.52
1:A:96:ILE:HG23	1:A:97:ALA:N	2.23	0.52
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.92	0.52
1:A:659:HIS:HA	2:B:1074:ASN:HD22	1.74	0.52
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.92	0.52
1:A:1220:PHE:CE2	1:A:1267:MET:HG3	2.45	0.52
1:A:1438:THR:O	1:A:1438:THR:HG22	2.10	0.52
2:B:546:SER:OG	2:B:632:ARG:N	2.38	0.52
5:E:32:GLN:NE2	5:E:36:GLU:CD	2.68	0.52
8:H:130:ARG:HH11	8:H:130:ARG:C	2.17	0.52
12:L:38:LEU:HD21	12:L:48:CYS:SG	2.50	0.52
1:A:338:GLY:O	2:B:1129:ARG:NH1	2.42	0.51
1:A:350:ARG:HH11	1:A:447:GLN:CG	2.23	0.51
1:A:446:ARG:HG2	1:A:447:GLN:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:CYS:SG	2:B:181:LEU:HD12	2.50	0.51
2:B:773:MET:CE	2:B:985:GLY:HA2	2.41	0.51
2:B:891:ASP:N	2:B:891:ASP:OD1	2.43	0.51
4:D:174:PRO:HA	4:D:177:VAL:HB	1.92	0.51
5:E:118:PRO:O	5:E:122:LYS:HB3	2.10	0.51
7:G:108:VAL:HG11	7:G:145:VAL:HG21	1.92	0.51
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.92	0.51
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.46	0.51
2:B:773:MET:HE3	2:B:985:GLY:HA2	1.91	0.51
4:D:51:ASN:O	4:D:53:SER:N	2.43	0.51
8:H:93:TYR:HB3	8:H:144:ILE:O	2.10	0.51
10:J:35:ALA:O	10:J:39:LEU:HD12	2.10	0.51
1:A:229:SER:OG	1:A:1416:ALA:HB2	2.10	0.51
1:A:741:ASN:HB3	1:A:744:LYS:HB3	1.92	0.51
1:A:919:ILE:HG13	1:A:925:LEU:HD12	1.92	0.51
2:B:540:SER:HB2	2:B:543:SER:HB2	1.93	0.51
2:B:837:ASP:OD1	2:B:1016:ALA:HB2	2.10	0.51
2:B:852:ARG:HH22	12:L:70:ARG:C	2.18	0.51
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.51
5:E:93:MET:SD	5:E:123:LEU:HD11	2.50	0.51
1:A:337:ARG:HE	1:A:839:ARG:HH21	1.58	0.51
1:A:598:LEU:HD22	8:H:25:ARG:CZ	2.41	0.51
1:A:961:ARG:O	1:A:961:ARG:HD3	2.09	0.51
1:A:1420:ASP:OD2	1:A:1422:ARG:HG3	2.11	0.51
2:B:274:PRO:O	2:B:275:TYR:HB2	2.09	0.51
2:B:683:SER:O	2:B:687:GLU:HB2	2.11	0.51
2:B:842:ASN:HB2	2:B:999:MET:HE2	1.92	0.51
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.46	0.51
3:C:46:ILE:HG12	3:C:157:CYS:HB3	1.93	0.51
3:C:124:LEU:HG	3:C:129:ILE:HG22	1.92	0.51
9:I:73:ARG:NH2	9:I:112:SER:OG	2.43	0.51
1:A:673:GLY:O	1:A:674:PRO:C	2.53	0.51
1:A:1096:SER:O	1:A:1100:ARG:HB3	2.10	0.51
2:B:50:SER:O	2:B:410:GLY:HA3	2.10	0.51
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.45	0.51
2:B:1023:VAL:HA	2:B:1026:LEU:HD12	1.93	0.51
5:E:153:HIS:C	5:E:154:ILE:HD12	2.35	0.51
1:A:911:SER:O	1:A:978:PRO:HB3	2.10	0.51
2:B:408:LEU:CD2	2:B:409:ALA:H	2.24	0.51
2:B:1162:ILE:HG23	2:B:1194:ILE:HG12	1.93	0.51
7:G:3:PHE:HZ	7:G:82:PHE:HE2	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:81:PRO:CD	7:G:157:ILE:HD11	2.40	0.51
8:H:5:LEU:HD13	8:H:135:LEU:CD2	2.40	0.51
1:A:306:ASN:N	1:A:324:SER:HB3	2.25	0.51
1:A:477:PRO:CG	1:A:521:MET:HG3	2.40	0.51
1:A:1217:LYS:O	1:A:1221:LYS:N	2.41	0.51
1:A:1291:VAL:HG23	1:A:1292:PRO:HD2	1.93	0.51
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.44	0.51
4:D:160:VAL:O	4:D:164:ILE:HG12	2.11	0.51
8:H:44:VAL:CG2	8:H:48:PRO:HA	2.40	0.51
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.41	0.51
11:K:55:LYS:O	11:K:78:THR:HG23	2.09	0.51
13:R:1:A:H62	14:T:27:DA:H62	1.58	0.51
1:A:1135:ARG:HG2	1:A:1282:VAL:CG1	2.40	0.51
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	1.93	0.51
18:A:1806:ATP:O1G	2:B:766:ARG:NH2	2.44	0.51
2:B:123:THR:HG23	2:B:205:ILE:HA	1.92	0.51
2:B:288:ALA:HB1	2:B:331:LEU:CD2	2.41	0.51
2:B:481:GLN:HG3	2:B:494:HIS:HE2	1.75	0.51
2:B:901:PRO:HA	2:B:949:VAL:CG1	2.39	0.51
2:B:996:ARG:NH2	3:C:38:ILE:HG23	2.26	0.51
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.75	0.51
8:H:100:THR:HG22	8:H:138:GLU:O	2.11	0.51
9:I:34:TYR:OH	9:I:36:GLU:OE1	2.29	0.51
1:A:107:CYS:HB2	1:A:148:CYS:SG	2.51	0.51
1:A:337:ARG:HE	1:A:839:ARG:NH2	2.08	0.51
1:A:506:ALA:HB3	1:A:509:LEU:HG	1.92	0.51
1:A:552:TRP:O	1:A:554:PRO:HD3	2.10	0.51
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.11	0.51
2:B:418:LYS:O	2:B:422:LYS:HG3	2.11	0.51
3:C:21:ILE:CG2	3:C:227:THR:HG23	2.41	0.51
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.92	0.51
4:D:25:ALA:HB3	7:G:84:GLY:CA	2.41	0.51
8:H:104:PHE:CE1	8:H:136:LYS:HA	2.46	0.51
10:J:48:ARG:HD2	10:J:48:ARG:C	2.35	0.51
1:A:420:ARG:O	1:A:424:ILE:HB	2.10	0.51
1:A:851:HIS:CD2	6:F:139:PRO:HG3	2.45	0.51
1:A:968:GLN:HA	1:A:973:ILE:HG12	1.92	0.51
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.45	0.51
2:B:911:ILE:O	2:B:912:ILE:HG13	2.10	0.51
2:B:916:THR:HB	2:B:935:ARG:HD2	1.93	0.51
3:C:79:GLN:HG3	3:C:127:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:VAL:HG11	10:J:5:VAL:HG22	1.92	0.51
5:E:112:TYR:HD1	5:E:112:TYR:H	1.58	0.51
8:H:11:GLN:HG3	8:H:12:VAL:N	2.25	0.51
9:I:75:CYS:HB2	9:I:108:HIS:CE1	2.46	0.51
9:I:92:ARG:HB2	9:I:95:THR:HG23	1.92	0.51
10:J:6:ARG:HA	10:J:12:LYS:O	2.11	0.51
11:K:1:MET:C	11:K:3:ALA:H	2.19	0.51
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.92	0.50
1:A:837:ILE:HG22	1:A:840:ARG:NH2	2.26	0.50
1:A:900:ASP:HB3	1:A:906:HIS:HB2	1.93	0.50
1:A:1393:ASN:OD1	1:A:1393:ASN:N	2.25	0.50
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.11	0.50
2:B:483:LEU:HD12	2:B:484:ASN:N	2.26	0.50
2:B:867:GLY:C	2:B:869:SER:H	2.17	0.50
6:F:81:THR:HG22	6:F:82:THR:N	2.26	0.50
8:H:77:ARG:NH1	8:H:78:SER:H	2.09	0.50
1:A:106:VAL:HG23	1:A:112:LYS:O	2.11	0.50
1:A:313:GLN:O	1:A:315:LEU:HD12	2.11	0.50
2:B:433:GLN:N	2:B:433:GLN:OE1	2.45	0.50
3:C:61:GLU:N	3:C:61:GLU:OE1	2.44	0.50
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.11	0.50
1:A:716:ASP:O	1:A:720:ARG:HG2	2.11	0.50
1:A:1029:ARG:O	1:A:1033:GLN:HB2	2.12	0.50
1:A:1220:PHE:HE2	1:A:1267:MET:HG3	1.77	0.50
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.93	0.50
3:C:136:ASP:HB2	3:C:141:GLY:H	1.77	0.50
3:C:170:TRP:O	3:C:172:PRO:HD3	2.11	0.50
1:A:497:THR:HG21	2:B:1149:GLU:CD	2.37	0.50
1:A:1120:LEU:HB2	1:A:1304:TRP:O	2.12	0.50
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.50
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.93	0.50
8:H:134:ASN:OD1	8:H:135:LEU:N	2.44	0.50
1:A:494:SER:OG	1:A:497:THR:HG23	2.11	0.50
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.94	0.50
2:B:287:ARG:O	2:B:327:ARG:HG3	2.11	0.50
2:B:603:LEU:HD23	2:B:608:ASP:HB2	1.92	0.50
2:B:610:ASN:O	2:B:613:VAL:HG22	2.11	0.50
1:A:249:SER:HB3	1:A:259:GLU:OE1	2.12	0.50
1:A:436:ILE:HG13	1:A:436:ILE:O	2.11	0.50
1:A:715:GLU:O	1:A:719:VAL:HG12	2.12	0.50
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:PRO:HG2	8:H:18:GLY:H	1.76	0.50
8:H:40:LEU:CB	8:H:123:MET:HA	2.42	0.50
1:A:99:ILE:HG23	1:A:211:PHE:CE2	2.46	0.50
1:A:566:ILE:O	8:H:96:VAL:HB	2.11	0.50
1:A:1117:THR:N	1:A:1328:TYR:O	2.44	0.50
1:A:1353:TYR:HD1	1:A:1368:MET:HE1	1.77	0.50
2:B:867:GLY:O	2:B:869:SER:N	2.39	0.50
2:B:1112:GLN:HB2	2:B:1117:GLN:O	2.11	0.50
10:J:24:LEU:HD22	10:J:39:LEU:CD1	2.41	0.50
11:K:1:MET:O	11:K:3:ALA:N	2.45	0.50
1:A:442:VAL:CG1	1:A:491:VAL:HG22	2.36	0.50
1:A:535:THR:HG21	1:A:617:VAL:CG2	2.42	0.50
8:H:113:ALA:HA	8:H:125:LEU:O	2.12	0.50
1:A:135:PHE:CD1	1:A:222:LEU:HG	2.46	0.50
1:A:446:ARG:NE	1:A:478:TYR:O	2.45	0.50
3:C:41:ILE:CG2	3:C:172:PRO:HG3	2.42	0.50
4:D:190:GLU:HG3	7:G:167:TYR:CG	2.46	0.50
5:E:19:VAL:O	5:E:23:VAL:HG23	2.12	0.50
1:A:529:CYS:HB2	1:A:751:SER:OG	2.11	0.49
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.37	0.49
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.94	0.49
3:C:68:GLY:HA3	3:C:169:LYS:HD2	1.93	0.49
3:C:248:ILE:HD13	11:K:101:LEU:HD12	1.92	0.49
5:E:72:PHE:HZ	5:E:155:ARG:HB3	1.77	0.49
5:E:151:PRO:HD2	5:E:153:HIS:HE1	1.77	0.49
1:A:575:LYS:HG3	8:H:119:GLY:O	2.12	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49
1:A:886:ILE:HG23	1:A:887:GLY:N	2.24	0.49
1:A:1438:THR:O	6:F:92:ARG:HD2	2.12	0.49
1:A:1444:MET:O	6:F:132:LEU:HA	2.12	0.49
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.44	0.49
2:B:1162:ILE:HD12	2:B:1163:CYS:O	2.11	0.49
3:C:169:LYS:HZ1	12:L:69:ALA:HB3	1.77	0.49
1:A:81:PHE:HE1	2:B:1205:GLN:HE21	1.60	0.49
1:A:408:ASP:OD1	1:A:409:SER:N	2.45	0.49
2:B:52:ASN:O	2:B:55:VAL:N	2.44	0.49
2:B:211:VAL:CG2	2:B:483:LEU:HB2	2.42	0.49
2:B:225:VAL:HG11	2:B:384:ARG:O	2.12	0.49
2:B:934:LYS:CD	2:B:935:ARG:H	2.23	0.49
2:B:1065:GLN:OE1	2:B:1066:SER:N	2.45	0.49
1:A:1103:GLU:OE2	1:A:1112:LYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:LYS:HB3	1:A:1237:ILE:CD1	2.41	0.49
1:A:1313:LEU:HD23	1:A:1338:VAL:HB	1.95	0.49
2:B:124:TYR:HD2	2:B:172:ILE:O	1.95	0.49
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.93	0.49
6:F:147:SER:OG	6:F:150:GLU:HG2	2.12	0.49
10:J:54:VAL:CG2	10:J:56:LEU:HD11	2.39	0.49
1:A:239:LEU:HG	1:A:240:PRO:HD2	1.94	0.49
1:A:445:ASN:ND2	1:A:455:MET:HE3	2.28	0.49
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.94	0.49
1:A:763:ALA:C	1:A:803:SER:HB3	2.38	0.49
1:A:1142:THR:HA	1:A:1273:LEU:HD13	1.94	0.49
8:H:18:GLY:O	8:H:20:TYR:N	2.39	0.49
8:H:26:ILE:HG22	8:H:40:LEU:HD23	1.95	0.49
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.95	0.49
1:A:576:GLN:HB2	8:H:119:GLY:HA3	1.94	0.49
1:A:1378:GLN:NE2	5:E:177:ARG:HH12	2.10	0.49
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.13	0.49
2:B:563:MET:CG	2:B:588:GLY:HA3	2.43	0.49
2:B:792:MET:O	2:B:793:ALA:HB2	2.12	0.49
5:E:117:THR:C	5:E:119:SER:H	2.19	0.49
12:L:48:CYS:HB3	12:L:51:CYS:SG	2.52	0.49
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.27	0.49
1:A:899:VAL:HG22	1:A:929:LEU:HD13	1.92	0.49
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.13	0.49
2:B:203:PHE:HB2	2:B:205:ILE:HD11	1.94	0.49
2:B:361:LEU:N	2:B:362:PRO:HD3	2.27	0.49
2:B:363:HIS:CD2	2:B:585:VAL:HG12	2.39	0.49
2:B:956:THR:HG23	12:L:46:VAL:HG21	1.95	0.49
2:B:983:ARG:HH11	2:B:1091:TYR:CB	2.25	0.49
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.95	0.49
1:A:343:LYS:HZ2	2:B:1151:LEU:HB3	1.77	0.49
1:A:683:ILE:CG2	1:A:801:GLU:HG3	2.39	0.49
1:A:697:ALA:CB	1:A:702:LEU:HB2	2.43	0.49
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.94	0.49
1:A:879:GLU:OE1	1:A:959:ASN:HB2	2.12	0.49
1:A:1167:GLU:O	1:A:1170:ILE:HG12	2.13	0.49
3:C:19:ASP:OD1	3:C:231:ASN:HB2	2.13	0.49
3:C:44:LEU:HG	3:C:45:ALA:N	2.27	0.49
5:E:59:SER:CB	5:E:81:GLU:HA	2.40	0.49
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.28	0.49
6:F:72:LYS:O	6:F:73:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HG2	1:A:6:TYR:N	2.28	0.49
1:A:8:SER:HB3	2:B:1178:ASN:OD1	2.12	0.49
1:A:55:ASP:N	1:A:56:PRO:HD3	2.28	0.49
1:A:740:LEU:C	1:A:740:LEU:HD12	2.38	0.49
1:A:899:VAL:HG11	1:A:929:LEU:HD22	1.93	0.49
2:B:362:PRO:C	2:B:364:ILE:H	2.21	0.49
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.29	0.49
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.95	0.49
8:H:59:ILE:HG22	8:H:60:ALA:N	2.27	0.49
1:A:13:THR:OG1	1:A:15:LYS:NZ	2.46	0.49
1:A:527:THR:O	1:A:653:VAL:HG11	2.13	0.49
1:A:532:ARG:CD	1:A:749:ALA:HB2	2.43	0.49
1:A:804:TYR:HH	1:A:816:HIS:CE1	2.30	0.49
1:A:930:ASP:O	1:A:934:LYS:N	2.40	0.49
1:A:1230:GLU:O	1:A:1233:ASP:HB2	2.13	0.49
2:B:486:TYR:CD1	2:B:1096:ARG:HD2	2.47	0.49
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.12	0.49
4:D:119:ARG:CD	4:D:120:GLU:H	2.25	0.49
7:G:145:VAL:HG12	7:G:163:ILE:HG22	1.95	0.49
1:A:345:VAL:HA	2:B:1154:ALA:O	2.13	0.48
1:A:597:LEU:HD23	8:H:103:LYS:HG2	1.94	0.48
1:A:1345:ARG:HG3	1:A:1376:THR:OG1	2.13	0.48
2:B:112:LEU:HD11	2:B:117:ALA:HB2	1.93	0.48
2:B:205:ILE:HD12	2:B:205:ILE:N	2.28	0.48
2:B:216:GLU:OE1	2:B:537:LYS:HE3	2.13	0.48
2:B:261:ARG:O	2:B:263:GLY:N	2.46	0.48
2:B:370:PHE:CD1	2:B:373:ARG:HD2	2.47	0.48
2:B:685:LEU:HA	2:B:690:VAL:HG12	1.94	0.48
8:H:76:THR:O	8:H:77:ARG:HB2	2.13	0.48
8:H:118:PHE:CZ	8:H:142:LEU:HD22	2.48	0.48
1:A:446:ARG:HH12	1:A:448:PRO:HG2	1.77	0.48
1:A:575:LYS:HB2	1:A:612:ILE:HG21	1.95	0.48
1:A:824:LEU:HD21	2:B:769:TYR:CE1	2.48	0.48
1:A:1140:HIS:HA	1:A:1274:ARG:O	2.14	0.48
1:A:1434:ALA:CB	1:A:1436:ILE:HD13	2.43	0.48
2:B:248:SER:N	2:B:418:LYS:HZ2	2.11	0.48
2:B:302:CYS:HB2	2:B:310:MET:CE	2.43	0.48
2:B:1165:ILE:O	2:B:1217:TYR:OH	2.26	0.48
2:B:1222:ARG:HG2	2:B:1223:ASP:N	2.27	0.48
3:C:183:TRP:O	3:C:185:LYS:HG3	2.13	0.48
1:A:46:THR:HG22	1:A:47:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLU:OE1	1:A:644:LYS:HD2	2.13	0.48
1:A:824:LEU:CD1	2:B:768:THR:HG21	2.43	0.48
1:A:1083:THR:HG22	1:A:1093:LYS:HG2	1.95	0.48
1:A:1291:VAL:HG12	1:A:1301:GLU:HG2	1.95	0.48
2:B:199:MET:HE1	2:B:491:THR:HG21	1.96	0.48
2:B:227:LYS:N	2:B:395:GLN:OE1	2.34	0.48
2:B:770:GLN:HG2	2:B:983:ARG:O	2.13	0.48
5:E:124:VAL:HB	5:E:125:PRO:CD	2.41	0.48
12:L:38:LEU:HD21	12:L:49:LYS:N	2.28	0.48
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.46	0.48
1:A:777:PHE:HD2	1:A:782:ARG:CA	2.25	0.48
2:B:128:LEU:HB2	2:B:168:GLY:H	1.77	0.48
2:B:449:ASN:OD1	2:B:450:ALA:N	2.46	0.48
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.38	0.48
2:B:542:MET:HG2	2:B:747:MET:HB3	1.95	0.48
2:B:1194:ILE:HD12	2:B:1196:ILE:HG23	1.95	0.48
3:C:43:THR:HG23	3:C:237:SER:HB3	1.94	0.48
8:H:139:ASN:O	8:H:140:ALA:HB2	2.14	0.48
11:K:87:LEU:O	11:K:87:LEU:HD22	2.13	0.48
1:A:216:VAL:O	1:A:220:THR:HG23	2.12	0.48
1:A:367:PRO:HA	1:A:463:ILE:O	2.13	0.48
1:A:834:THR:HA	1:A:837:ILE:HG12	1.94	0.48
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.14	0.48
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.26	0.48
2:B:128:LEU:HD23	2:B:168:GLY:C	2.38	0.48
2:B:167:ILE:HD12	2:B:167:ILE:N	2.28	0.48
2:B:210:LYS:HG3	2:B:461:LEU:O	2.13	0.48
2:B:313:MET:O	2:B:316:PRO:HD2	2.13	0.48
2:B:579:ARG:NH2	2:B:621:GLU:O	2.46	0.48
1:A:337:ARG:CZ	1:A:839:ARG:NE	2.76	0.48
1:A:340:LEU:HD22	1:A:1429:ILE:HA	1.96	0.48
1:A:511:ILE:HA	1:A:521:MET:HE3	1.94	0.48
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.96	0.48
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	1.96	0.48
2:B:448:ILE:HD12	2:B:448:ILE:O	2.14	0.48
3:C:17:ASN:O	3:C:18:VAL:HG23	2.14	0.48
5:E:124:VAL:HG12	5:E:132:ILE:HB	1.96	0.48
7:G:59:GLY:HA3	7:G:70:PHE:CE2	2.47	0.48
8:H:6:PHE:HB3	8:H:59:ILE:HG13	1.96	0.48
1:A:247:ARG:HD2	1:A:263:THR:OG1	2.14	0.48
1:A:834:THR:O	1:A:837:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:ARG:HG2	1:A:1391:ARG:O	2.13	0.48
1:A:1450:LEU:HD23	6:F:108:PHE:HZ	1.79	0.48
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.48	0.48
6:F:96:THR:O	6:F:100:GLN:HG3	2.13	0.48
7:G:26:LEU:HD12	7:G:56:ILE:HD13	1.96	0.48
1:A:563:PRO:HB3	1:A:572:TRP:CZ2	2.49	0.48
1:A:852:TYR:CD1	1:A:1060:PRO:HB2	2.48	0.48
1:A:1144:LYS:HG3	1:A:1268:LEU:HB3	1.96	0.48
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.77	0.48
1:A:1398:MET:N	1:A:1426:GLU:OE2	2.46	0.48
1:A:1399:ARG:NH2	1:A:1417:GLU:OE2	2.46	0.48
2:B:102:VAL:HG12	2:B:110:HIS:HB3	1.94	0.48
2:B:409:ALA:O	2:B:413:LEU:HG	2.14	0.48
2:B:597:MET:HE3	2:B:601:ARG:NH1	2.29	0.48
2:B:624:LEU:HD12	2:B:626:ILE:HD11	1.95	0.48
2:B:999:MET:CG	2:B:1000:PRO:HD2	2.41	0.48
7:G:81:PRO:CG	7:G:157:ILE:HD11	2.43	0.48
1:A:216:VAL:HG23	1:A:217:LYS:HG3	1.95	0.48
1:A:984:LYS:O	1:A:988:LEU:HB2	2.14	0.48
2:B:640:VAL:HG13	2:B:651:LEU:N	2.28	0.48
2:B:1106:ARG:CZ	2:B:1109:GLY:HA3	2.43	0.48
2:B:1107:ALA:O	2:B:1109:GLY:N	2.47	0.48
4:D:5:THR:HG22	7:G:9:LEU:HD13	1.96	0.48
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.49	0.48
11:K:40:HIS:NE2	11:K:63:VAL:HG21	2.29	0.48
1:A:923:LEU:HD12	1:A:924:LYS:N	2.29	0.48
3:C:115:SER:CB	3:C:142:VAL:H	2.23	0.48
3:C:259:LEU:HA	3:C:262:LEU:HB2	1.96	0.48
7:G:3:PHE:CZ	7:G:82:PHE:HE2	2.31	0.48
10:J:2:ILE:HD12	10:J:57:ILE:CD1	2.43	0.48
12:L:40:LEU:HD12	12:L:44:ASP:HB3	1.95	0.48
1:A:697:ALA:HB2	1:A:702:LEU:HD22	1.95	0.47
1:A:720:ARG:O	1:A:724:GLU:HB3	2.14	0.47
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.96	0.47
2:B:199:MET:HE1	2:B:491:THR:CG2	2.44	0.47
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.40	0.47
2:B:1207:LEU:HB3	2:B:1212:ILE:CG2	2.43	0.47
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.44	0.47
8:H:4:THR:HA	8:H:60:ALA:HB2	1.96	0.47
8:H:9:ILE:HD12	8:H:9:ILE:N	2.29	0.47
1:A:121:LEU:HB3	1:A:141:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:H	2:B:1107:ALA:HA	1.80	0.47
1:A:1084:PHE:HE2	2:B:769:TYR:CE2	2.32	0.47
1:A:1169:ILE:HD13	1:A:1229:SER:OG	2.14	0.47
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.14	0.47
2:B:780:VAL:HG23	2:B:799:PRO:HG2	1.95	0.47
5:E:35:VAL:O	5:E:37:LEU:N	2.47	0.47
5:E:198:ILE:HD12	5:E:212:ARG:HG3	1.95	0.47
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.43	0.47
1:A:81:PHE:CD1	1:A:243:PRO:HD3	2.50	0.47
1:A:99:ILE:HG23	1:A:211:PHE:HE2	1.79	0.47
1:A:407:ARG:HG3	1:A:413:ILE:CD1	2.42	0.47
1:A:479:ASN:ND2	18:A:1806:ATP:O3'	2.45	0.47
1:A:590:ARG:HH12	1:A:592:ASP:CG	2.21	0.47
1:A:1001:ARG:CD	6:F:83:PRO:HD3	2.44	0.47
1:A:1425:SER:O	1:A:1429:ILE:HD12	2.14	0.47
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.95	0.47
3:C:22:LEU:HD13	3:C:230:MET:CE	2.44	0.47
6:F:144:GLU:O	6:F:144:GLU:HG3	2.13	0.47
8:H:93:TYR:CD2	8:H:145:ARG:HB2	2.49	0.47
1:A:730:GLY:CA	1:A:759:ALA:HB2	2.45	0.47
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.23	0.47
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.79	0.47
1:A:1287:TYR:OH	1:A:1307:GLU:OE2	2.30	0.47
1:A:1333:ILE:H	1:A:1333:ILE:HD12	1.79	0.47
7:G:143:ILE:CG2	7:G:145:VAL:HG13	2.43	0.47
10:J:12:LYS:HD3	10:J:12:LYS:C	2.36	0.47
12:L:48:CYS:CB	12:L:51:CYS:SG	3.00	0.47
1:A:41:MET:HE2	1:A:41:MET:HB2	1.76	0.47
1:A:267:ALA:O	1:A:271:LYS:HG3	2.14	0.47
1:A:456:MET:CE	1:A:510:GLN:HB2	2.44	0.47
1:A:661:GLY:HA3	2:B:1081:LEU:HD22	1.95	0.47
1:A:779:PHE:HB2	1:A:782:ARG:HG3	1.97	0.47
1:A:871:ASP:O	1:A:873:MET:HE2	2.14	0.47
1:A:1015:VAL:O	1:A:1016:THR:C	2.57	0.47
1:A:1445:ILE:HG22	6:F:131:PRO:O	2.15	0.47
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.47	0.47
2:B:597:MET:HE3	2:B:601:ARG:HH11	1.78	0.47
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.49	0.47
2:B:843:GLN:N	2:B:994:TYR:O	2.45	0.47
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.30	0.47
4:D:47:LEU:HD23	4:D:48:ILE:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:CYS:SG	4:D:194:LEU:HD12	2.54	0.47
6:F:86:THR:HG22	6:F:88:TYR:H	1.78	0.47
1:A:351:THR:HG22	1:A:468:PHE:CE2	2.49	0.47
1:A:578:LEU:HD23	1:A:578:LEU:O	2.14	0.47
1:A:587:HIS:HB2	1:A:969:GLN:OE1	2.14	0.47
1:A:592:ASP:OD2	1:A:604:GLY:HA2	2.15	0.47
1:A:646:PHE:O	1:A:650:GLN:HG3	2.15	0.47
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.96	0.47
2:B:349:ILE:C	2:B:351:TYR:N	2.73	0.47
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.30	0.47
2:B:1029:CYS:HB3	2:B:1086:PHE:CZ	2.50	0.47
2:B:1161:HIS:O	2:B:1171:VAL:HB	2.15	0.47
2:B:1190:ASP:C	2:B:1191:ILE:HD12	2.40	0.47
3:C:84:ARG:HD3	11:K:11:LEU:HD11	1.95	0.47
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.50	0.47
9:I:49:ILE:HG22	9:I:49:ILE:O	2.15	0.47
11:K:114:LEU:HD23	11:K:114:LEU:C	2.39	0.47
1:A:44:THR:HG1	1:A:46:THR:HG1	1.61	0.47
1:A:107:CYS:HB3	1:A:110:CYS:HB2	1.95	0.47
1:A:524:VAL:HG22	1:A:525:GLN:N	2.30	0.47
1:A:532:ARG:HG3	1:A:533:LYS:N	2.28	0.47
1:A:635:ARG:HD2	1:A:879:GLU:OE2	2.14	0.47
1:A:722:LEU:HB3	1:A:799:PHE:CE1	2.49	0.47
1:A:902:LEU:HG	1:A:926:GLN:HG2	1.96	0.47
1:A:1084:PHE:HD1	1:A:1084:PHE:H	1.61	0.47
1:A:1153:TYR:HB2	1:A:1192:LEU:HB3	1.97	0.47
1:A:1342:GLU:OE1	5:E:212:ARG:HD2	2.15	0.47
2:B:132:VAL:HG23	2:B:165:VAL:HG21	1.96	0.47
2:B:269:ILE:CG2	2:B:282:ILE:HG12	2.45	0.47
2:B:288:ALA:O	2:B:331:LEU:HD21	2.15	0.47
2:B:323:VAL:O	2:B:324:ILE:HD12	2.14	0.47
2:B:449:ASN:ND2	2:B:452:THR:HG23	2.30	0.47
2:B:485:ARG:NH1	2:B:788:ARG:HH12	2.13	0.47
2:B:492:LEU:O	2:B:496:ARG:HG3	2.14	0.47
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.49	0.47
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.97	0.47
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	1.96	0.47
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.15	0.47
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.50	0.47
3:C:37:MET:HE3	3:C:244:VAL:HG13	1.96	0.47
4:D:59:ILE:HG21	4:D:145:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:ARG:HG3	5:E:35:VAL:HG12	1.95	0.47
5:E:109:ILE:HD12	5:E:109:ILE:N	2.29	0.47
1:A:295:LEU:O	1:A:298:PHE:HB3	2.15	0.47
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.97	0.47
1:A:775:ILE:HG23	1:A:818:MET:CE	2.43	0.47
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.15	0.47
3:C:22:LEU:O	3:C:227:THR:HA	2.15	0.47
3:C:31:ASN:O	3:C:35:ARG:HG3	2.14	0.47
1:A:335:ARG:HG2	1:A:340:LEU:HD12	1.95	0.47
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.97	0.47
1:A:481:ASP:O	1:A:485:ASP:HB2	2.14	0.47
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.15	0.47
1:A:971:PHE:CD2	1:A:1040:GLN:HG3	2.50	0.47
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.97	0.47
2:B:768:THR:HG22	2:B:768:THR:O	2.14	0.47
3:C:66:ARG:H	3:C:66:ARG:HG2	1.54	0.47
9:I:101:PHE:HE1	9:I:112:SER:HB2	1.80	0.47
1:A:83:HIS:HA	1:A:239:LEU:O	2.14	0.47
1:A:107:CYS:SG	1:A:110:CYS:N	2.76	0.47
1:A:897:TYR:HB3	1:A:936:LEU:HD13	1.97	0.47
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.97	0.47
3:C:182:PRO:HD2	3:C:210:GLU:CD	2.40	0.47
5:E:71:LYS:O	5:E:73:PRO:HD3	2.15	0.47
8:H:6:PHE:HD2	8:H:130:ARG:HD3	1.79	0.47
10:J:3:VAL:CG2	10:J:18:TRP:HB2	2.44	0.47
1:A:731:ARG:CB	1:A:755:PHE:HZ	2.27	0.46
1:A:1134:ILE:HG22	1:A:1306:LEU:HD22	1.96	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:CD1	2.42	0.46
2:B:35:SER:OG	2:B:811:TYR:OH	2.20	0.46
2:B:378:LEU:O	2:B:382:ILE:HG13	2.15	0.46
3:C:52:GLU:OE1	3:C:154:LYS:HD2	2.15	0.46
3:C:133:ILE:CD1	3:C:237:SER:HA	2.45	0.46
4:D:63:LEU:HB3	4:D:129:LEU:HD21	1.96	0.46
5:E:4:GLU:HB3	5:E:7:ARG:NH1	2.29	0.46
5:E:32:GLN:OE1	5:E:32:GLN:CA	2.62	0.46
7:G:15:PRO:HA	7:G:18:PHE:CD2	2.50	0.46
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.16	0.46
18:A:1806:ATP:H8	18:A:1806:ATP:C5'	2.28	0.46
5:E:12:LEU:HG	5:E:55:ARG:NH2	2.30	0.46
5:E:12:LEU:CD1	5:E:55:ARG:HE	2.24	0.46
5:E:91:LYS:HA	5:E:94:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:13:LEU:O	7:G:67:SER:HB2	2.15	0.46
8:H:132:LEU:HG	8:H:133:ASN:N	2.30	0.46
9:I:64:SER:O	9:I:66:PRO:HD3	2.15	0.46
1:A:205:GLU:O	1:A:209:ASN:N	2.42	0.46
1:A:818:MET:HG2	2:B:514:LEU:O	2.15	0.46
1:A:902:LEU:HD21	1:A:923:LEU:HA	1.98	0.46
1:A:981:LEU:CD2	1:A:1039:LYS:HD2	2.45	0.46
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.97	0.46
2:B:1082:MET:HE3	3:C:190:ASP:HB2	1.97	0.46
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.51	0.46
4:D:60:LYS:O	4:D:64:VAL:HG12	2.15	0.46
4:D:220:LEU:H	4:D:220:LEU:CD1	2.22	0.46
7:G:126:ASN:O	7:G:128:PRO:HD3	2.15	0.46
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.30	0.46
1:A:1224:LEU:HG	1:A:1225:PHE:N	2.31	0.46
1:A:1277:GLU:HG2	1:A:1278:ASN:N	2.30	0.46
1:A:1436:ILE:O	2:B:1144:ALA:HB2	2.15	0.46
2:B:1060:ARG:HE	3:C:202:PRO:HG3	1.80	0.46
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.46	0.46
7:G:122:ASN:HB3	7:G:129:SER:O	2.16	0.46
9:I:34:TYR:OH	9:I:36:GLU:HB3	2.14	0.46
1:A:176:LYS:HB3	1:A:176:LYS:HE2	1.58	0.46
1:A:265:LYS:O	1:A:269:ILE:HG13	2.16	0.46
1:A:448:PRO:O	1:A:450:LEU:HG	2.16	0.46
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.15	0.46
1:A:1128:GLN:O	1:A:1131:ALA:N	2.48	0.46
2:B:515:HIS:O	2:B:518:HIS:HB2	2.16	0.46
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.96	0.46
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.51	0.46
1:A:75:ASN:O	1:A:76:GLU:CB	2.62	0.46
1:A:350:ARG:HH11	1:A:447:GLN:HG2	1.81	0.46
1:A:824:LEU:HD21	2:B:769:TYR:OH	2.15	0.46
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.49	0.46
1:A:1281:ARG:O	1:A:1282:VAL:HG23	2.16	0.46
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.51	0.46
14:T:21:DC:H2''	14:T:22:DT:H5'	1.98	0.46
1:A:41:MET:HA	1:A:50:ILE:HG22	1.97	0.46
1:A:47:ARG:HD3	1:A:62:ASP:OD1	2.16	0.46
1:A:341:MET:HE1	1:A:1428:VAL:HB	1.97	0.46
1:A:551:TYR:CE1	11:K:74:ARG:HD3	2.51	0.46
1:A:605:MET:HE2	1:A:607:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:PHE:HA	2:B:58:THR:HB	1.98	0.46
3:C:29:MET:HE2	11:K:94:ILE:HG23	1.97	0.46
6:F:130:ILE:HB	6:F:148:VAL:HG11	1.98	0.46
9:I:25:LEU:CB	9:I:38:ALA:HB2	2.46	0.46
1:A:456:MET:HB3	1:A:507:VAL:CG2	2.46	0.46
1:A:672:ASP:CA	1:A:676:MET:HG3	2.46	0.46
1:A:1305:VAL:C	1:A:1306:LEU:HD12	2.40	0.46
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.14	0.46
2:B:243:ALA:HB2	2:B:250:PHE:O	2.15	0.46
2:B:301:ILE:HD12	2:B:301:ILE:N	2.31	0.46
2:B:642:ASP:OD1	2:B:642:ASP:N	2.49	0.46
3:C:241:ASP:OD1	3:C:241:ASP:N	2.37	0.46
5:E:13:TRP:CE3	5:E:39:LEU:HB2	2.51	0.46
5:E:39:LEU:O	5:E:43:LYS:HG3	2.16	0.46
1:A:337:ARG:CZ	1:A:839:ARG:HE	2.29	0.46
1:A:349:ALA:O	2:B:1128:LEU:HD22	2.15	0.46
1:A:353:ILE:HG21	1:A:487:MET:CG	2.44	0.46
1:A:446:ARG:NH1	18:A:1806:ATP:O2'	2.48	0.46
1:A:566:ILE:O	1:A:567:LYS:HB2	2.15	0.46
1:A:941:LYS:O	1:A:945:GLU:HG3	2.15	0.46
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.97	0.46
2:B:601:ARG:HG2	2:B:605:ARG:NH1	2.31	0.46
2:B:655:LYS:HA	2:B:658:ILE:HB	1.98	0.46
2:B:797:TYR:HB2	2:B:852:ARG:O	2.15	0.46
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.96	0.46
7:G:61:ILE:HD12	7:G:68:ALA:HB2	1.97	0.46
7:G:153:GLN:HG3	7:G:153:GLN:O	2.15	0.46
8:H:26:ILE:O	8:H:39:THR:HA	2.16	0.46
9:I:103:CYS:SG	9:I:107:SER:N	2.88	0.46
12:L:38:LEU:HG	12:L:49:LYS:HB2	1.98	0.46
1:A:105:CYS:SG	1:A:139:TRP:HA	2.55	0.46
1:A:888:GLY:O	1:A:1297:GLU:HA	2.16	0.46
1:A:899:VAL:CG2	1:A:929:LEU:HD13	2.46	0.46
1:A:1039:LYS:HE2	1:A:1043:ASP:CG	2.40	0.46
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.98	0.46
1:A:1151:GLU:HA	9:I:44:TYR:O	2.14	0.46
1:A:1167:GLU:HA	1:A:1170:ILE:HD13	1.97	0.46
2:B:258:LEU:HD23	2:B:258:LEU:C	2.40	0.46
11:K:45:LEU:HD21	11:K:94:ILE:HG21	1.98	0.46
1:A:308:ILE:HG22	1:A:309:ALA:H	1.81	0.45
1:A:634:THR:HG23	1:A:639:PRO:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ALA:O	1:A:737:LEU:HG	2.16	0.45
1:A:901:LEU:HB2	1:A:926:GLN:HB2	1.96	0.45
1:A:1089:VAL:O	1:A:1091:SER:N	2.49	0.45
2:B:124:TYR:HB2	2:B:204:ILE:HB	1.98	0.45
2:B:778:MET:HE2	2:B:794:ASN:CG	2.42	0.45
2:B:861:ASP:CG	2:B:914:LYS:HE2	2.41	0.45
5:E:93:MET:CE	5:E:116:ILE:HG12	2.46	0.45
5:E:168:TYR:C	5:E:169:ARG:HG3	2.41	0.45
7:G:157:ILE:O	7:G:157:ILE:CG1	2.64	0.45
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.16	0.45
1:A:533:LYS:HE2	1:A:745:GLN:OE1	2.16	0.45
1:A:1037:LEU:HD22	1:A:1042:PHE:HA	1.98	0.45
2:B:498:THR:O	2:B:536:VAL:HG13	2.15	0.45
2:B:790:ASP:OD1	2:B:790:ASP:N	2.42	0.45
2:B:839:MET:HE2	2:B:839:MET:HB3	1.85	0.45
2:B:1224:PHE:HD2	5:E:174:GLN:HE22	1.64	0.45
5:E:112:TYR:HB3	5:E:116:ILE:HD12	1.98	0.45
6:F:147:SER:O	6:F:150:GLU:HG2	2.17	0.45
11:K:51:LEU:HD23	11:K:59:ALA:HB3	1.97	0.45
1:A:306:ASN:ND2	1:A:313:GLN:HG3	2.32	0.45
1:A:350:ARG:HG2	1:A:486:GLU:HG2	1.99	0.45
1:A:645:LEU:CD1	1:A:649:ILE:HD11	2.46	0.45
1:A:697:ALA:CA	1:A:702:LEU:HB2	2.47	0.45
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.16	0.45
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.31	0.45
2:B:114:PRO:HG2	2:B:115:GLN:H	1.80	0.45
2:B:632:ARG:CZ	2:B:632:ARG:HB2	2.46	0.45
2:B:975:GLN:OE1	2:B:1100:ASP:CG	2.59	0.45
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.52	0.45
2:B:1172:ILE:O	2:B:1172:ILE:HG13	2.14	0.45
3:C:50:GLU:CB	12:L:64:LEU:HD23	2.42	0.45
4:D:118:THR:C	4:D:119:ARG:HG3	2.41	0.45
7:G:60:ARG:NH2	7:G:63:PRO:HD3	2.32	0.45
8:H:18:GLY:C	8:H:20:TYR:H	2.22	0.45
8:H:33:GLN:HB2	8:H:35:GLN:NE2	2.31	0.45
1:A:108:MET:HG2	1:A:171:GLN:OE1	2.16	0.45
1:A:239:LEU:HG	1:A:240:PRO:CD	2.47	0.45
1:A:560:ILE:N	1:A:560:ILE:HD12	2.31	0.45
1:A:690:VAL:CG2	1:A:721:PHE:HB2	2.47	0.45
6:F:83:PRO:HA	6:F:146:TRP:CZ3	2.52	0.45
11:K:107:THR:O	11:K:111:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH1	2:B:1127:GLY:O	2.50	0.45
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.97	0.45
1:A:852:TYR:CE2	6:F:136:ARG:HB3	2.51	0.45
1:A:1130:GLN:O	1:A:1134:ILE:HD13	2.16	0.45
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.17	0.45
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.32	0.45
2:B:274:PRO:HB2	2:B:359:GLU:CB	2.47	0.45
2:B:322:PHE:CZ	9:I:30:ARG:HB3	2.51	0.45
2:B:843:GLN:HB2	2:B:993:THR:HB	1.98	0.45
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.98	0.45
4:D:154:PHE:CE2	4:D:163:VAL:HG11	2.52	0.45
5:E:101:GLN:HG3	5:E:127:ILE:HD12	1.99	0.45
8:H:10:PHE:CB	8:H:28:ALA:HB1	2.42	0.45
8:H:18:GLY:C	8:H:20:TYR:N	2.75	0.45
1:A:7:SER:OG	2:B:1193:GLN:OE1	2.27	0.45
1:A:716:ASP:O	1:A:719:VAL:HG12	2.16	0.45
1:A:1031:VAL:HG13	1:A:1037:LEU:CD1	2.47	0.45
2:B:431:TYR:CE1	2:B:447:ALA:HB3	2.52	0.45
2:B:784:ASN:O	2:B:788:ARG:HG2	2.16	0.45
2:B:1162:ILE:HA	2:B:1168:LEU:O	2.16	0.45
2:B:1207:LEU:HB3	2:B:1212:ILE:HG22	1.98	0.45
3:C:60:ASP:CG	12:L:60:ARG:HH22	2.25	0.45
3:C:124:LEU:O	3:C:127:ARG:NE	2.50	0.45
7:G:81:PRO:HG2	7:G:157:ILE:HD11	1.98	0.45
9:I:54:GLU:HA	9:I:90:GLN:HG3	1.99	0.45
10:J:6:ARG:HG2	10:J:13:VAL:HG13	1.99	0.45
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.98	0.45
1:A:1053:PHE:O	1:A:1056:SER:N	2.49	0.45
2:B:237:VAL:CG2	2:B:257:LYS:HG2	2.42	0.45
2:B:349:ILE:O	2:B:351:TYR:N	2.49	0.45
2:B:737:THR:O	2:B:737:THR:HG22	2.17	0.45
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.81	0.45
10:J:64:ASN:CB	10:J:65:PRO:CD	2.94	0.45
11:K:1:MET:HG2	11:K:2:ASN:HD22	1.81	0.45
11:K:73:LEU:HD21	11:K:75:ILE:HD11	1.98	0.45
1:A:910:PRO:HG3	1:A:917:SER:N	2.32	0.45
1:A:1435:PRO:O	1:A:1436:ILE:HD12	2.16	0.45
2:B:58:THR:HG22	2:B:58:THR:O	2.16	0.45
2:B:100:PRO:O	2:B:180:TYR:OH	2.33	0.45
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.98	0.45
2:B:1158:PHE:CD1	2:B:1160:VAL:HG22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:ILE:HD12	3:C:21:ILE:N	2.32	0.45
3:C:166:GLU:O	3:C:167:HIS:HB2	2.16	0.45
8:H:103:LYS:HD2	8:H:104:PHE:H	1.81	0.45
10:J:7:CYS:N	10:J:12:LYS:O	2.34	0.45
11:K:47:ARG:NH1	11:K:51:LEU:HD11	2.32	0.45
1:A:101:LYS:HD3	1:A:139:TRP:CE2	2.51	0.45
1:A:511:ILE:HA	1:A:521:MET:CE	2.47	0.45
1:A:535:THR:O	1:A:616:VAL:HG22	2.17	0.45
1:A:1325:THR:HA	5:E:147:HIS:HA	1.98	0.45
2:B:100:PRO:HA	2:B:126:SER:HA	1.98	0.45
2:B:189:LEU:O	2:B:192:LEU:N	2.50	0.45
2:B:269:ILE:HG22	2:B:282:ILE:HG12	1.98	0.45
2:B:997:GLU:OE1	3:C:39:ALA:HB2	2.17	0.45
3:C:66:ARG:O	3:C:69:LEU:N	2.50	0.45
1:A:550:LEU:HB3	1:A:556:TRP:CZ2	2.52	0.45
1:A:883:LEU:HD12	1:A:952:ALA:O	2.17	0.45
1:A:994:GLN:HG2	1:A:1022:LEU:HD23	1.98	0.45
2:B:218:SER:HA	2:B:404:LYS:HA	1.98	0.45
2:B:287:ARG:CG	2:B:292:ILE:HG13	2.46	0.45
2:B:394:ASP:CG	9:I:91:ARG:HD2	2.42	0.45
5:E:3:GLN:NE2	5:E:5:ASN:HB2	2.32	0.45
7:G:81:PRO:HG3	7:G:106:MET:SD	2.57	0.45
8:H:30:SER:CB	8:H:36:CYS:HB3	2.47	0.45
9:I:106:CYS:HB2	9:I:108:HIS:HD2	1.81	0.45
1:A:622:VAL:O	1:A:622:VAL:HG22	2.16	0.44
1:A:821:ARG:HE	1:A:821:ARG:HB2	1.55	0.44
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.17	0.44
2:B:174:LEU:HD12	2:B:174:LEU:N	2.31	0.44
2:B:734:HIS:O	2:B:736:THR:HG23	2.18	0.44
3:C:155:LEU:C	3:C:155:LEU:HD12	2.43	0.44
5:E:198:ILE:C	5:E:199:ILE:HD12	2.42	0.44
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.17	0.44
1:A:1113:THR:O	1:A:1113:THR:CG2	2.58	0.44
2:B:62:ILE:HD12	2:B:417:PHE:HD2	1.82	0.44
2:B:266:ALA:O	2:B:268:THR:HG22	2.17	0.44
2:B:1095:LEU:O	2:B:1097:HIS:N	2.42	0.44
3:C:65:HIS:NE2	3:C:69:LEU:HD11	2.32	0.44
3:C:259:LEU:HD13	3:C:262:LEU:CD1	2.47	0.44
8:H:124:ARG:HH21	8:H:126:GLU:HG3	1.82	0.44
10:J:45:CYS:O	10:J:48:ARG:HG3	2.17	0.44
1:A:107:CYS:SG	1:A:110:CYS:HB2	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:LEU:HD13	1:A:659:HIS:CE1	2.53	0.44
1:A:701:LEU:HD21	9:I:114:GLN:CB	2.39	0.44
3:C:19:ASP:OD1	3:C:231:ASN:ND2	2.51	0.44
4:D:25:ALA:HB3	7:G:84:GLY:HA3	2.00	0.44
5:E:14:ARG:HH12	5:E:142:VAL:HG22	1.83	0.44
8:H:56:THR:HG22	8:H:57:VAL:N	2.31	0.44
9:I:19:ASP:C	9:I:21:GLU:H	2.25	0.44
9:I:40:SER:OG	9:I:41:PRO:HD2	2.18	0.44
10:J:60:PHE:C	10:J:62:ARG:H	2.26	0.44
1:A:884:ASP:HB2	1:A:897:TYR:OH	2.18	0.44
2:B:510:LYS:HB2	2:B:513:GLN:CG	2.28	0.44
2:B:545:ILE:HD11	2:B:633:VAL:HG22	1.98	0.44
2:B:1190:ASP:O	2:B:1191:ILE:HD12	2.17	0.44
1:A:636:GLU:HG3	1:A:636:GLU:O	2.17	0.44
1:A:867:ILE:HG13	1:A:870:GLU:C	2.43	0.44
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.58	0.44
1:A:1291:VAL:CG1	1:A:1301:GLU:HG2	2.47	0.44
2:B:21:GLU:HA	2:B:656:GLY:HA3	1.99	0.44
2:B:240:ILE:CG2	2:B:381:MET:HE1	2.47	0.44
2:B:408:LEU:HD22	2:B:409:ALA:H	1.83	0.44
2:B:582:VAL:HB	2:B:587:HIS:NE2	2.32	0.44
2:B:655:LYS:O	2:B:658:ILE:HG22	2.17	0.44
8:H:43:ASN:OD1	8:H:46:LEU:HG	2.18	0.44
1:A:5:GLN:HG2	1:A:6:TYR:H	1.82	0.44
1:A:172:PRO:HB2	1:A:183:GLY:CA	2.44	0.44
1:A:215:SER:HB3	1:A:218:ASP:CG	2.42	0.44
1:A:407:ARG:HD2	1:A:430:TRP:CH2	2.52	0.44
1:A:810:PRO:HB3	2:B:745:PRO:HB3	2.00	0.44
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.46	0.44
2:B:31:TRP:NE1	2:B:807:ARG:HD3	2.31	0.44
2:B:755:ILE:H	2:B:755:ILE:HG13	1.50	0.44
2:B:841:MET:HG3	2:B:990:ILE:CD1	2.48	0.44
5:E:26:ARG:HH12	5:E:133:GLU:CD	2.25	0.44
7:G:98:GLY:HA3	7:G:110:VAL:O	2.17	0.44
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.82	0.44
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.53	0.44
1:A:185:TRP:HB2	1:A:198:GLU:HB3	1.99	0.44
1:A:338:GLY:CA	2:B:1129:ARG:HH12	2.30	0.44
1:A:902:LEU:O	1:A:903:ASN:HB2	2.18	0.44
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.48	0.44
2:B:307:ASP:OD2	2:B:310:MET:HB2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:GLY:C	2:B:532:ALA:H	2.24	0.44
2:B:857:ARG:NH2	2:B:942:ARG:HD3	2.33	0.44
11:K:44:ASN:HA	11:K:61:TYR:CE1	2.53	0.44
1:A:382:PRO:HG3	1:A:428:TYR:CE1	2.53	0.44
1:A:1370:LEU:O	1:A:1374:VAL:N	2.49	0.44
2:B:407:ASP:HB3	2:B:412:LEU:CD1	2.48	0.44
2:B:820:GLY:N	2:B:1091:TYR:OH	2.44	0.44
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.85	0.44
4:D:186:ASP:O	4:D:211:LEU:HD13	2.18	0.44
4:D:220:LEU:HD12	4:D:220:LEU:N	2.24	0.44
5:E:93:MET:O	5:E:97:VAL:HG23	2.17	0.44
8:H:42:ILE:HG23	8:H:95:TYR:CE2	2.53	0.44
11:K:11:LEU:HD23	11:K:11:LEU:HA	1.83	0.44
1:A:329:LEU:HB2	1:A:1406:VAL:HG22	2.00	0.44
1:A:566:ILE:C	1:A:567:LYS:HG2	2.43	0.44
2:B:217:ARG:O	2:B:405:ARG:N	2.30	0.44
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.72	0.44
3:C:8:VAL:HG12	3:C:9:LYS:H	1.82	0.44
4:D:192:LYS:NZ	4:D:204:ASP:OD1	2.49	0.44
1:A:119:ASN:HB3	1:A:122:MET:HB2	2.00	0.43
1:A:338:GLY:C	2:B:1129:ARG:HH12	2.26	0.43
1:A:378:GLU:O	1:A:431:LYS:HA	2.18	0.43
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.99	0.43
1:A:714:PHE:O	1:A:718:VAL:HG23	2.17	0.43
1:A:1146:VAL:HG21	1:A:1197:LEU:HD22	1.99	0.43
2:B:219:ALA:HB2	2:B:405:ARG:CG	2.45	0.43
2:B:293:PRO:HG2	2:B:296:GLU:OE1	2.18	0.43
2:B:758:PHE:HE2	2:B:1027:ILE:HG22	1.82	0.43
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.17	0.43
2:B:826:ALA:O	2:B:1011:ILE:HA	2.17	0.43
2:B:959:ASP:HB2	2:B:961:LEU:HG	2.00	0.43
4:D:138:ASN:ND2	7:G:35:GLU:HG3	2.33	0.43
7:G:57:GLN:NE2	7:G:71:ASN:O	2.51	0.43
9:I:59:VAL:HG23	9:I:61:ASP:H	1.83	0.43
11:K:29:ASN:O	11:K:76:GLN:HG3	2.18	0.43
1:A:446:ARG:CG	1:A:447:GLN:N	2.81	0.43
1:A:946:VAL:HG22	5:E:201:LYS:HB3	2.00	0.43
1:A:1005:GLU:OE2	1:A:1009:ASN:ND2	2.51	0.43
1:A:1377:THR:HA	5:E:212:ARG:HH22	1.81	0.43
2:B:555:ILE:HA	2:B:558:LEU:HD12	1.99	0.43
2:B:770:GLN:HG2	2:B:983:ARG:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:MET:HE1	7:G:79:PHE:HA	2.00	0.43
8:H:10:PHE:O	8:H:55:LEU:HB2	2.18	0.43
1:A:1139:GLU:OE1	1:A:1282:VAL:HB	2.17	0.43
1:A:1422:ARG:NH2	2:B:1223:ASP:O	2.40	0.43
1:A:1438:THR:O	1:A:1438:THR:CG2	2.65	0.43
2:B:173:MET:O	2:B:176:SER:OG	2.26	0.43
2:B:865:LYS:HA	2:B:871:THR:HG22	2.00	0.43
2:B:886:LYS:HE3	2:B:936:ASP:OD2	2.18	0.43
2:B:912:ILE:HD11	2:B:964:VAL:CG1	2.48	0.43
5:E:93:MET:CE	5:E:123:LEU:HD11	2.49	0.43
7:G:27:LYS:HE2	7:G:51:TYR:CE1	2.53	0.43
7:G:106:MET:HE3	7:G:108:VAL:HG23	1.97	0.43
7:G:111:THR:C	7:G:115:MET:HE3	2.43	0.43
12:L:61:THR:C	12:L:63:ARG:H	2.26	0.43
1:A:3:GLY:O	1:A:4:GLN:HB2	2.18	0.43
1:A:343:LYS:O	2:B:1130:PHE:N	2.47	0.43
1:A:360:GLU:HA	1:A:360:GLU:OE2	2.18	0.43
1:A:391:LEU:HD23	1:A:400:PRO:C	2.42	0.43
1:A:419:LYS:HG3	1:A:420:ARG:H	1.83	0.43
1:A:472:LEU:HD22	2:B:835:GLN:CD	2.44	0.43
1:A:810:PRO:HB2	2:B:705:MET:SD	2.59	0.43
1:A:840:ARG:HG2	1:A:1402:PHE:CE2	2.53	0.43
1:A:1146:VAL:CG2	1:A:1202:MET:HE1	2.47	0.43
2:B:282:ILE:HD12	2:B:283:VAL:N	2.34	0.43
2:B:604:ARG:C	2:B:606:LYS:N	2.76	0.43
2:B:640:VAL:HG13	2:B:651:LEU:CA	2.48	0.43
2:B:898:LEU:HD23	2:B:898:LEU:HA	1.86	0.43
3:C:21:ILE:HG23	3:C:227:THR:HG23	2.00	0.43
3:C:115:SER:HB3	3:C:141:GLY:HA3	2.01	0.43
3:C:241:ASP:HB3	11:K:109:TRP:CZ2	2.52	0.43
4:D:118:THR:O	4:D:121:LYS:N	2.42	0.43
5:E:72:PHE:CZ	5:E:155:ARG:HB3	2.52	0.43
5:E:128:PRO:HB2	5:E:129:PRO:HD3	2.01	0.43
8:H:12:VAL:HG22	8:H:50:ALA:O	2.19	0.43
10:J:24:LEU:HD22	10:J:39:LEU:HD12	2.01	0.43
1:A:53:LEU:O	1:A:54:ASN:HB2	2.18	0.43
1:A:76:GLU:HG3	2:B:1159:ARG:NH2	2.31	0.43
1:A:126:LEU:HD21	1:A:221:SER:HB2	2.01	0.43
1:A:224:PHE:HB3	1:A:225:ASN:H	1.72	0.43
1:A:343:LYS:CE	2:B:1151:LEU:HB3	2.47	0.43
1:A:351:THR:HB	2:B:1103:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:GLU:O	2:B:262:GLU:HG2	2.18	0.43
2:B:809:MET:HE2	2:B:814:PHE:CD2	2.54	0.43
2:B:941:LEU:HG	2:B:942:ARG:N	2.32	0.43
2:B:1172:ILE:HD12	2:B:1174:LYS:HG3	2.01	0.43
3:C:71:PRO:C	3:C:72:LEU:HD12	2.43	0.43
12:L:43:THR:HG22	12:L:43:THR:O	2.18	0.43
1:A:344:ARG:NH1	2:B:1120:GLU:HA	2.32	0.43
1:A:658:LEU:HD22	2:B:1074:ASN:ND2	2.32	0.43
1:A:787:PHE:CD1	1:A:796:SER:HB2	2.53	0.43
1:A:922:ASP:OD1	1:A:924:LYS:HG3	2.18	0.43
2:B:902:GLY:O	12:L:65:VAL:HG11	2.19	0.43
2:B:992:ILE:CD1	11:K:66:PRO:HB2	2.48	0.43
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.00	0.43
5:E:164:LEU:O	5:E:164:LEU:HG	2.17	0.43
11:K:38:GLU:CD	11:K:42:LEU:HD12	2.44	0.43
13:R:4:G:H2'	13:R:5:A:C8	2.52	0.43
14:T:25:DC:H2''	14:T:26:DG:H8	1.82	0.43
1:A:474:VAL:C	1:A:477:PRO:HD2	2.43	0.43
1:A:597:LEU:HD12	1:A:597:LEU:HA	1.80	0.43
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.54	0.43
1:A:709:THR:CG2	1:A:712:GLU:H	2.31	0.43
1:A:830:LYS:HD3	1:A:1094:VAL:HG11	2.01	0.43
1:A:1313:LEU:HD23	1:A:1338:VAL:CB	2.49	0.43
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.52	0.43
5:E:132:ILE:HD12	5:E:132:ILE:N	2.30	0.43
6:F:81:THR:HG22	6:F:136:ARG:NH1	2.34	0.43
6:F:81:THR:CG2	6:F:136:ARG:NH1	2.82	0.43
7:G:154:VAL:HG12	7:G:155:SER:N	2.34	0.43
8:H:58:THR:HG22	8:H:59:ILE:N	2.32	0.43
1:A:10:PRO:HD2	2:B:1191:ILE:O	2.19	0.43
1:A:645:LEU:HG	1:A:649:ILE:HD11	2.01	0.43
1:A:687:LYS:HE3	1:A:795:GLU:OE2	2.19	0.43
1:A:791:ASP:OD1	1:A:793:SER:OG	2.21	0.43
1:A:800:VAL:HA	1:A:812:GLU:HG2	2.00	0.43
1:A:821:ARG:NH2	2:B:524:PRO:O	2.51	0.43
1:A:840:ARG:HD2	1:A:1384:VAL:O	2.18	0.43
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.49	0.43
1:A:1269:GLU:H	1:A:1269:GLU:HG2	1.62	0.43
2:B:214:ALA:HB3	2:B:498:THR:HA	1.99	0.43
2:B:620:ARG:NH1	9:I:89:GLN:OE1	2.51	0.43
2:B:997:GLU:HG2	2:B:998:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1058:LEU:O	2:B:1062:HIS:HD2	2.02	0.43
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.43
5:E:61:GLN:HG2	5:E:62:ALA:H	1.84	0.43
5:E:82:PHE:CD1	5:E:82:PHE:N	2.87	0.43
7:G:38:CYS:SG	7:G:39:THR:N	2.92	0.43
7:G:93:SER:HB2	7:G:100:GLU:CB	2.47	0.43
7:G:101:VAL:HG12	7:G:103:VAL:HG23	2.00	0.43
9:I:8:ARG:HG2	9:I:34:TYR:CE1	2.53	0.43
12:L:62:LYS:H	12:L:62:LYS:HG2	1.60	0.43
1:A:403:LYS:HB3	1:A:404:TYR:HD1	1.83	0.43
1:A:1111:MET:HE3	1:A:1111:MET:HB3	1.78	0.43
2:B:100:PRO:HG3	2:B:172:ILE:HG13	2.01	0.43
2:B:1038:SER:HB3	2:B:1062:HIS:CE1	2.54	0.43
3:C:86:CYS:SG	3:C:87:PHE:N	2.89	0.43
3:C:224:GLN:HG3	3:C:225:ALA:H	1.84	0.43
4:D:141:LEU:HD12	4:D:141:LEU:O	2.19	0.43
6:F:79:ARG:HG3	6:F:79:ARG:NH1	2.33	0.43
7:G:89:GLY:HA3	7:G:103:VAL:CG2	2.48	0.43
10:J:6:ARG:HA	10:J:13:VAL:HA	2.01	0.43
1:A:115:LEU:CB	1:A:122:MET:HG3	2.48	0.43
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.32	0.43
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.54	0.43
1:A:1068:ALA:CB	1:A:1367:HIS:HA	2.48	0.43
1:A:1193:LEU:HD12	1:A:1193:LEU:HA	1.71	0.43
2:B:190:TYR:CE2	10:J:62:ARG:HG3	2.54	0.43
2:B:332:ASP:C	2:B:334:ILE:N	2.75	0.43
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.48	0.43
2:B:850:LEU:HG	2:B:851:PHE:HD2	1.84	0.43
2:B:1168:LEU:HB2	2:B:1170:THR:HG22	2.01	0.43
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.54	0.42
1:A:673:GLY:O	1:A:675:THR:N	2.52	0.42
1:A:716:ASP:HA	1:A:719:VAL:HG12	2.00	0.42
1:A:1079:MET:SD	1:A:1359:ASP:HB3	2.59	0.42
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	2.01	0.42
1:A:1197:LEU:HB3	1:A:1202:MET:CE	2.49	0.42
2:B:51:PHE:O	2:B:54:PHE:HB3	2.19	0.42
2:B:605:ARG:NE	2:B:639:ILE:HD13	2.33	0.42
4:D:118:THR:O	4:D:120:GLU:N	2.52	0.42
7:G:30:LEU:HD22	7:G:72:VAL:CG1	2.48	0.42
9:I:75:CYS:HB2	9:I:108:HIS:HE1	1.83	0.42
10:J:10:CYS:SG	10:J:43:ARG:NE	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HD2	1:A:74:MET:HG3	2.00	0.42
1:A:370:ILE:O	1:A:374:LEU:HG	2.19	0.42
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.53	0.42
1:A:1062:GLU:OE2	6:F:88:TYR:OH	2.37	0.42
1:A:1212:VAL:O	1:A:1216:ILE:HG12	2.18	0.42
18:A:1806:ATP:C5'	18:A:1806:ATP:C8	3.02	0.42
2:B:211:VAL:O	2:B:480:SER:HA	2.19	0.42
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.01	0.42
2:B:453:ILE:O	2:B:457:LEU:HB2	2.19	0.42
2:B:571:PRO:C	2:B:573:GLN:H	2.26	0.42
2:B:807:ARG:N	2:B:1045:SER:OG	2.43	0.42
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.54	0.42
7:G:1:MET:HB2	7:G:3:PHE:CZ	2.54	0.42
10:J:19:GLU:H	10:J:19:GLU:HG3	1.40	0.42
12:L:66:GLN:HG3	12:L:67:PHE:N	2.34	0.42
1:A:488:ASN:CG	2:B:1128:LEU:HD23	2.44	0.42
1:A:551:TYR:CE2	11:K:62:LYS:HG2	2.54	0.42
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.19	0.42
1:A:1226:VAL:C	1:A:1227:ILE:HG13	2.44	0.42
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.83	0.42
2:B:113:TYR:CB	2:B:114:PRO:HD2	2.49	0.42
2:B:197:PHE:O	2:B:488:TYR:OH	2.26	0.42
2:B:225:VAL:O	2:B:396:ASP:HB2	2.19	0.42
2:B:365:THR:HG21	2:B:370:PHE:HD2	1.82	0.42
2:B:707:PRO:HG2	2:B:708:GLU:H	1.84	0.42
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	2.00	0.42
2:B:1058:LEU:O	2:B:1061:GLU:HB3	2.20	0.42
2:B:1156:ASP:OD1	2:B:1197:PRO:HB3	2.19	0.42
3:C:236:GLY:O	3:C:237:SER:C	2.61	0.42
8:H:76:THR:HG22	8:H:77:ARG:H	1.84	0.42
1:A:40:THR:HG23	1:A:259:GLU:CG	2.47	0.42
1:A:185:TRP:HZ3	1:A:200:ARG:CB	2.32	0.42
1:A:473:SER:O	1:A:521:MET:HG2	2.19	0.42
1:A:662:PHE:O	2:B:828:ALA:HA	2.19	0.42
1:A:765:VAL:HB	1:A:800:VAL:CG1	2.50	0.42
1:A:960:ILE:HG21	1:A:1025:ARG:CD	2.46	0.42
1:A:1267:MET:O	1:A:1271:ILE:HB	2.19	0.42
2:B:202:TYR:CD2	2:B:209:GLU:HB3	2.55	0.42
2:B:465:ASN:HA	2:B:476:ARG:O	2.19	0.42
2:B:549:THR:HG22	2:B:550:ASP:N	2.35	0.42
2:B:653:VAL:HA	2:B:689:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.53	0.42
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.01	0.42
7:G:34:VAL:HG13	7:G:45:ILE:HG21	2.01	0.42
8:H:32:THR:HG22	8:H:33:GLN:HG3	2.02	0.42
9:I:59:VAL:HG23	9:I:61:ASP:HB2	2.01	0.42
9:I:103:CYS:C	9:I:105:SER:H	2.27	0.42
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.50	0.42
1:A:47:ARG:HD3	1:A:62:ASP:CG	2.45	0.42
1:A:690:VAL:HG11	1:A:718:VAL:HG13	2.01	0.42
1:A:850:VAL:CG2	1:A:1064:VAL:HG11	2.49	0.42
1:A:899:VAL:HG13	1:A:929:LEU:HB3	2.02	0.42
1:A:933:TYR:O	1:A:937:VAL:HG23	2.20	0.42
1:A:1450:LEU:HD23	6:F:108:PHE:CZ	2.54	0.42
2:B:222:ILE:O	2:B:240:ILE:HA	2.18	0.42
2:B:230:ALA:N	2:B:231:PRO:CD	2.83	0.42
2:B:581:PHE:CE1	2:B:586:TRP:HB2	2.54	0.42
2:B:884:ARG:HA	2:B:934:LYS:O	2.19	0.42
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.54	0.42
2:B:1220:ARG:HG2	2:B:1221:SER:N	2.35	0.42
3:C:37:MET:CE	3:C:244:VAL:HG13	2.49	0.42
3:C:46:ILE:O	3:C:169:LYS:HE3	2.19	0.42
3:C:89:GLU:O	3:C:90:ASP:HB3	2.20	0.42
4:D:176:GLU:OE2	4:D:198:LEU:HD23	2.20	0.42
4:D:191:ALA:HB2	4:D:211:LEU:HD11	2.02	0.42
7:G:30:LEU:O	7:G:34:VAL:HB	2.19	0.42
8:H:38:LEU:HB2	8:H:125:LEU:HD12	2.02	0.42
11:K:56:VAL:HG23	11:K:77:THR:HG22	2.00	0.42
12:L:61:THR:C	12:L:63:ARG:N	2.77	0.42
1:A:472:LEU:HD11	2:B:835:GLN:HB3	2.02	0.42
1:A:1155:ASP:OD2	1:A:1161:THR:N	2.52	0.42
2:B:206:ASN:OD1	2:B:458:LYS:HD3	2.19	0.42
2:B:332:ASP:O	2:B:334:ILE:N	2.52	0.42
2:B:466:TRP:N	2:B:476:ARG:O	2.41	0.42
2:B:1171:VAL:HG21	2:B:1191:ILE:HG13	2.01	0.42
4:D:7:THR:HG23	7:G:42:PHE:CE1	2.54	0.42
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.48	0.42
1:A:315:LEU:HB3	1:A:318:SER:HB2	2.01	0.42
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.91	0.42
1:A:694:THR:HG22	1:A:698:GLN:NE2	2.35	0.42
2:B:46:GLN:CD	2:B:46:GLN:H	2.28	0.42
2:B:217:ARG:O	2:B:217:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:GLY:HA2	2:B:241:ARG:HB2	2.02	0.42
2:B:762:ASN:HD21	2:B:984:HIS:HB3	1.84	0.42
2:B:802:PRO:HG3	2:B:1091:TYR:CE2	2.55	0.42
2:B:911:ILE:C	2:B:911:ILE:HD12	2.45	0.42
3:C:67:LEU:O	3:C:70:ILE:HB	2.20	0.42
3:C:121:VAL:O	3:C:121:VAL:HG23	2.18	0.42
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.55	0.42
7:G:89:GLY:CA	7:G:103:VAL:HG22	2.50	0.42
1:A:92:HIS:NE2	1:A:304:MET:SD	2.93	0.42
1:A:446:ARG:HG2	1:A:447:GLN:H	1.85	0.42
1:A:605:MET:HE2	1:A:607:ILE:HG13	2.02	0.42
1:A:1277:GLU:C	1:A:1279:ILE:H	2.28	0.42
1:A:1376:THR:HG22	5:E:212:ARG:HH22	1.84	0.42
2:B:521:LEU:HB3	2:B:633:VAL:HG11	2.00	0.42
2:B:613:VAL:HG23	2:B:613:VAL:O	2.20	0.42
2:B:618:ASP:O	2:B:622:LYS:N	2.53	0.42
2:B:1071:VAL:HG11	2:B:1080:LYS:HD3	2.01	0.42
2:B:1117:GLN:HB2	2:B:1118:PRO:HD2	2.00	0.42
3:C:57:VAL:HG23	3:C:58:LEU:CD2	2.49	0.42
8:H:118:PHE:HZ	8:H:142:LEU:HD22	1.84	0.42
11:K:38:GLU:HB3	11:K:71:PHE:HE2	1.83	0.42
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.19	0.42
1:A:665:GLY:HA3	2:B:1086:PHE:CD1	2.55	0.42
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.20	0.42
1:A:1202:MET:HE3	1:A:1209:MET:HE1	2.01	0.42
1:A:1438:THR:HG23	6:F:92:ARG:CB	2.44	0.42
2:B:604:ARG:NH2	2:B:614:SER:HA	2.35	0.42
6:F:111:LEU:HD21	6:F:114:GLU:O	2.19	0.42
8:H:113:ALA:HB2	8:H:126:GLU:HA	2.01	0.42
1:A:412:ARG:HH12	2:B:1108:ARG:CD	2.32	0.42
1:A:419:LYS:CG	1:A:420:ARG:N	2.83	0.42
1:A:697:ALA:HB2	1:A:702:LEU:CG	2.50	0.42
1:A:1150:SER:O	9:I:45:ARG:HA	2.19	0.42
2:B:209:GLU:OE1	2:B:485:ARG:NH1	2.52	0.42
2:B:270:LYS:HG2	2:B:281:PRO:HA	2.01	0.42
2:B:453:ILE:HD12	2:B:453:ILE:N	2.35	0.42
2:B:490:SER:HA	2:B:775:LYS:HG2	2.01	0.42
2:B:634:TYR:CD2	2:B:692:TYR:HB3	2.54	0.42
2:B:705:MET:HB3	2:B:706:GLN:H	1.74	0.42
2:B:769:TYR:C	2:B:771:SER:N	2.78	0.42
2:B:848:ARG:HA	3:C:69:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1077:THR:HA	11:K:44:ASN:ND2	2.34	0.42
5:E:199:ILE:HD12	5:E:199:ILE:N	2.34	0.42
9:I:98:VAL:HG23	9:I:100:PHE:HE1	1.84	0.42
10:J:8:PHE:H	10:J:49:MET:CE	2.25	0.42
1:A:332:LYS:H	1:A:337:ARG:HB3	1.85	0.41
1:A:694:THR:HG22	1:A:698:GLN:HE21	1.85	0.41
1:A:1092:LYS:HA	1:A:1095:THR:HB	2.01	0.41
1:A:1353:TYR:CD1	1:A:1368:MET:HE1	2.54	0.41
2:B:217:ARG:NH2	2:B:405:ARG:HG3	2.35	0.41
2:B:235:SER:HB2	2:B:258:LEU:CD2	2.48	0.41
2:B:318:VAL:HG12	2:B:322:PHE:HB2	2.01	0.41
2:B:394:ASP:HB2	9:I:91:ARG:HH11	1.85	0.41
2:B:736:THR:O	2:B:737:THR:OG1	2.33	0.41
2:B:778:MET:SD	2:B:853:SER:HB2	2.60	0.41
2:B:1072:MET:HE3	2:B:1072:MET:HB3	1.87	0.41
3:C:246:ARG:HA	3:C:249:ASP:HB3	2.02	0.41
4:D:55:ALA:HB3	4:D:148:LEU:HD21	2.01	0.41
5:E:80:VAL:HG12	5:E:82:PHE:CE1	2.55	0.41
6:F:109:VAL:HB	6:F:124:GLU:HG3	2.02	0.41
7:G:5:LYS:HA	7:G:5:LYS:HD2	1.86	0.41
7:G:91:VAL:HG12	7:G:139:ILE:O	2.20	0.41
8:H:59:ILE:O	8:H:60:ALA:HB3	2.20	0.41
12:L:50:ASP:O	12:L:51:CYS:C	2.63	0.41
1:A:96:ILE:CG2	1:A:97:ALA:N	2.83	0.41
1:A:179:LEU:HD13	1:A:311:GLN:NE2	2.35	0.41
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.96	0.41
1:A:449:SER:HB2	2:B:1133:MET:HB3	2.01	0.41
1:A:551:TYR:CE1	11:K:74:ARG:HB2	2.56	0.41
1:A:575:LYS:HB2	1:A:612:ILE:CG2	2.49	0.41
1:A:598:LEU:HD12	8:H:124:ARG:HB2	2.02	0.41
1:A:700:ASN:C	1:A:702:LEU:N	2.78	0.41
1:A:1364:ASN:HD22	1:A:1366:ARG:HD2	1.85	0.41
18:A:1806:ATP:PG	2:B:766:ARG:HH21	2.42	0.41
2:B:185:THR:H	2:B:188:ASP:HB2	1.86	0.41
2:B:349:ILE:C	2:B:351:TYR:H	2.28	0.41
2:B:529:GLU:H	2:B:529:GLU:HG3	1.39	0.41
2:B:1142:GLY:O	2:B:1144:ALA:N	2.53	0.41
4:D:43:GLU:HB2	4:D:44:GLU:H	1.58	0.41
4:D:175:PHE:HZ	7:G:85:GLU:HB2	1.86	0.41
5:E:13:TRP:HB2	5:E:42:PHE:CE2	2.55	0.41
5:E:15:ALA:HA	5:E:140:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:CD	2:B:1220:ARG:HA	2.46	0.41
1:A:19:PHE:O	1:A:1416:ALA:HA	2.20	0.41
1:A:30:ILE:H	1:A:30:ILE:HG13	1.74	0.41
1:A:250:ILE:HG13	1:A:251:SER:N	2.35	0.41
1:A:566:ILE:O	1:A:567:LYS:CB	2.68	0.41
1:A:575:LYS:HB2	1:A:612:ILE:HB	2.03	0.41
1:A:588:LEU:O	1:A:606:LEU:HD12	2.20	0.41
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.55	0.41
2:B:796:LEU:HD23	2:B:799:PRO:HA	2.02	0.41
2:B:1162:ILE:CG2	2:B:1194:ILE:HG12	2.49	0.41
6:F:82:THR:O	6:F:82:THR:HG23	2.20	0.41
6:F:110:ASP:O	6:F:112:GLU:N	2.53	0.41
10:J:37:SER:N	10:J:47:ARG:HH12	2.19	0.41
11:K:21:ILE:CD1	11:K:84:LYS:HE3	2.50	0.41
1:A:130:ASP:N	1:A:130:ASP:OD1	2.52	0.41
1:A:365:GLY:O	1:A:468:PHE:HA	2.21	0.41
1:A:507:VAL:N	1:A:508:PRO:CD	2.83	0.41
1:A:515:GLN:NE2	1:A:1071:SER:HA	2.25	0.41
1:A:679:ILE:HG23	1:A:729:ALA:CB	2.50	0.41
1:A:709:THR:HG23	1:A:711:ARG:N	2.35	0.41
1:A:795:GLU:CD	1:A:795:GLU:H	2.29	0.41
2:B:126:SER:HB3	2:B:127:GLY:H	1.72	0.41
2:B:857:ARG:O	2:B:967:ARG:HA	2.20	0.41
3:C:18:VAL:O	3:C:231:ASN:HA	2.20	0.41
6:F:86:THR:CG2	6:F:88:TYR:HD2	2.34	0.41
6:F:132:LEU:O	6:F:148:VAL:HG23	2.20	0.41
7:G:1:MET:O	7:G:2:PHE:C	2.63	0.41
7:G:46:LEU:HD23	7:G:46:LEU:HA	1.85	0.41
7:G:51:TYR:CD1	7:G:51:TYR:C	2.98	0.41
8:H:41:ASP:O	8:H:42:ILE:HG13	2.20	0.41
1:A:34:LYS:CG	1:A:36:ARG:HG3	2.50	0.41
1:A:353:ILE:HA	1:A:468:PHE:O	2.20	0.41
1:A:361:LEU:HD22	1:A:646:PHE:CD2	2.55	0.41
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.41
1:A:647:GLY:O	1:A:651:LYS:HD2	2.20	0.41
1:A:694:THR:HA	1:A:714:PHE:CE1	2.56	0.41
1:A:767:GLN:HA	1:A:799:PHE:HA	2.02	0.41
1:A:998:LEU:HB2	1:A:1001:ARG:NH1	2.35	0.41
1:A:1270:ASN:OD1	1:A:1270:ASN:N	2.52	0.41
2:B:130:VAL:HG12	2:B:167:ILE:HD11	2.02	0.41
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:ARG:HB3	2:B:781:PHE:CD2	2.55	0.41
2:B:638:PHE:HD2	2:B:741:CYS:HB3	1.84	0.41
2:B:982:SER:OG	2:B:986:GLN:HB2	2.20	0.41
5:E:31:THR:O	5:E:35:VAL:HG23	2.21	0.41
7:G:11:ILE:HD11	7:G:30:LEU:HB2	2.03	0.41
7:G:98:GLY:HA2	7:G:115:MET:HE1	2.02	0.41
7:G:111:THR:HB	7:G:114:LEU:CD2	2.49	0.41
9:I:101:PHE:CE1	9:I:112:SER:HB2	2.55	0.41
1:A:107:CYS:CB	1:A:110:CYS:HB2	2.50	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.90	0.41
1:A:148:CYS:HB3	1:A:167:CYS:O	2.20	0.41
1:A:335:ARG:HD2	2:B:1203:LEU:HB2	2.01	0.41
1:A:445:ASN:HB2	1:A:454:SER:O	2.21	0.41
1:A:508:PRO:HB3	1:A:643:ALA:HB2	2.01	0.41
1:A:777:PHE:HD2	1:A:782:ARG:C	2.28	0.41
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.28	0.41
1:A:1147:THR:HB	9:I:48:LEU:HD22	2.01	0.41
1:A:1234:GLU:HG2	1:A:1235:LYS:N	2.36	0.41
1:A:1371:LEU:HG	1:A:1375:MET:HE2	2.01	0.41
2:B:774:GLY:HA2	2:B:1093:GLN:HE22	1.86	0.41
2:B:870:ILE:O	2:B:870:ILE:HG13	2.21	0.41
2:B:1169:MET:C	2:B:1171:VAL:H	2.29	0.41
3:C:3:GLU:N	3:C:7:GLN:CD	2.79	0.41
3:C:66:ARG:O	3:C:67:LEU:C	2.62	0.41
3:C:195:GLN:HA	3:C:195:GLN:OE1	2.21	0.41
7:G:116:PRO:HG2	7:G:119:LEU:HD13	2.01	0.41
1:A:26:GLU:O	1:A:30:ILE:HG13	2.21	0.41
1:A:567:LYS:HG3	8:H:96:VAL:HG21	2.02	0.41
1:A:573:SER:HB3	1:A:576:GLN:HB2	2.03	0.41
1:A:683:ILE:O	1:A:687:LYS:HG3	2.20	0.41
1:A:777:PHE:HD2	1:A:782:ARG:HA	1.86	0.41
1:A:1003:LYS:HG2	1:A:1004:ASN:H	1.85	0.41
2:B:202:TYR:CE2	2:B:209:GLU:HB3	2.56	0.41
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.56	0.41
2:B:800:GLN:HB3	10:J:52:THR:OG1	2.20	0.41
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	2.02	0.41
3:C:43:THR:HG22	3:C:44:LEU:N	2.34	0.41
4:D:5:THR:CG2	7:G:9:LEU:HD13	2.51	0.41
4:D:29:LEU:HG	7:G:82:PHE:CE2	2.56	0.41
5:E:178:ILE:HD11	5:E:182:ASP:CG	2.46	0.41
1:A:74:MET:HB3	1:A:75:ASN:H	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:N	1:A:469:ARG:O	2.45	0.41
2:B:101:MET:SD	2:B:111:ALA:HA	2.60	0.41
2:B:308:TRP:CZ3	9:I:45:ARG:HB3	2.56	0.41
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.21	0.41
2:B:521:LEU:HB3	2:B:633:VAL:HG12	2.01	0.41
2:B:566:LEU:HD22	2:B:586:TRP:O	2.20	0.41
2:B:570:VAL:O	2:B:570:VAL:CG2	2.68	0.41
2:B:616:ILE:HG23	2:B:700:SER:OG	2.20	0.41
2:B:955:THR:OG1	2:B:956:THR:N	2.53	0.41
2:B:958:GLN:H	2:B:958:GLN:HG2	1.68	0.41
1:A:93:VAL:HG21	1:A:305:ASP:HB3	2.03	0.41
1:A:279:LEU:HD23	1:A:279:LEU:O	2.21	0.41
1:A:350:ARG:HH11	1:A:447:GLN:HG3	1.85	0.41
1:A:354:SER:HB2	1:A:469:ARG:NH1	2.34	0.41
1:A:527:THR:HG23	1:A:653:VAL:HB	2.02	0.41
1:A:940:ARG:HG2	1:A:941:LYS:HE3	2.02	0.41
1:A:986:ILE:HG22	1:A:987:VAL:N	2.35	0.41
1:A:1111:MET:SD	1:A:1331:SER:HA	2.61	0.41
2:B:426:LYS:HE3	2:B:430:ARG:HE	1.86	0.41
2:B:817:LEU:N	2:B:818:PRO:HD3	2.35	0.41
2:B:980:PHE:CE1	2:B:1094:ARG:HG3	2.56	0.41
2:B:1072:MET:SD	2:B:1085:ILE:HB	2.61	0.41
2:B:1156:ASP:HB2	2:B:1198:TYR:N	2.29	0.41
3:C:34:ARG:O	3:C:38:ILE:HG13	2.20	0.41
3:C:133:ILE:HD11	3:C:237:SER:HA	2.03	0.41
4:D:27:LEU:HD11	4:D:173:HIS:CB	2.41	0.41
4:D:183:LEU:HD21	7:G:86:VAL:HB	2.02	0.41
5:E:14:ARG:NH2	5:E:141:VAL:HG12	2.36	0.41
12:L:38:LEU:CD2	12:L:48:CYS:SG	3.09	0.41
12:L:60:ARG:HG2	12:L:61:THR:O	2.21	0.41
1:A:602:ASP:HB2	8:H:20:TYR:OH	2.20	0.41
2:B:805:THR:HA	2:B:809:MET:SD	2.61	0.41
2:B:1175:LEU:H	2:B:1175:LEU:HG	1.60	0.41
4:D:207:LEU:HD12	4:D:207:LEU:O	2.21	0.41
5:E:119:SER:O	5:E:123:LEU:HB3	2.21	0.41
7:G:85:GLU:O	7:G:85:GLU:HG3	2.21	0.41
11:K:57:LEU:HD12	11:K:76:GLN:HG2	2.03	0.41
14:T:24:DT:C3'	14:T:25:DC:H5''	2.51	0.41
1:A:32:VAL:O	1:A:57:ARG:HD2	2.20	0.40
1:A:54:ASN:C	1:A:56:PRO:HD3	2.46	0.40
1:A:472:LEU:HD11	2:B:835:GLN:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:CG2	1:A:478:TYR:HE2	2.32	0.40
1:A:492:PRO:HB3	1:A:497:THR:OG1	2.20	0.40
1:A:699:ALA:C	1:A:701:LEU:H	2.29	0.40
1:A:834:THR:OG1	1:A:1077:THR:HA	2.21	0.40
1:A:899:VAL:HG13	1:A:929:LEU:HD13	2.03	0.40
1:A:907:THR:HG21	1:A:920:LEU:HG	2.03	0.40
1:A:1015:VAL:O	1:A:1018:PHE:N	2.54	0.40
1:A:1063:MET:HG3	2:B:1139:ILE:O	2.20	0.40
1:A:1143:LEU:HD12	1:A:1143:LEU:HA	1.91	0.40
1:A:1161:THR:HG22	1:A:1161:THR:O	2.21	0.40
2:B:214:ALA:HB3	2:B:497:ARG:O	2.21	0.40
2:B:293:PRO:HB3	9:I:11:ASN:HB3	2.02	0.40
3:C:193:TYR:CD2	3:C:197:SER:HB3	2.57	0.40
5:E:71:LYS:C	5:E:73:PRO:HD3	2.45	0.40
6:F:79:ARG:HG3	6:F:79:ARG:HH11	1.86	0.40
8:H:129:TYR:CG	8:H:130:ARG:N	2.89	0.40
10:J:5:VAL:O	10:J:6:ARG:HB2	2.20	0.40
11:K:94:ILE:HG22	11:K:98:LEU:CD1	2.52	0.40
1:A:83:HIS:HD2	1:A:238:CYS:SG	2.45	0.40
1:A:575:LYS:NZ	1:A:602:ASP:OD2	2.52	0.40
1:A:867:ILE:HG13	1:A:871:ASP:N	2.36	0.40
2:B:44:VAL:O	2:B:45:SER:C	2.64	0.40
2:B:693:ILE:HD11	2:B:740:HIS:NE2	2.36	0.40
3:C:33:LEU:HD22	3:C:33:LEU:HA	1.86	0.40
3:C:204:SER:N	3:C:207:CYS:SG	2.94	0.40
4:D:51:ASN:ND2	4:D:54:GLU:H	2.19	0.40
4:D:192:LYS:HD3	4:D:199:ASN:HA	2.03	0.40
7:G:46:LEU:HB2	7:G:77:VAL:HG12	2.03	0.40
7:G:60:ARG:HH22	7:G:63:PRO:HD3	1.86	0.40
1:A:1303:GLU:CD	1:A:1326:ARG:HH22	2.29	0.40
2:B:464:GLY:HA2	2:B:480:SER:H	1.87	0.40
2:B:899:ILE:O	2:B:952:VAL:HG21	2.21	0.40
3:C:36:VAL:HG23	11:K:41:THR:HG23	2.03	0.40
3:C:71:PRO:O	3:C:72:LEU:HD12	2.21	0.40
3:C:142:VAL:HG13	10:J:15:GLY:HA3	2.04	0.40
3:C:159:ALA:O	3:C:160:LYS:HG3	2.21	0.40
1:A:353:ILE:CG2	1:A:487:MET:HB2	2.51	0.40
1:A:548:ASN:O	1:A:552:TRP:HD1	2.04	0.40
1:A:808:LEU:HD13	2:B:760:ASP:O	2.21	0.40
1:A:826:ASP:OD1	1:A:830:LYS:HD2	2.20	0.40
1:A:1138:ILE:HG22	1:A:1276:VAL:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:PRO:HG3	1:A:1190:PRO:HB3	2.02	0.40
2:B:292:ILE:N	2:B:293:PRO:CD	2.84	0.40
2:B:885:MET:H	2:B:885:MET:HG2	1.64	0.40
2:B:1078:GLY:HA3	3:C:31:ASN:HB2	2.03	0.40
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.49	0.40
4:D:198:LEU:HB2	4:D:199:ASN:H	1.56	0.40
1:A:54:ASN:OD1	1:A:247:ARG:NH1	2.48	0.40
1:A:470:LEU:C	1:A:470:LEU:HD12	2.46	0.40
1:A:567:LYS:HE3	8:H:91:ASP:HB2	2.04	0.40
1:A:849:MET:HB2	1:A:1062:GLU:O	2.22	0.40
1:A:1106:ASN:N	1:A:1106:ASN:HD22	2.19	0.40
2:B:801:LYS:O	10:J:52:THR:HB	2.22	0.40
2:B:831:SER:OG	2:B:833:TYR:HD1	2.05	0.40
2:B:1029:CYS:SG	2:B:1090:THR:OG1	2.74	0.40
2:B:1157:ALA:H	2:B:1197:PRO:HA	1.86	0.40
3:C:258:ILE:O	3:C:262:LEU:HB2	2.21	0.40
4:D:36:LYS:HE3	4:D:44:GLU:OE2	2.21	0.40
4:D:187:THR:HG22	4:D:189:ASP:H	1.87	0.40
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.22	0.40
8:H:38:LEU:HD12	8:H:39:THR:N	2.36	0.40
12:L:42:ARG:O	12:L:43:THR:C	2.64	0.40
12:L:55:ILE:O	12:L:56:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1376/1733 (79%)	1168 (85%)	166 (12%)	42 (3%)	3	20
2	B	1036/1224 (85%)	854 (82%)	141 (14%)	41 (4%)	2	16
3	C	263/318 (83%)	223 (85%)	29 (11%)	11 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	155/221 (70%)	134 (86%)	14 (9%)	7 (4%)	2	13
5	E	200/215 (93%)	178 (89%)	17 (8%)	5 (2%)	4	24
6	F	83/155 (54%)	76 (92%)	5 (6%)	2 (2%)	4	24
7	G	169/171 (99%)	137 (81%)	24 (14%)	8 (5%)	2	12
8	H	107/146 (73%)	80 (75%)	18 (17%)	9 (8%)	0	4
9	I	111/122 (91%)	85 (77%)	24 (22%)	2 (2%)	6	30
10	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	2	12
11	K	112/120 (93%)	96 (86%)	13 (12%)	3 (3%)	4	22
12	L	41/70 (59%)	19 (46%)	15 (37%)	7 (17%)	0	0
All	All	3716/4565 (81%)	3103 (84%)	473 (13%)	140 (4%)	2	16

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	433	GLU
1	A	567	LYS
1	A	672	ASP
1	A	674	PRO
1	A	1016	THR
1	A	1377	THR
2	B	58	THR
2	B	245	GLU
2	B	262	GLU
2	B	277	LYS
2	B	467	GLY
2	B	705	MET
2	B	711	GLU
2	B	1156	ASP
2	B	1223	ASP
3	C	184	ASN
4	D	52	LEU
4	D	53	SER
5	E	36	GLU
8	H	17	PRO
8	H	34	ASP
10	J	2	ILE
12	L	51	CYS
1	A	40	THR

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	76	GLU
1	A	151	ASP
1	A	701	LEU
1	A	846	GLU
1	A	1107	VAL
1	A	1108	ALA
1	A	1437	GLY
2	B	24	PRO
2	B	260	GLY
2	B	333	PHE
2	B	576	ASP
2	B	707	PRO
2	B	737	THR
2	B	867	GLY
2	B	1046	PRO
2	B	1096	ARG
3	C	216	GLY
4	D	119	ARG
4	D	138	ASN
6	F	111	LEU
7	G	63	PRO
8	H	12	VAL
8	H	119	GLY
10	J	64	ASN
11	K	2	ASN
11	K	69	ALA
12	L	46	VAL
12	L	49	LYS
1	A	52	GLY
1	A	58	LEU
1	A	309	ALA
1	A	332	LYS
1	A	1090	ALA
1	A	1099	PRO
1	A	1120	LEU
1	A	1140	HIS
1	A	1164	PRO
1	A	1229	SER
1	A	1435	PRO
2	B	108	VAL
2	B	126	SER

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Mol	Chain	Res	Type
2	B	350	GLN
2	B	793	ALA
2	B	868	MET
2	B	1080	LYS
2	B	1082	MET
2	B	1108	ARG
2	B	1157	ALA
3	C	60	ASP
3	C	167	HIS
3	C	227	THR
4	D	218	GLU
5	E	29	PHE
6	F	72	LYS
7	G	44	TYR
7	G	154	VAL
8	H	128	ASN
1	A	131	SER
1	A	286	HIS
1	A	448	PRO
1	A	600	PRO
1	A	703	THR
1	A	972	HIS
1	A	1331	SER
1	A	1358	SER
1	A	1376	THR
2	B	106	ASP
2	B	365	THR
2	B	572	HIS
2	B	1214	PRO
5	E	104	ASN
7	G	2	PHE
8	H	35	GLN
9	I	47	GLU
10	J	6	ARG
12	L	38	LEU
1	A	54	ASN
1	A	958	VAL
1	A	1273	LEU
2	B	471	LYS
2	B	571	PRO
2	B	792	MET
2	B	987	LYS

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Mol	Chain	Res	Type
2	B	1017	ILE
2	B	1037	LEU
2	B	1143	ALA
3	C	65	HIS
3	C	90	ASP
3	C	231	ASN
4	D	43	GLU
4	D	198	LEU
5	E	3	GLN
7	G	20	PRO
7	G	165	GLU
8	H	140	ALA
9	I	19	ASP
11	K	81	TYR
12	L	43	THR
2	B	177	LYS
2	B	469	GLN
2	B	727	LYS
3	C	214	ASN
12	L	59	ALA
1	A	73	GLY
1	A	986	ILE
7	G	34	VAL
8	H	48	PRO
8	H	59	ILE
12	L	55	ILE
5	E	124	VAL
3	C	6	PRO
7	G	136	VAL
1	A	570	PRO
3	C	18	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1213/1520 (80%)	1100 (91%)	113 (9%)	8	31
2	B	917/1061 (86%)	822 (90%)	95 (10%)	7	26
3	C	232/274 (85%)	215 (93%)	17 (7%)	13	39
4	D	143/200 (72%)	121 (85%)	22 (15%)	2	12
5	E	189/197 (96%)	159 (84%)	30 (16%)	2	11
6	F	74/137 (54%)	62 (84%)	12 (16%)	2	11
7	G	152/152 (100%)	134 (88%)	18 (12%)	5	21
8	H	104/128 (81%)	93 (89%)	11 (11%)	6	25
9	I	105/116 (90%)	91 (87%)	14 (13%)	4	17
10	J	60/65 (92%)	50 (83%)	10 (17%)	2	11
11	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
12	L	38/57 (67%)	24 (63%)	14 (37%)	0	0
All	All	3326/4009 (83%)	2961 (89%)	365 (11%)	6	23

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	41	MET
1	A	49	LYS
1	A	58	LEU
1	A	84	ILE
1	A	126	LEU
1	A	130	ASP
1	A	148	CYS
1	A	164	ARG
1	A	170	THR
1	A	176	LYS
1	A	205	GLU
1	A	206	GLU
1	A	232	GLU
1	A	239	LEU
1	A	261	ASP
1	A	308	ILE
1	A	344	ARG
1	A	360	GLU

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Mol	Chain	Res	Type
1	A	370	ILE
1	A	385	ILE
1	A	393	ARG
1	A	398	GLU
1	A	399	HIS
1	A	427	GLN
1	A	442	VAL
1	A	447	GLN
1	A	450	LEU
1	A	451	HIS
1	A	462	VAL
1	A	472	LEU
1	A	481	ASP
1	A	483	ASP
1	A	485	ASP
1	A	512	VAL
1	A	515	GLN
1	A	538	ASP
1	A	544	ASP
1	A	559	VAL
1	A	569	LYS
1	A	575	LYS
1	A	586	ILE
1	A	588	LEU
1	A	597	LEU
1	A	598	LEU
1	A	601	LYS
1	A	602	ASP
1	A	626	ASN
1	A	635	ARG
1	A	658	LEU
1	A	660	ASN
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	677	ARG
1	A	681	GLU
1	A	710	LEU
1	A	727	ASP
1	A	756	ILE
1	A	768	GLN
1	A	833	GLU

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Mol	Chain	Res	Type
1	A	841	LEU
1	A	864	ILE
1	A	867	ILE
1	A	883	LEU
1	A	885	THR
1	A	890	ASP
1	A	932	GLU
1	A	963	ILE
1	A	964	ILE
1	A	980	ASP
1	A	988	LEU
1	A	1003	LYS
1	A	1007	ILE
1	A	1012	ARG
1	A	1037	LEU
1	A	1043	ASP
1	A	1089	VAL
1	A	1116	LEU
1	A	1138	ILE
1	A	1169	ILE
1	A	1172	LEU
1	A	1188	GLN
1	A	1195	LEU
1	A	1203	ASN
1	A	1226	VAL
1	A	1232	ASN
1	A	1233	ASP
1	A	1258	HIS
1	A	1266	THR
1	A	1267	MET
1	A	1269	GLU
1	A	1271	ILE
1	A	1280	GLU
1	A	1289	ARG
1	A	1295	THR
1	A	1322	ILE
1	A	1327	ILE
1	A	1334	ASP
1	A	1341	ILE
1	A	1356	ILE
1	A	1358	SER
1	A	1372	VAL

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Mol	Chain	Res	Type
1	A	1375	MET
1	A	1378	GLN
1	A	1384	VAL
1	A	1393	ASN
1	A	1394	THR
1	A	1403	GLU
1	A	1422	ARG
1	A	1424	VAL
1	A	1450	LEU
1	A	1454	MET
2	B	20	ASP
2	B	25	ILE
2	B	90	ILE
2	B	92	PHE
2	B	102	VAL
2	B	112	LEU
2	B	123	THR
2	B	126	SER
2	B	181	LEU
2	B	192	LEU
2	B	199	MET
2	B	209	GLU
2	B	249	ARG
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG
2	B	268	THR
2	B	272	THR
2	B	273	LEU
2	B	276	ILE
2	B	279	ASP
2	B	280	ILE
2	B	284	ILE
2	B	292	ILE
2	B	302	CYS
2	B	332	ASP
2	B	356	LEU
2	B	367	LEU
2	B	371	GLU
2	B	396	ASP
2	B	408	LEU
2	B	412	LEU

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Mol	Chain	Res	Type
2	B	416	LEU
2	B	433	GLN
2	B	446	LEU
2	B	452	THR
2	B	463	THR
2	B	465	ASN
2	B	466	TRP
2	B	468	GLU
2	B	527	THR
2	B	529	GLU
2	B	531	GLN
2	B	537	LYS
2	B	539	LEU
2	B	547	VAL
2	B	561	TRP
2	B	585	VAL
2	B	587	HIS
2	B	589	VAL
2	B	592	ASN
2	B	603	LEU
2	B	616	ILE
2	B	626	ILE
2	B	629	ASP
2	B	635	ARG
2	B	653	VAL
2	B	658	ILE
2	B	694	ASP
2	B	696	GLU
2	B	710	LEU
2	B	743	ILE
2	B	755	ILE
2	B	760	ASP
2	B	766	ARG
2	B	787	VAL
2	B	790	ASP
2	B	797	TYR
2	B	815	ARG
2	B	841	MET
2	B	844	SER
2	B	875	GLU
2	B	891	ASP
2	B	915	THR

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Mol	Chain	Res	Type
2	B	973	ILE
2	B	1007	VAL
2	B	1021	MET
2	B	1050	ILE
2	B	1072	MET
2	B	1087	PHE
2	B	1093	GLN
2	B	1112	GLN
2	B	1124	ARG
2	B	1132	GLU
2	B	1145	SER
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1162	ILE
2	B	1170	THR
2	B	1175	LEU
2	B	1203	LEU
2	B	1212	ILE
2	B	1218	THR
2	B	1223	ASP
3	C	27	LEU
3	C	48	SER
3	C	54	ASN
3	C	58	LEU
3	C	66	ARG
3	C	118	LEU
3	C	124	LEU
3	C	129	ILE
3	C	138	GLU
3	C	166	GLU
3	C	231	ASN
3	C	240	VAL
3	C	241	ASP
3	C	243	VAL
3	C	252	GLN
3	C	259	LEU
3	C	262	LEU
4	D	8	PHE
4	D	27	LEU
4	D	29	LEU
4	D	34	GLN

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Mol	Chain	Res	Type
4	D	38	ILE
4	D	40	HIS
4	D	43	GLU
4	D	47	LEU
4	D	48	ILE
4	D	50	LEU
4	D	63	LEU
4	D	122	GLU
4	D	124	GLU
4	D	130	LEU
4	D	150	ASN
4	D	158	GLU
4	D	165	GLN
4	D	177	VAL
4	D	187	THR
4	D	198	LEU
4	D	199	ASN
4	D	200	ASN
5	E	2	ASP
5	E	29	PHE
5	E	32	GLN
5	E	41	ASP
5	E	57	MET
5	E	60	PHE
5	E	65	THR
5	E	82	PHE
5	E	84	ASP
5	E	85	GLU
5	E	88	VAL
5	E	94	LYS
5	E	112	TYR
5	E	116	ILE
5	E	123	LEU
5	E	124	VAL
5	E	131	THR
5	E	132	ILE
5	E	134	THR
5	E	149	LEU
5	E	156	LEU
5	E	164	LEU
5	E	165	LEU
5	E	167	ARG

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Mol	Chain	Res	Type
5	E	172	GLU
5	E	175	LEU
5	E	178	ILE
5	E	190	LEU
5	E	196	VAL
5	E	207	ARG
6	F	79	ARG
6	F	90	ARG
6	F	97	ARG
6	F	109	VAL
6	F	118	LEU
6	F	119	ARG
6	F	127	GLU
6	F	133	VAL
6	F	138	LEU
6	F	151	LEU
6	F	153	VAL
6	F	155	LEU
7	G	2	PHE
7	G	11	ILE
7	G	35	GLU
7	G	47	CYS
7	G	54	ILE
7	G	56	ILE
7	G	61	ILE
7	G	77	VAL
7	G	88	ASP
7	G	90	THR
7	G	96	GLN
7	G	106	MET
7	G	108	VAL
7	G	119	LEU
7	G	139	ILE
7	G	157	ILE
7	G	165	GLU
7	G	171	ILE
8	H	26	ILE
8	H	27	GLU
8	H	33	GLN
8	H	40	LEU
8	H	63	LEU
8	H	91	ASP

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Mol	Chain	Res	Type
8	H	107	VAL
8	H	114	VAL
8	H	130	ARG
8	H	131	ASN
8	H	135	LEU
9	I	8	ARG
9	I	13	MET
9	I	26	LEU
9	I	31	THR
9	I	35	VAL
9	I	54	GLU
9	I	72	ASP
9	I	73	ARG
9	I	93	LYS
9	I	98	VAL
9	I	104	LEU
9	I	106	CYS
9	I	109	ILE
9	I	114	GLN
10	J	3	VAL
10	J	7	CYS
10	J	9	SER
10	J	12	LYS
10	J	13	VAL
10	J	19	GLU
10	J	22	LEU
10	J	24	LEU
10	J	30	LEU
10	J	61	LEU
11	K	25	THR
11	K	45	LEU
11	K	50	LEU
11	K	56	VAL
11	K	87	LEU
11	K	98	LEU
11	K	101	LEU
11	K	112	GLN
11	K	113	THR
12	L	28	LYS
12	L	30	ILE
12	L	33	GLU
12	L	37	LYS

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Mol	Chain	Res	Type
12	L	39	SER
12	L	42	ARG
12	L	46	VAL
12	L	47	ARG
12	L	48	CYS
12	L	51	CYS
12	L	57	LEU
12	L	64	LEU
12	L	65	VAL
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	109	HIS
1	A	316	GLN
1	A	390	GLN
1	A	445	ASN
1	A	447	GLN
1	A	471	ASN
1	A	479	ASN
1	A	515	GLN
1	A	603	ASN
1	A	611	GLN
1	A	626	ASN
1	A	650	GLN
1	A	717	ASN
1	A	767	GLN
1	A	768	GLN
1	A	935	GLN
1	A	975	HIS
1	A	1004	ASN
1	A	1009	ASN
1	A	1106	ASN
1	A	1258	HIS
1	A	1364	ASN
1	A	1387	HIS
2	B	110	HIS
2	B	363	HIS
2	B	383	ASN
2	B	465	ASN

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Mol	Chain	Res	Type
2	B	538	ASN
2	B	776	GLN
2	B	835	GLN
2	B	1025	HIS
2	B	1062	HIS
2	B	1084	GLN
2	B	1179	GLN
3	C	7	GLN
3	C	252	GLN
5	E	143	ASN
7	G	113	HIS
8	H	11	GLN
9	I	22	ASN
9	I	51	ASN
9	I	79	HIS
9	I	83	ASN
9	I	108	HIS
11	K	104	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U
13	R	3	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	ATP	A	1806	17	32,33,33	0.59	0	48,52,52	0.76	2 (4%)
16	GOL	A	1803	-	5,5,5	1.02	0	5,5,5	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ATP	A	1806	17	-	6/22/38/38	0/3/3/3
16	GOL	A	1803	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1806	ATP	O2A-PA-O3A	2.77	114.77	107.27
18	A	1806	ATP	O3A-PA-O1A	-2.42	103.41	110.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1806	ATP	C5'-O5'-PA-O2A
18	A	1806	ATP	C5'-O5'-PA-O3A
18	A	1806	ATP	C3'-C4'-C5'-O5'
18	A	1806	ATP	O4'-C4'-C5'-O5'
16	A	1803	GOL	C1-C2-C3-O3
18	A	1806	ATP	C4'-C5'-O5'-PA

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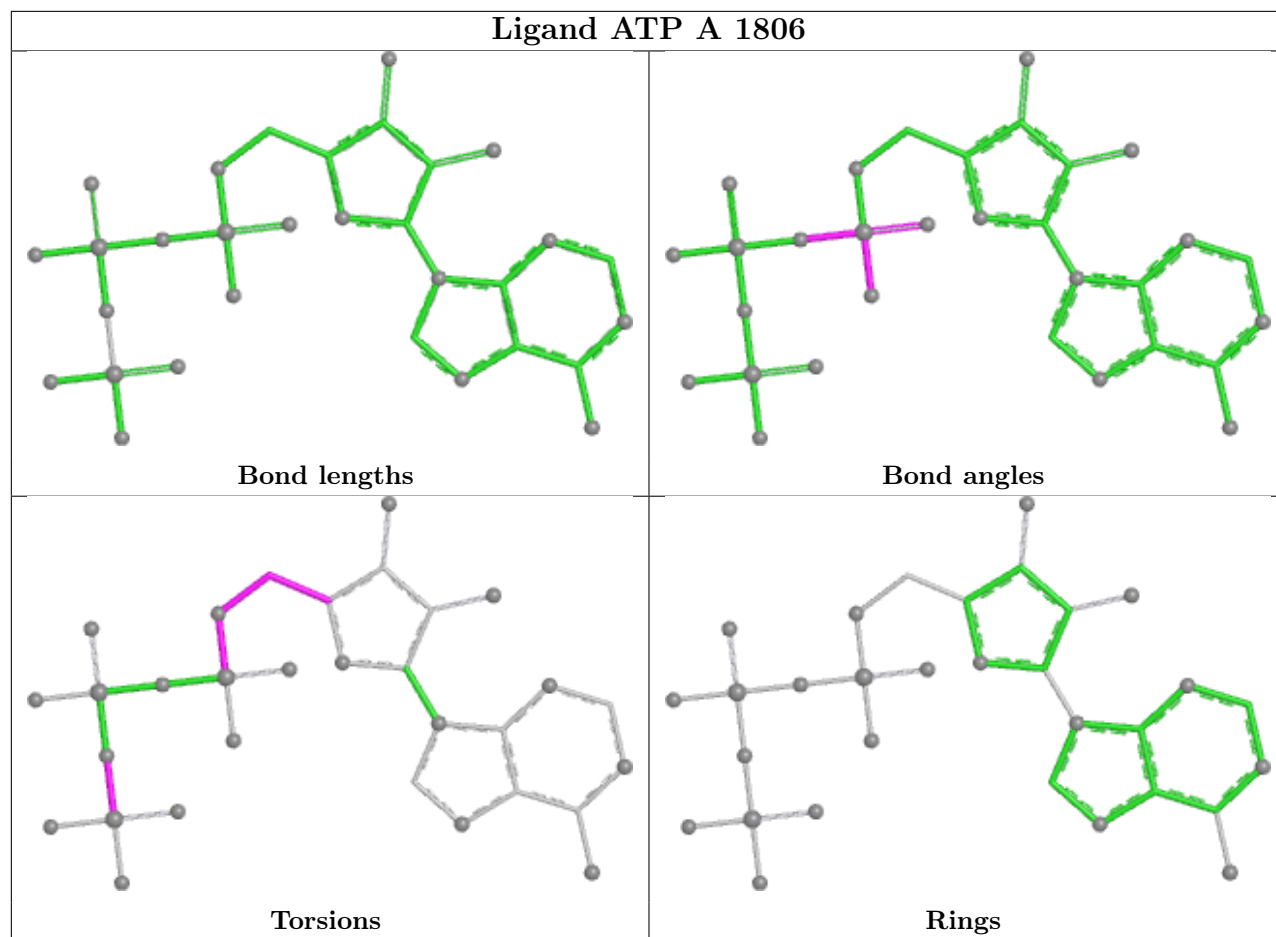
Mol	Chain	Res	Type	Atoms
16	A	1803	GOL	O2-C2-C3-O3
18	A	1806	ATP	PB-O3B-PG-O2G

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1806	ATP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1396/1733 (80%)	-0.01	24 (1%) 69 51	40, 92, 158, 219	0
2	B	1060/1224 (86%)	0.08	36 (3%) 48 32	30, 99, 165, 276	0
3	C	265/318 (83%)	0.01	3 (1%) 78 62	60, 98, 143, 188	0
4	D	161/221 (72%)	0.19	4 (2%) 58 40	74, 107, 159, 212	0
5	E	206/215 (95%)	0.19	4 (1%) 66 48	61, 124, 184, 234	0
6	F	85/155 (54%)	-0.25	1 (1%) 76 59	46, 73, 106, 132	0
7	G	171/171 (100%)	-0.03	2 (1%) 76 59	70, 96, 150, 175	0
8	H	117/146 (80%)	0.56	10 (8%) 16 13	95, 135, 180, 221	0
9	I	113/122 (92%)	0.44	6 (5%) 32 22	99, 139, 200, 222	0
10	J	65/70 (92%)	-0.07	1 (1%) 72 53	70, 95, 138, 181	0
11	K	114/120 (95%)	-0.21	1 (0%) 81 67	57, 97, 143, 170	0
12	L	43/70 (61%)	0.85	6 (13%) 6 6	80, 128, 180, 197	0
13	R	10/10 (100%)	0.24	0 100 100	98, 113, 170, 205	0
14	T	14/14 (100%)	0.20	0 100 100	86, 106, 203, 205	0
All	All	3820/4589 (83%)	0.06	98 (2%) 57 39	30, 99, 166, 276	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	6.7
9	I	110	PHE	6.4
2	B	916	THR	5.2
9	I	76	PRO	5.0
2	B	731	VAL	4.9
11	K	114	LEU	4.5
4	D	220	LEU	4.5
8	H	107	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	359	GLU	4.2
9	I	77	LYS	4.1
2	B	251	ILE	4.0
2	B	246	LYS	3.9
12	L	53	HIS	3.9
1	A	1088	GLY	3.7
8	H	139	ASN	3.6
3	C	94	LYS	3.6
12	L	39	SER	3.5
9	I	84	VAL	3.5
2	B	111	ALA	3.5
8	H	50	ALA	3.2
5	E	53	PRO	3.2
2	B	735	ALA	3.1
8	H	127	GLY	3.1
2	B	248	SER	3.1
2	B	712	PRO	3.1
5	E	117	THR	3.0
1	A	788	SER	3.0
2	B	1169	MET	3.0
1	A	165	GLY	3.0
2	B	349	ILE	3.0
4	D	155	ARG	2.9
2	B	90	ILE	2.9
2	B	468	GLU	2.8
2	B	934	LYS	2.8
3	C	149	LYS	2.8
1	A	257	ARG	2.7
8	H	89	LEU	2.7
8	H	12	VAL	2.7
5	E	139	ALA	2.7
12	L	54	ARG	2.6
2	B	266	ALA	2.6
2	B	484	ASN	2.6
1	A	1169	ILE	2.6
1	A	447	GLN	2.6
2	B	335	GLY	2.6
6	F	155	LEU	2.6
2	B	27	ALA	2.6
2	B	486	TYR	2.5
1	A	1096	SER	2.5
2	B	865	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	483	ASP	2.5
1	A	1127	ASP	2.4
7	G	21	ARG	2.4
10	J	65	PRO	2.4
1	A	975	HIS	2.4
5	E	105	PHE	2.4
12	L	38	LEU	2.4
9	I	52	ILE	2.3
1	A	446	ARG	2.3
9	I	109	ILE	2.3
2	B	431	TYR	2.3
12	L	52	GLY	2.3
2	B	303	TYR	2.3
3	C	151	GLN	2.3
2	B	681	TRP	2.2
1	A	1140	HIS	2.2
2	B	587	HIS	2.2
8	H	136	LYS	2.2
1	A	115	LEU	2.2
1	A	153	PRO	2.2
1	A	1010	ALA	2.2
2	B	597	MET	2.2
8	H	55	LEU	2.2
7	G	155	SER	2.2
1	A	672	ASP	2.1
1	A	706	HIS	2.1
12	L	57	LEU	2.1
2	B	24	PRO	2.1
4	D	3	VAL	2.1
1	A	1141	THR	2.1
8	H	132	LEU	2.1
1	A	1095	THR	2.1
2	B	884	ARG	2.1
2	B	665	GLU	2.1
2	B	91	SER	2.1
2	B	1019	SER	2.1
1	A	587	HIS	2.1
1	A	1161	THR	2.1
2	B	868	MET	2.1
2	B	948	ILE	2.0
2	B	1170	THR	2.0
2	B	876	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	57	ARG	2.0
2	B	1173	ALA	2.0
8	H	113	ALA	2.0
2	B	1224	PHE	2.0
1	A	969	GLN	2.0
4	D	124	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

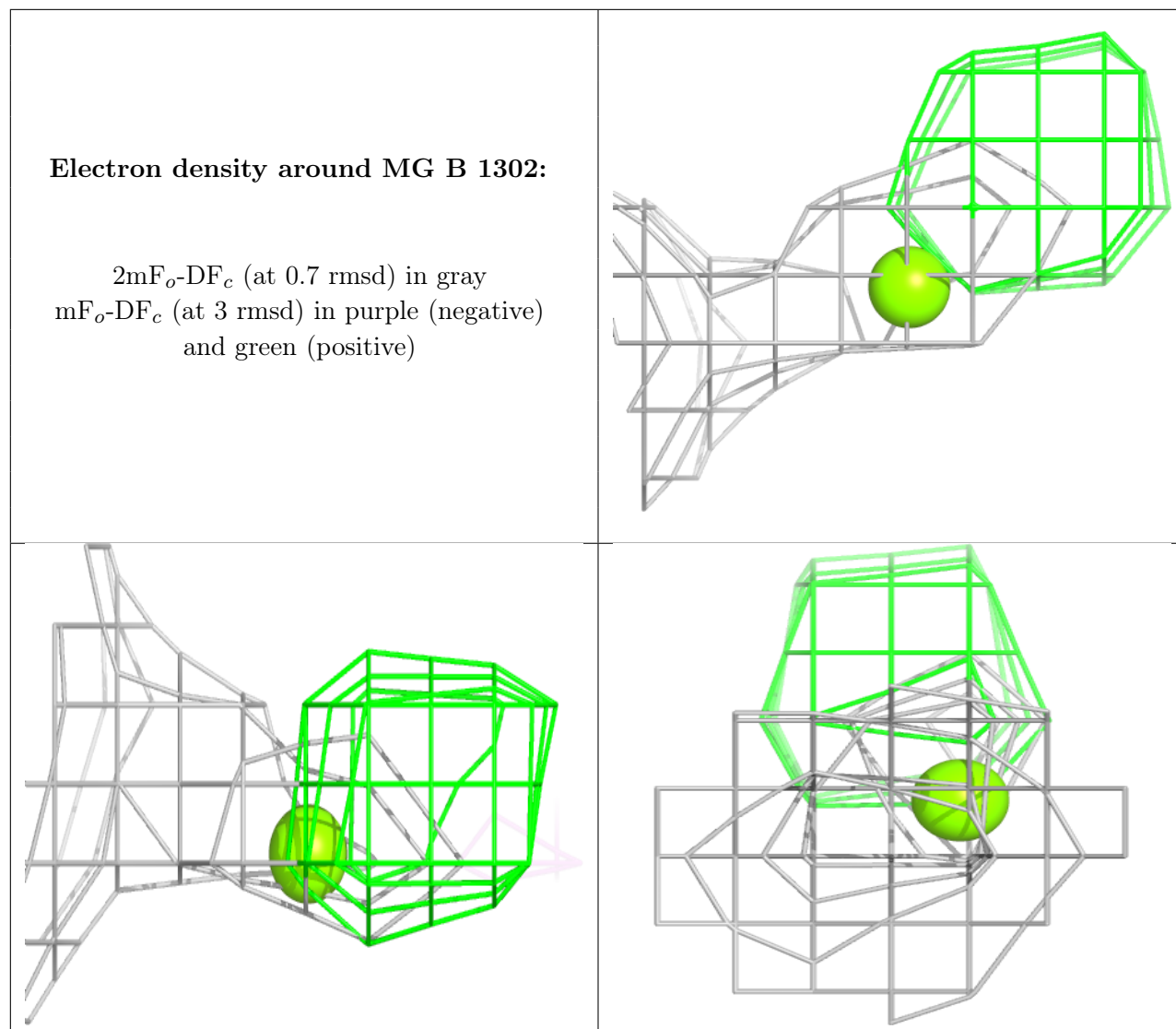
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MG	B	1302	1/1	0.77	0.64	92,92,92,92	0
17	MG	A	1805	1/1	0.81	0.15	105,105,105,105	0
15	ZN	A	1801	1/1	0.84	0.09	213,213,213,213	0
18	ATP	A	1806	31/31	0.92	0.12	112,118,133,155	0
15	ZN	L	101	1/1	0.93	0.07	173,173,173,173	0
17	MG	A	1804	1/1	0.94	0.09	94,94,94,94	0
15	ZN	A	1802	1/1	0.97	0.03	56,56,56,56	0
16	GOL	A	1803	6/6	0.97	0.12	103,110,116,118	0
15	ZN	I	201	1/1	0.98	0.10	103,103,103,103	0
15	ZN	C	401	1/1	0.99	0.04	69,69,69,69	0
15	ZN	B	1301	1/1	0.99	0.02	61,61,61,61	0
15	ZN	I	202	1/1	0.99	0.02	181,181,181,181	0
15	ZN	J	101	1/1	1.00	0.01	79,79,79,79	0

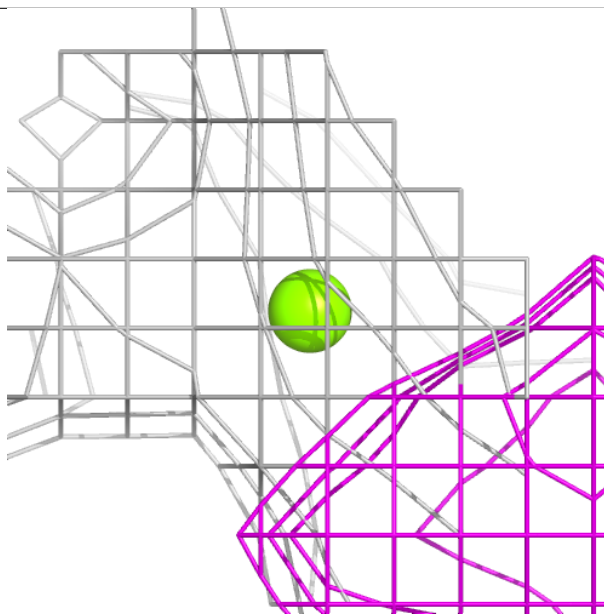
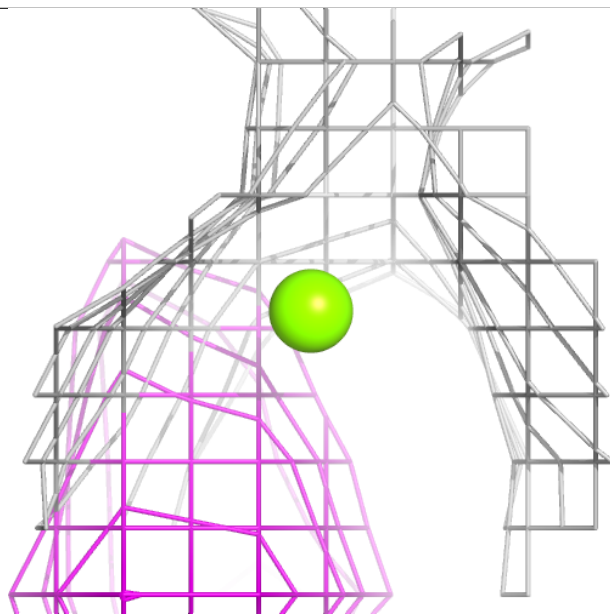
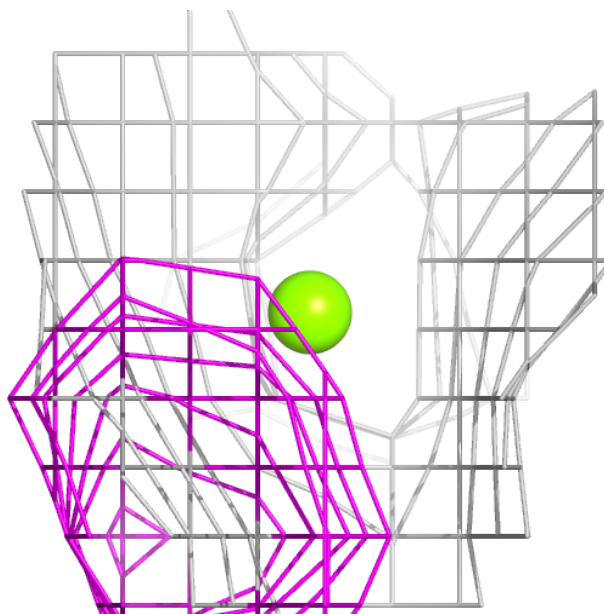
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.



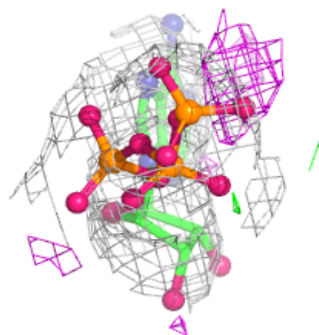
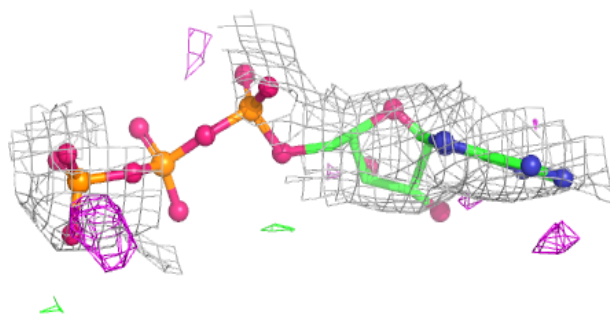
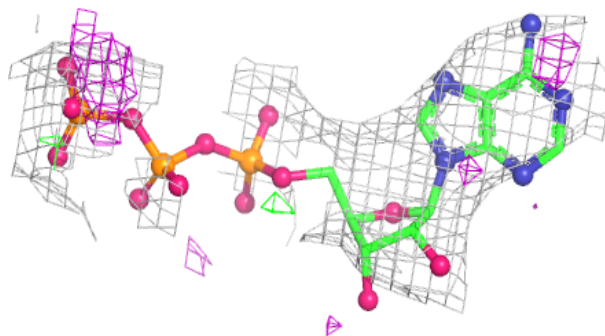
Electron density around MG A 1805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



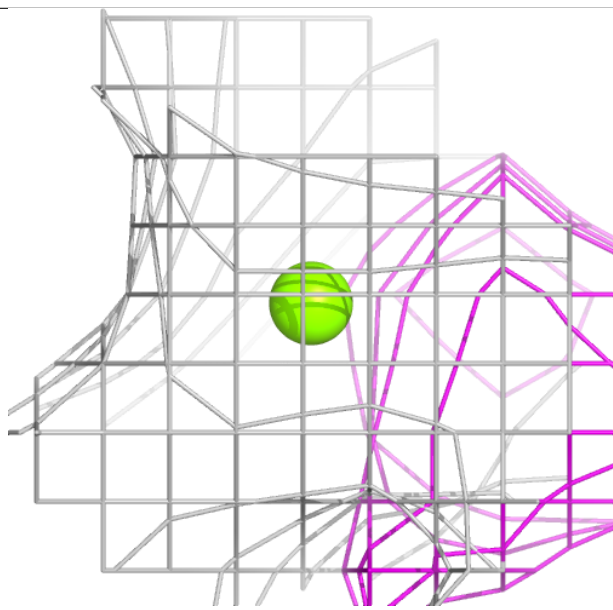
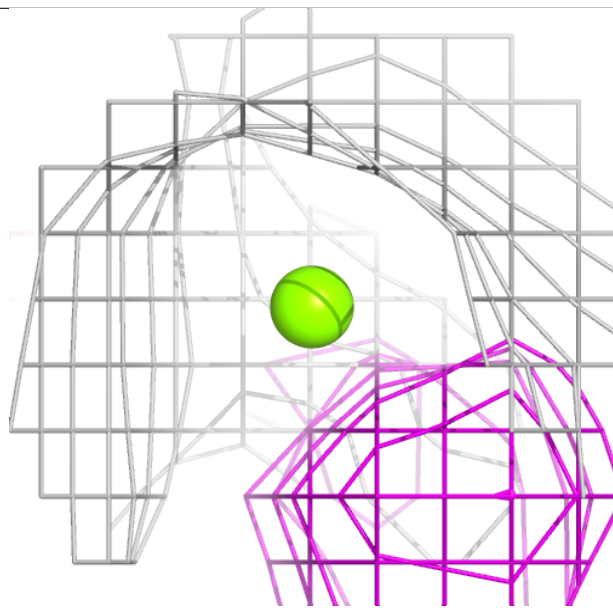
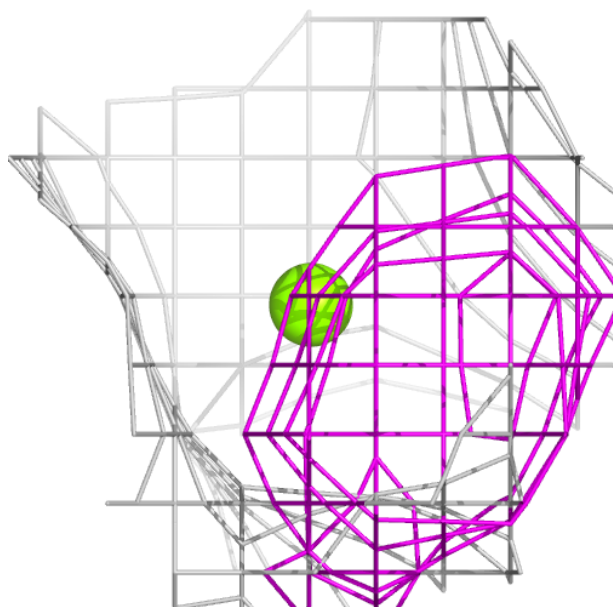
Electron density around ATP A 1806:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 1804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.