Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 11:01 AM EST

PDB ID	:	4XLN
Title	:	Crystal structure of T. aquaticus transcription initiation complex containing bubble promoter and RNA
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2015-01-13
Resolution	:	4.00 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:

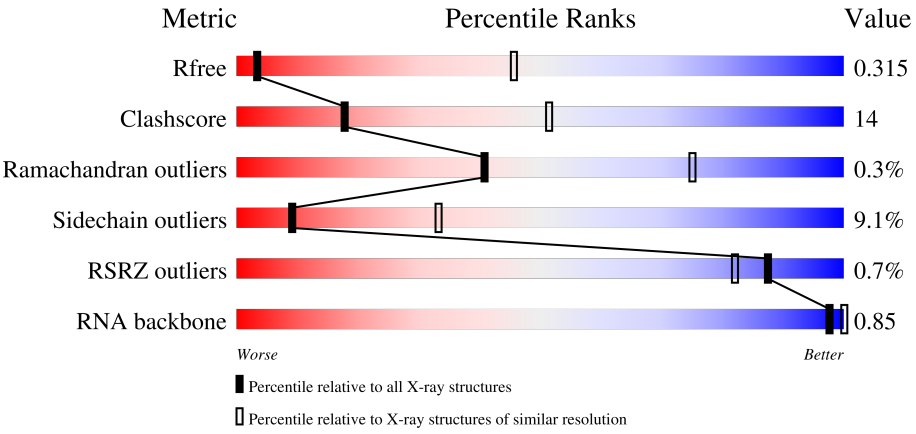
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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 <=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	314	47% 23% · 28%
1	B	314	46% 22% · 28%
1	G	314	% 47% 23% · 28%
1	H	314	46% 22% · 28%

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Mol	Chain	Length	Quality of chain
2	C	1119	59% 36%
2	I	1119	61% 35%
3	D	1524	63% 31%
3	J	1524	59% 28% 10%
4	E	99	63% 27% 6%
4	K	99	61% 29% 6%
5	F	347	62% 34%
5	L	347	63% 33%
6	O	48	8% 69% 27%
6	R	48	65% 35%
7	P	48	8% 65% 29% 6%
7	S	48	60% 29% 10%
8	Q	4	75% 25%
8	T	4	50% 50%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 58255 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	347	Total	C	N	O	S	0	0	0
			2801	1767	505	525	4			
5	L	347	Total	C	N	O	S	0	0	0
			2801	1767	505	525	4			

- Molecule 6 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
6	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
7	S	43	Total	C	N	O	P	0	0	0
			882	421	164	255	42			

- Molecule 8 is a RNA chain called RNA (5'-D(P*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
8	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	J	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

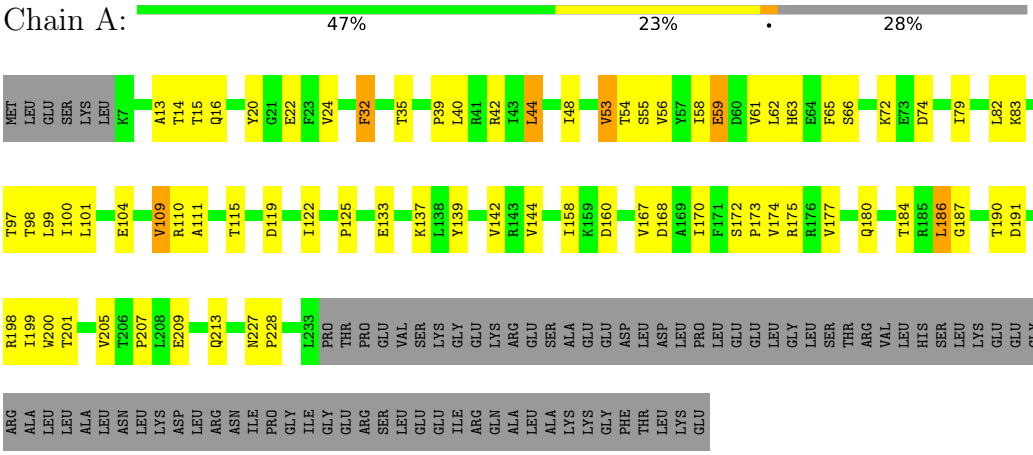
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Mg 1 1	0	0
10	J	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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.

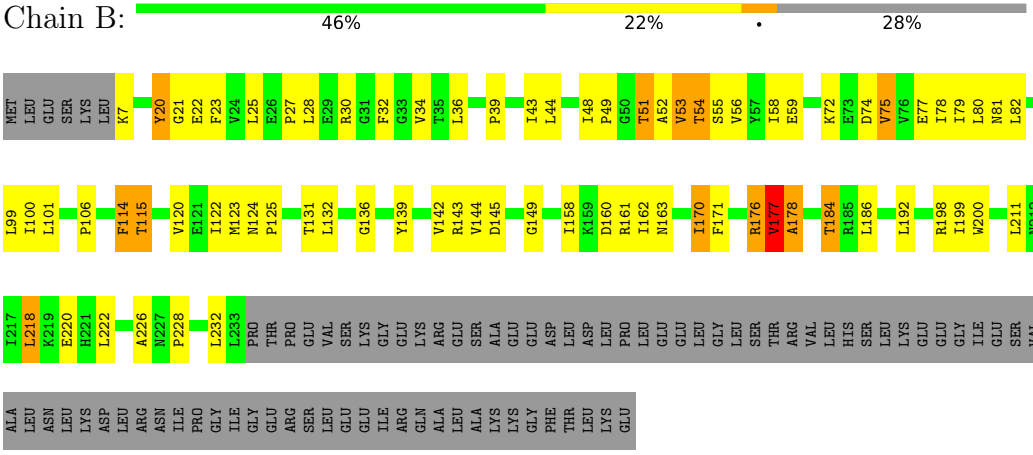
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



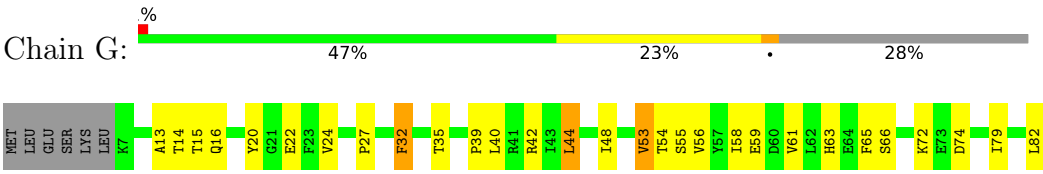
• Molecule 1: DNA-directed RNA polymerase subunit alpha

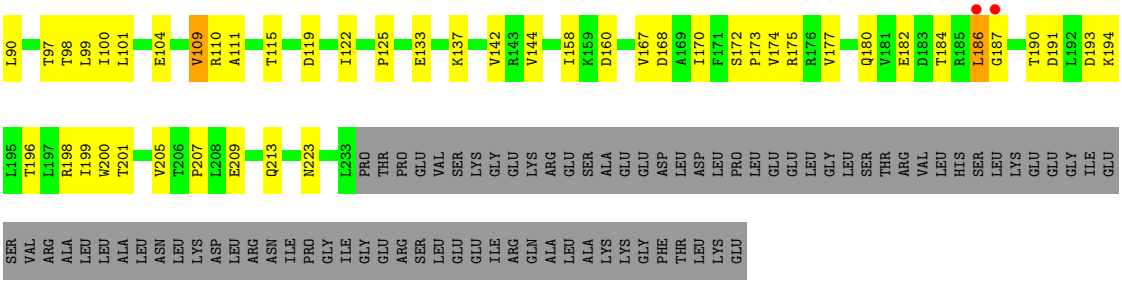
Chain B:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

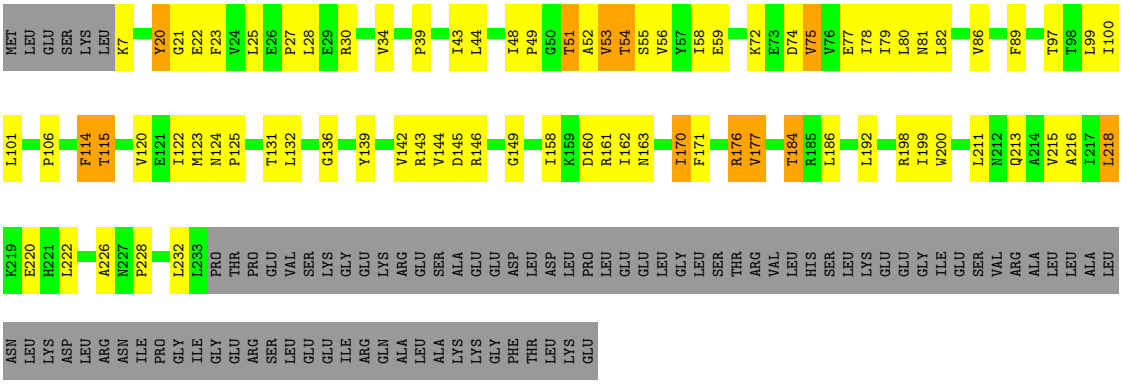
Chain G:





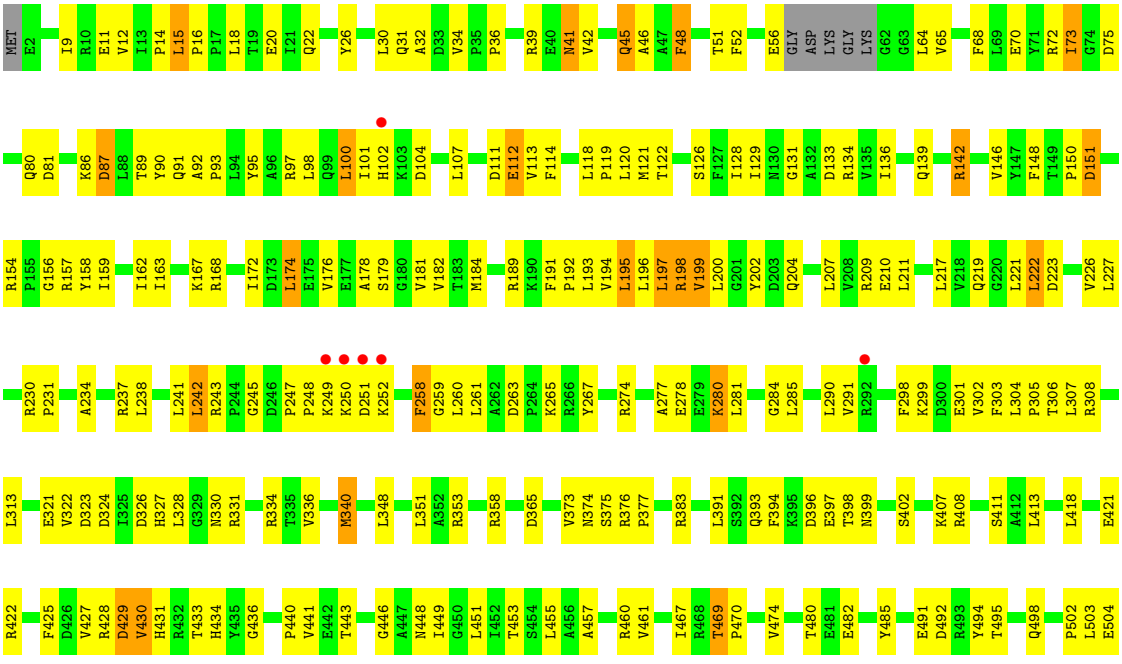
• Molecule 1: DNA-directed RNA polymerase subunit alpha

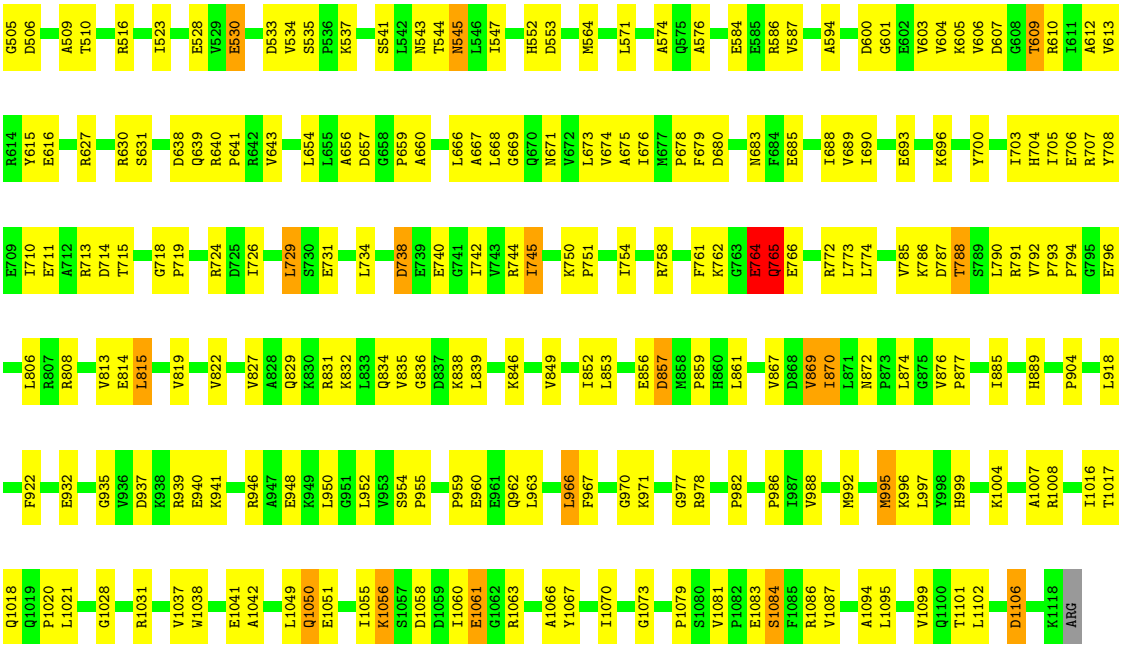
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

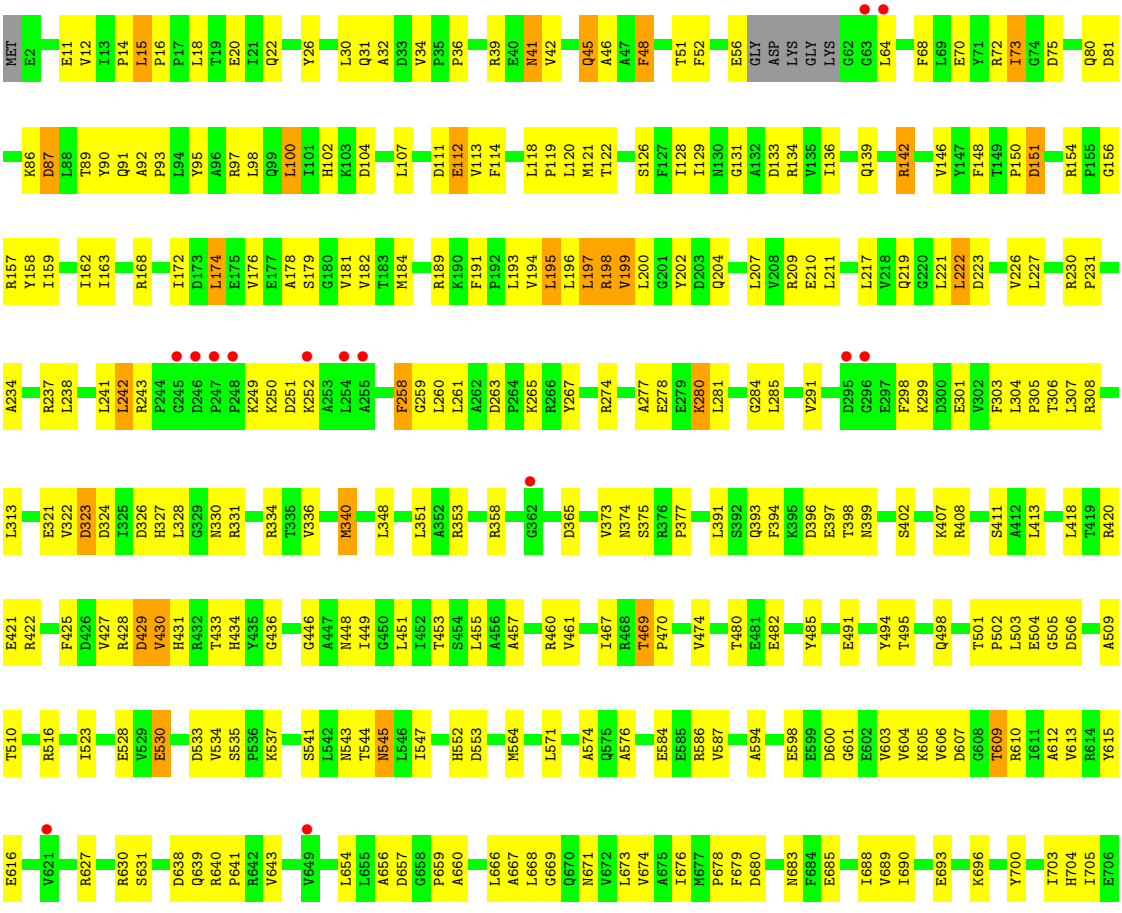
Chain C:

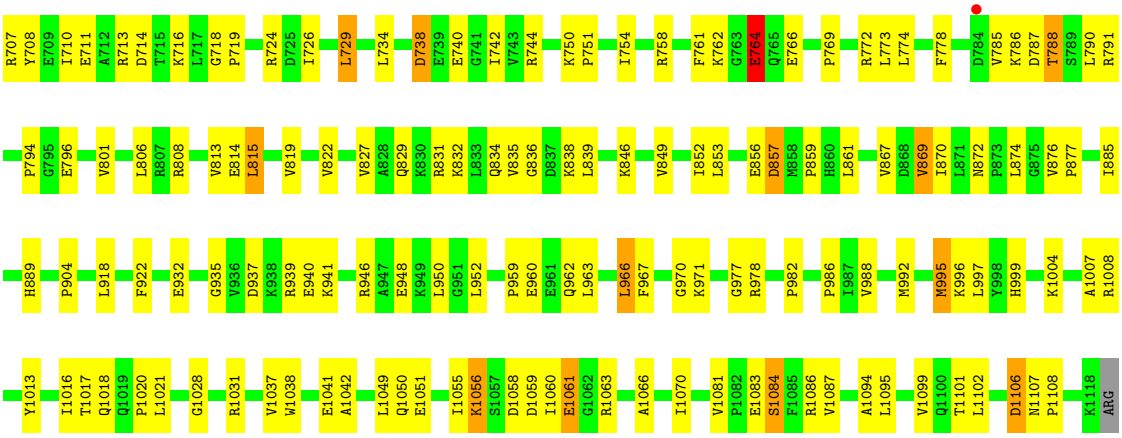




• Molecule 2: DNA-directed RNA polymerase subunit beta

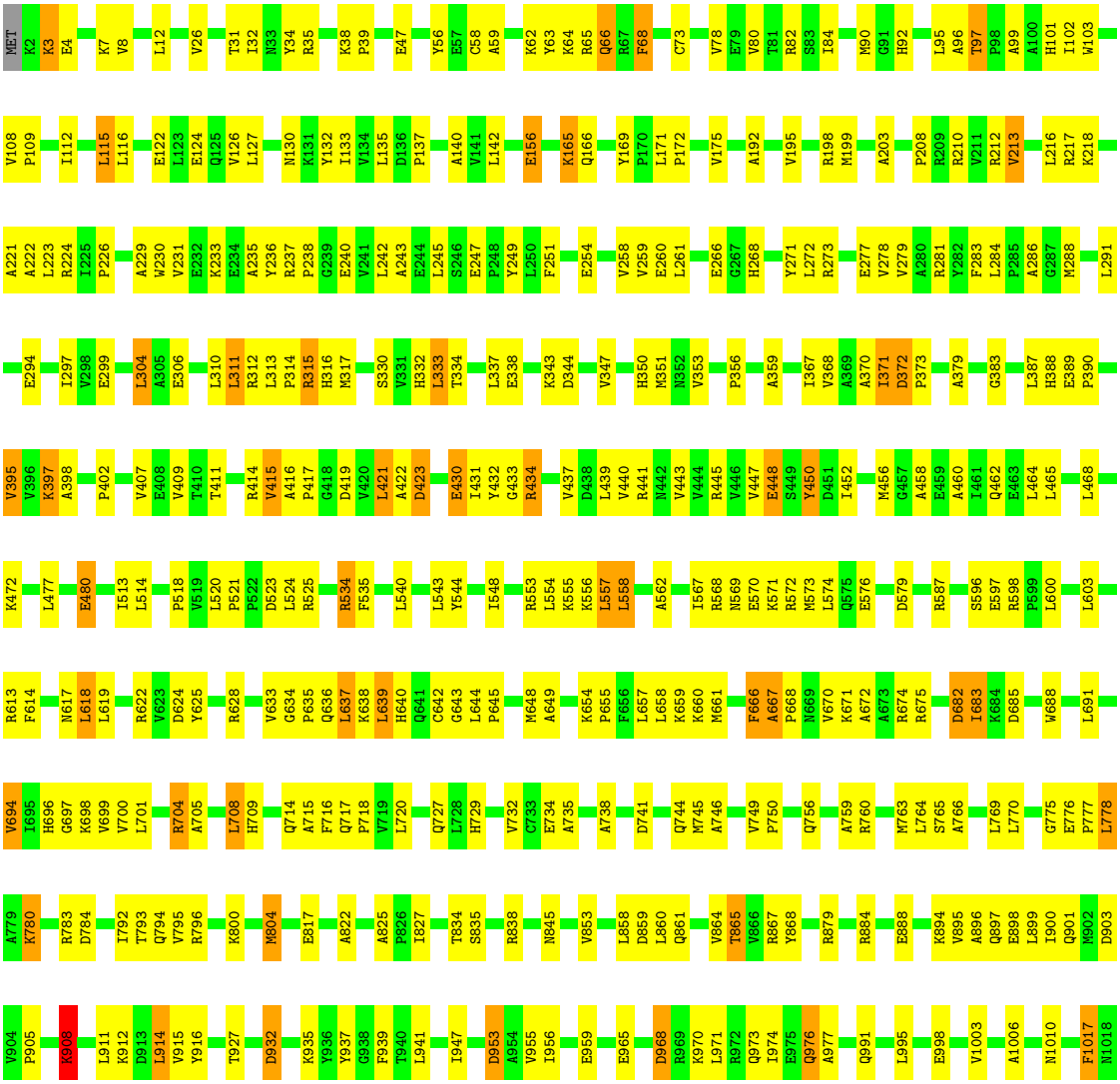
Chain I:

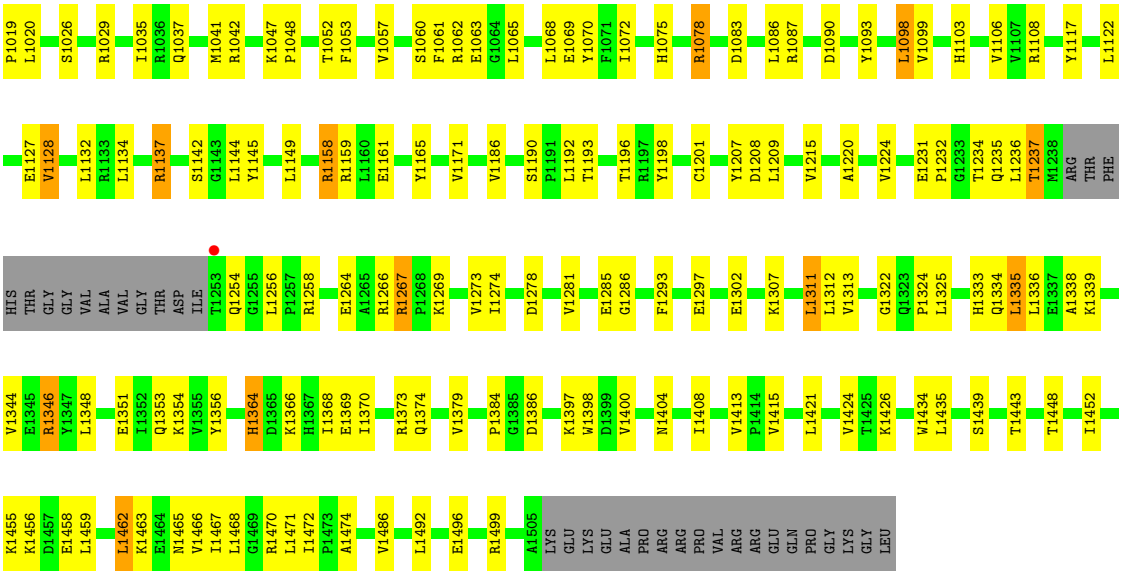




• Molecule 3: DNA-directed RNA polymerase subunit beta'

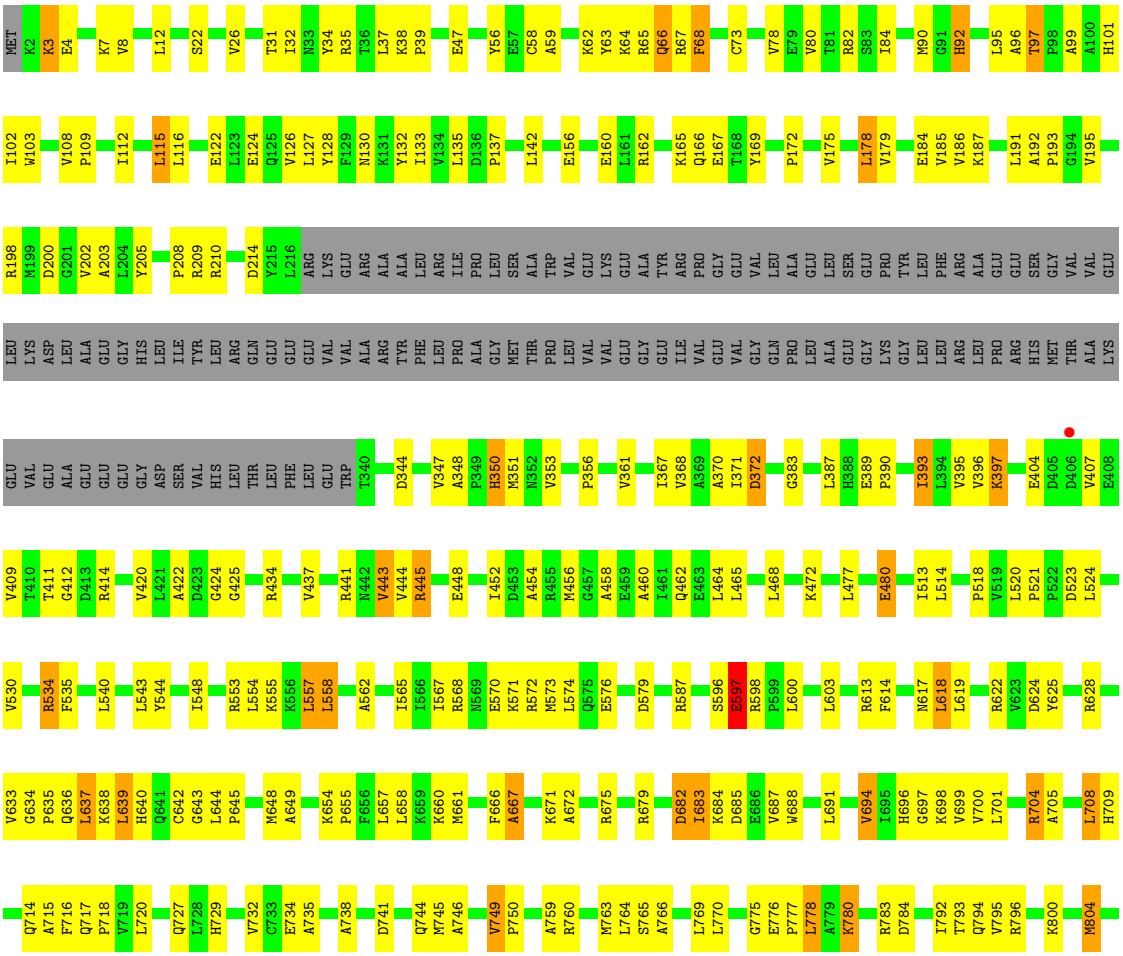
Chain D:

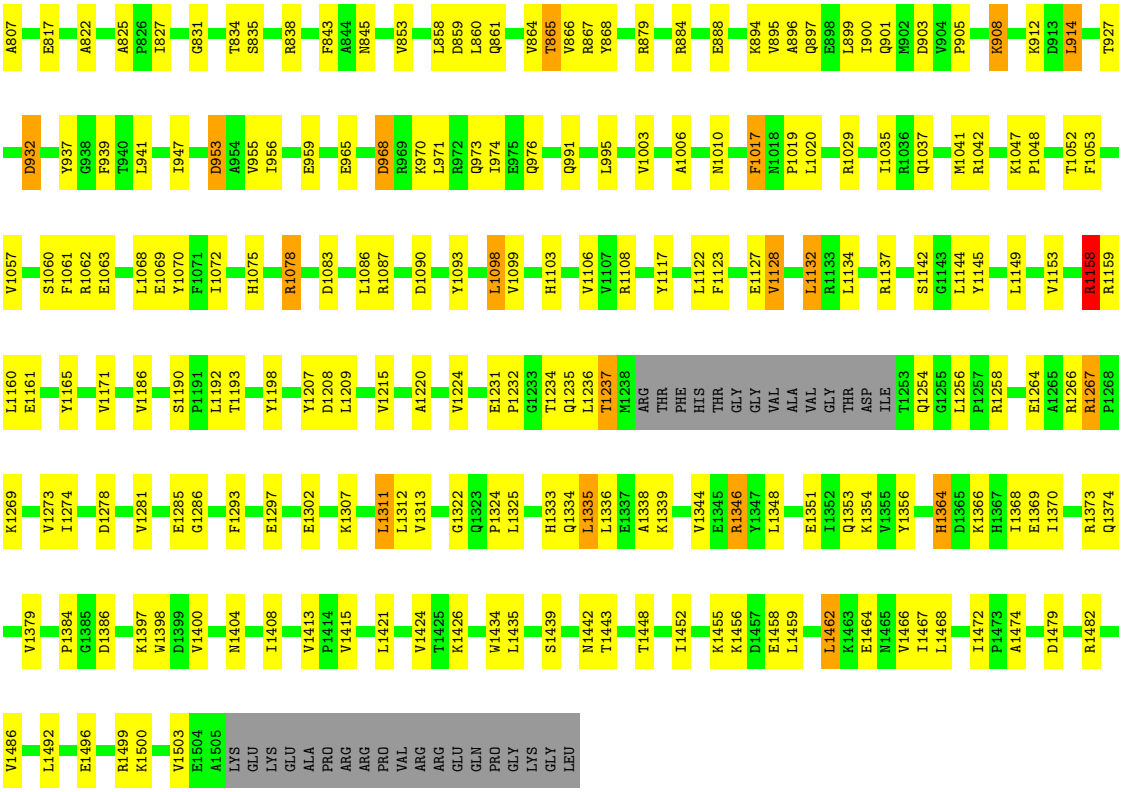




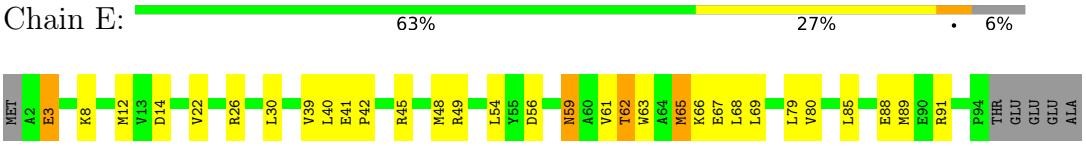
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:

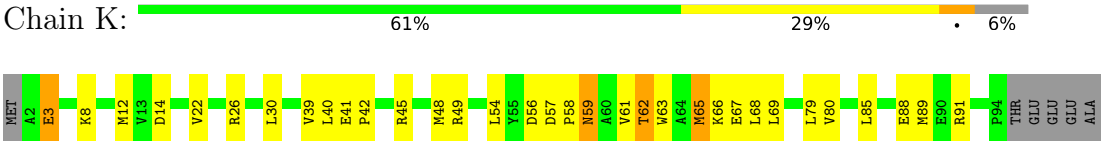




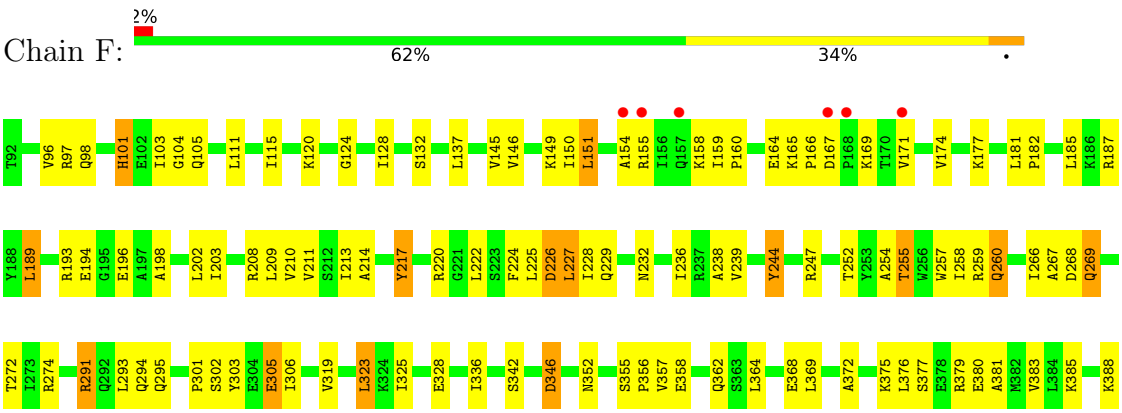
• Molecule 4: DNA-directed RNA polymerase subunit omega

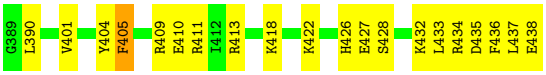


• Molecule 4: DNA-directed RNA polymerase subunit omega

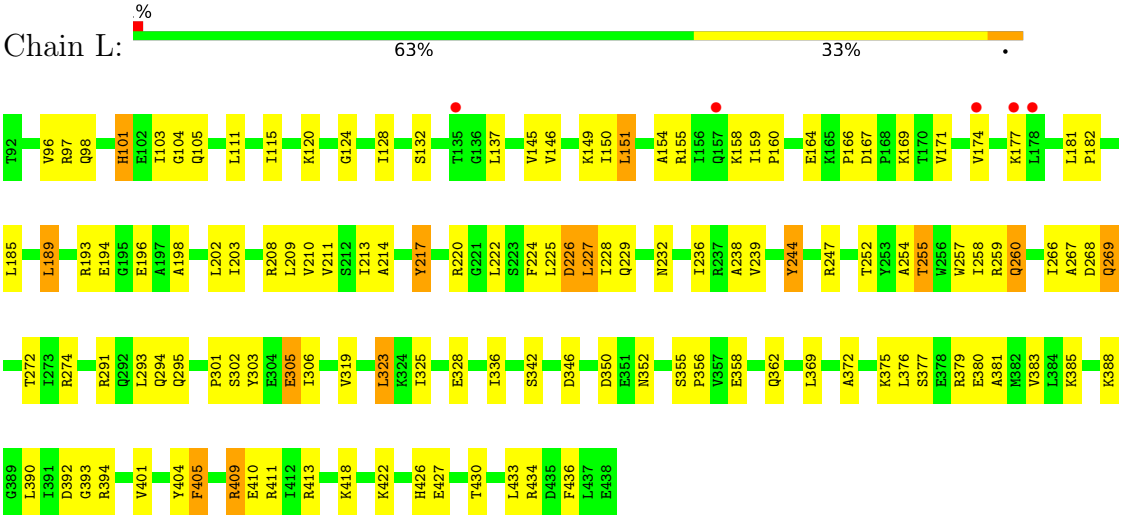


• Molecule 5: RNA polymerase sigma factor SigA

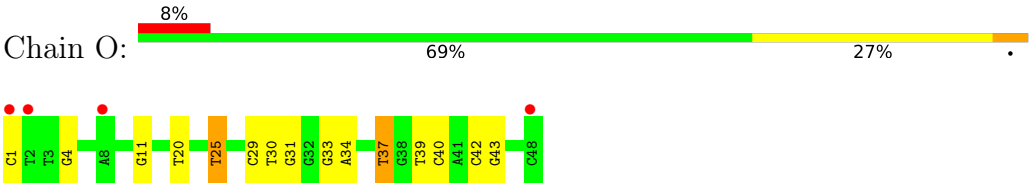




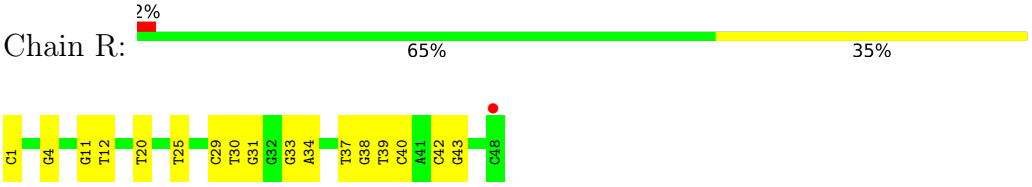
• Molecule 5: RNA polymerase sigma factor SigA



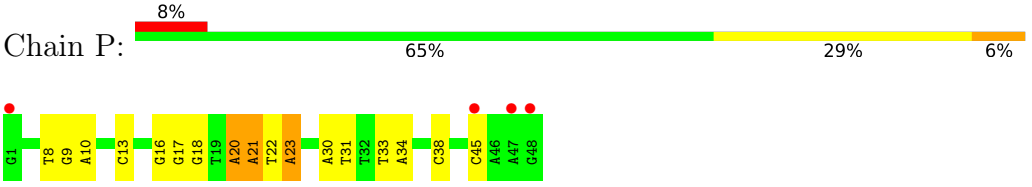
• Molecule 6: DNA (48-MER)



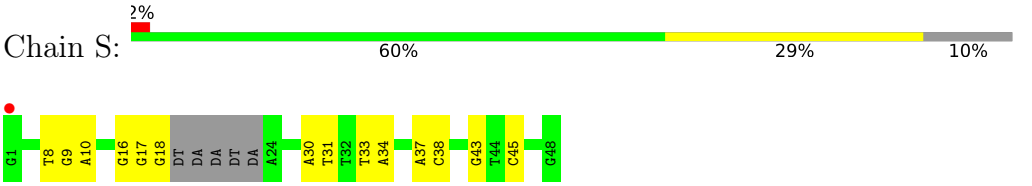
• Molecule 6: DNA (48-MER)



• Molecule 7: DNA (48-MER)



• Molecule 7: DNA (48-MER)



• Molecule 8: RNA (5'-D(P*UP*CP*GP*A)-3')

Chain Q:

• Molecule 8: RNA (5'-D(P*UP*CP*GP*A)-3')

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	289.26Å 289.26Å 536.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 4.00 34.96 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.96-4.00) 99.0 (34.96-4.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.280 , 0.315 0.280 , 0.315	Depositor DCC
R_{free} test set	9497 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	99.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 116.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	58255	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, 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	0.23	0/1804	0.46	0/2455
1	B	0.25	0/1804	0.50	1/2455 (0.0%)
1	G	0.24	0/1804	0.46	0/2455
1	H	0.24	0/1804	0.49	0/2455
2	C	0.25	1/8905 (0.0%)	0.48	3/12040 (0.0%)
2	I	0.26	1/8905 (0.0%)	0.48	2/12040 (0.0%)
3	D	0.24	0/11963	0.48	4/16165 (0.0%)
3	J	0.24	1/10959 (0.0%)	0.47	3/14802 (0.0%)
4	E	0.21	0/783	0.38	0/1054
4	K	0.21	0/783	0.38	0/1054
5	F	0.23	0/2843	0.53	4/3822 (0.1%)
5	L	0.23	0/2843	0.55	4/3822 (0.1%)
6	O	0.44	0/1109	1.07	4/1712 (0.2%)
6	R	0.44	0/1109	1.07	3/1712 (0.2%)
7	P	0.48	0/1106	1.11	5/1706 (0.3%)
7	S	0.44	0/989	1.01	0/1523
8	Q	0.15	0/94	0.67	0/144
8	T	0.16	0/94	0.67	0/144
All	All	0.26	3/59701 (0.0%)	0.55	33/81560 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
2	C	0	2
2	I	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	764	GLU	CD-OE2	8.42	1.34	1.25
2	C	764	GLU	CB-CG	-6.22	1.40	1.52
3	J	597	GLU	CB-CG	5.05	1.61	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	291	ARG	NE-CZ-NH2	-12.83	113.89	120.30
5	L	291	ARG	NE-CZ-NH1	12.47	126.54	120.30
5	F	291	ARG	NE-CZ-NH1	-11.97	114.31	120.30
5	F	291	ARG	NE-CZ-NH2	11.77	126.18	120.30
2	I	764	GLU	C-N-CA	8.19	142.16	121.70
7	P	21	DA	O4'-C1'-N9	7.90	113.53	108.00
6	O	25	DT	C5-C4-O4	-7.00	120.00	124.90
6	R	25	DT	C5-C4-O4	-6.98	120.01	124.90
7	P	23	DA	O4'-C4'-C3'	-6.92	101.73	104.50
1	B	178	ALA	N-CA-C	-6.40	93.72	111.00
5	L	291	ARG	CD-NE-CZ	6.36	132.50	123.60
7	P	23	DA	C1'-O4'-C4'	-6.29	103.81	110.10
3	J	1158	ARG	NE-CZ-NH1	6.16	123.38	120.30
5	L	151	LEU	CA-CB-CG	6.15	129.46	115.30
5	F	151	LEU	CA-CB-CG	6.15	129.44	115.30
6	O	37	DT	C5-C4-O4	-5.96	120.73	124.90
3	D	534	ARG	CB-CG-CD	5.85	126.81	111.60
7	P	23	DA	C4'-C3'-C2'	-5.82	97.87	103.10
2	C	765	GLN	N-CA-C	-5.73	95.52	111.00
2	C	764	GLU	C-N-CA	5.67	135.87	121.70
3	J	534	ARG	CG-CD-NE	-5.66	99.91	111.80
3	D	311	LEU	CA-CB-CG	5.62	128.22	115.30
6	O	37	DT	N3-C4-O4	5.59	123.26	119.90
5	F	291	ARG	CD-NE-CZ	5.58	131.41	123.60
6	R	25	DT	N3-C4-O4	5.49	123.19	119.90
2	C	195	LEU	CA-CB-CG	5.13	127.11	115.30
2	I	195	LEU	CA-CB-CG	5.13	127.10	115.30
3	J	1286	GLY	N-CA-C	-5.11	100.32	113.10
3	D	1286	GLY	N-CA-C	-5.09	100.37	113.10
3	D	908	LYS	CA-CB-CG	5.07	124.54	113.40
7	P	20	DA	O4'-C1'-N9	-5.06	104.46	108.00
6	O	25	DT	N3-C4-O4	5.04	122.93	119.90
6	R	37	DT	C5-C4-O4	-5.02	121.39	124.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	177	VAL	Mainchain,Peptide
2	C	178	ALA	Peptide
2	C	764	GLU	Peptide
2	I	178	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	1799	57	0
1	B	1770	0	1799	55	0
1	G	1770	0	1799	59	0
1	H	1770	0	1799	55	0
2	C	8739	0	8841	295	0
2	I	8739	0	8841	282	0
3	D	11761	0	11976	343	0
3	J	10779	0	10993	314	0
4	E	768	0	784	18	0
4	K	768	0	784	20	0
5	F	2801	0	2881	97	0
5	L	2801	0	2881	87	0
6	O	988	0	544	17	0
6	R	988	0	544	16	0
7	P	985	0	543	17	0
7	S	882	0	487	14	0
8	Q	85	0	43	0	0
8	T	85	0	43	1	0
9	D	2	0	0	0	0
9	J	2	0	0	0	0
10	D	1	0	0	0	0
10	J	1	0	0	0	0
All	All	58255	0	57381	1567	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 14.

All (1567) 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)
1:G:14:THR:HB	1:G:22:GLU:HB2	1.54	0.90
1:A:14:THR:HB	1:A:22:GLU:HB2	1.54	0.89
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.54	0.88
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.56	0.88
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.56	0.85
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.56	0.84
2:I:358:ARG:HH12	2:I:374:ASN:HB2	1.42	0.83
3:J:407:VAL:HG22	3:J:409:VAL:H	1.44	0.83
2:C:358:ARG:HH12	2:C:374:ASN:HB2	1.42	0.82
3:D:1158:ARG:HG3	3:D:1158:ARG:HH11	1.44	0.82
3:J:1267:ARG:H	3:J:1267:ARG:HE	1.25	0.81
3:D:1267:ARG:H	3:D:1267:ARG:HE	1.25	0.81
3:J:1158:ARG:HG3	3:J:1158:ARG:HH11	1.47	0.79
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.66	0.78
1:G:99:LEU:HB2	1:G:142:VAL:HG22	1.64	0.77
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.65	0.77
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.67	0.76
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.66	0.76
3:D:245:LEU:HD12	3:D:311:LEU:HD21	1.67	0.76
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	1.67	0.76
2:I:494:TYR:HB3	2:I:530:GLU:HG3	1.68	0.76
3:J:1047:LYS:HG2	3:J:1048:PRO:HD2	1.67	0.76
3:D:407:VAL:HG22	3:D:409:VAL:H	1.50	0.76
2:C:494:TYR:HB3	2:C:530:GLU:HG3	1.68	0.75
3:D:7:LYS:HE2	3:D:1456:LYS:HD2	1.67	0.75
3:J:7:LYS:HE2	3:J:1456:LYS:HD2	1.67	0.75
2:C:154:ARG:HG2	2:C:156:GLY:H	1.52	0.75
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.67	0.75
7:P:9:DG:H2"	7:P:10:DA:H5'	1.68	0.74
2:C:16:PRO:HB2	2:C:460:ARG:HH21	1.52	0.74
2:I:16:PRO:HB2	2:I:460:ARG:HH21	1.52	0.74
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.67	0.74
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.70	0.74
1:G:42:ARG:HH12	2:I:857:ASP:HB3	1.52	0.74
2:I:710:ILE:HD12	2:I:790:LEU:HB2	1.69	0.73
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.69	0.73
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.71	0.73
1:G:56:VAL:HG13	1:G:142:VAL:HG12	1.70	0.73
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.52	0.73
2:I:154:ARG:HG2	2:I:156:GLY:H	1.52	0.73
7:S:9:DG:H2"	7:S:10:DA:H5'	1.68	0.73
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:397:LYS:HD3	3:J:448:GLU:HB3	1.70	0.72
2:I:971:LYS:HG2	2:I:988:VAL:HG12	1.70	0.72
2:C:971:LYS:HG2	2:C:988:VAL:HG12	1.70	0.72
1:B:186:LEU:HB2	1:B:192:LEU:HD21	1.72	0.72
3:J:82:ARG:HG3	3:J:84:ILE:HG22	1.70	0.72
3:J:1254:GLN:HB3	3:J:1258:ARG:HB2	1.70	0.72
2:I:603:VAL:HA	2:I:613:VAL:HG12	1.72	0.71
3:J:974:ILE:HG12	3:J:991:GLN:HE21	1.55	0.71
1:H:186:LEU:HB2	1:H:192:LEU:HD21	1.72	0.71
2:I:700:TYR:HD2	2:I:996:LYS:HB2	1.56	0.71
3:J:412:GLY:HA2	3:J:434:ARG:HE	1.55	0.71
3:D:371:ILE:HD12	5:F:247:ARG:HD3	1.73	0.71
2:I:704:HIS:HD2	2:I:831:ARG:HD2	1.55	0.71
2:C:603:VAL:HA	2:C:613:VAL:HG12	1.73	0.70
3:D:90:MET:HG2	3:D:521:PRO:HD3	1.72	0.70
2:I:313:LEU:HD13	2:I:321:GLU:HA	1.72	0.70
2:C:376:ARG:NE	7:P:22:DT:OP2	2.23	0.70
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.73	0.70
5:L:104:GLY:HA2	5:L:208:ARG:HH12	1.57	0.70
3:D:974:ILE:HG12	3:D:991:GLN:HE21	1.55	0.70
3:J:90:MET:HG2	3:J:521:PRO:HD3	1.72	0.70
2:C:700:TYR:HD2	2:C:996:LYS:HB2	1.56	0.70
3:D:171:LEU:HD22	3:D:172:PRO:HD2	1.73	0.69
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.73	0.69
1:B:53:VAL:HA	1:B:144:VAL:HA	1.74	0.69
2:C:313:LEU:HD13	2:C:321:GLU:HA	1.72	0.69
5:F:104:GLY:HA2	5:F:208:ARG:HH12	1.57	0.69
1:H:53:VAL:HA	1:H:144:VAL:HA	1.74	0.69
2:I:587:VAL:HG11	2:I:666:LEU:HD22	1.75	0.69
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.75	0.69
5:F:222:LEU:HG	5:F:226:ASP:HB3	1.75	0.69
2:I:874:LEU:HD13	3:J:783:ARG:HB3	1.75	0.69
1:B:59:GLU:HG3	1:B:139:TYR:HB3	1.76	0.68
3:D:415:VAL:HG11	3:D:432:TYR:HA	1.75	0.68
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.75	0.68
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.58	0.68
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.75	0.68
1:H:59:GLU:HG3	1:H:139:TYR:HB3	1.76	0.68
2:I:714:ASP:HA	2:I:719:PRO:HA	1.75	0.67
2:C:714:ASP:HA	2:C:719:PRO:HA	1.75	0.67
2:C:1051:GLU:HG2	2:C:1055:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1008:ARG:HH11	2:I:1028:GLY:HA2	1.58	0.67
2:C:195:LEU:HB2	2:C:226:VAL:HG11	1.76	0.67
3:D:1142:SER:O	3:D:1364:HIS:ND1	2.28	0.67
5:L:222:LEU:HG	5:L:226:ASP:HB3	1.75	0.67
1:B:49:PRO:HD2	1:B:213:GLN:HE22	1.58	0.67
2:C:1083:GLU:O	2:C:1086:ARG:N	2.28	0.67
3:J:1142:SER:O	3:J:1364:HIS:ND1	2.28	0.67
2:I:690:ILE:HG13	2:I:852:ILE:HG23	1.77	0.66
2:C:690:ILE:HG13	2:C:852:ILE:HG23	1.77	0.66
3:D:567:ILE:HG22	3:D:571:LYS:HE3	1.78	0.66
2:I:971:LYS:HB3	2:I:986:PRO:HB2	1.75	0.66
2:I:1051:GLU:HG2	2:I:1055:ILE:HD12	1.76	0.66
2:C:245:GLY:HA3	5:F:97:ARG:HE	1.60	0.66
2:I:195:LEU:HB2	2:I:226:VAL:HG11	1.76	0.66
3:J:367:ILE:HG22	3:J:368:VAL:HG23	1.78	0.66
2:I:1037:VAL:HG13	2:I:1049:LEU:HD11	1.77	0.66
3:J:567:ILE:HG22	3:J:571:LYS:HE3	1.78	0.66
1:H:49:PRO:HD2	1:H:213:GLN:HE22	1.59	0.66
2:I:1083:GLU:O	2:I:1086:ARG:N	2.28	0.66
1:A:184:THR:HB	1:A:194:LYS:HB3	1.77	0.65
3:J:1346:ARG:HH11	3:J:1346:ARG:HB3	1.61	0.65
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.76	0.65
3:D:350:HIS:HB3	3:D:371:ILE:HG22	1.77	0.65
3:D:1144:LEU:HD21	3:D:1186:VAL:HG21	1.78	0.65
3:J:1322:GLY:HA3	3:J:1339:LYS:HG3	1.78	0.65
1:G:56:VAL:HG21	1:G:82:LEU:HD13	1.78	0.65
1:G:184:THR:HB	1:G:194:LYS:HB3	1.77	0.65
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.77	0.65
1:B:72:LYS:HB2	1:B:131:THR:HB	1.77	0.65
3:D:439:LEU:HD11	5:F:187:ARG:HB2	1.77	0.65
3:J:1144:LEU:HD21	3:J:1186:VAL:HG21	1.79	0.65
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.77	0.65
2:C:754:ILE:HG13	2:C:791:ARG:HG2	1.79	0.64
2:C:1018:GLN:HG2	2:C:1083:GLU:HG2	1.80	0.64
3:J:208:PRO:HA	3:J:390:PRO:HA	1.78	0.64
7:S:8:DT:H2"	7:S:9:DG:H5"	1.78	0.64
2:C:874:LEU:O	3:D:1029:ARG:HG2	1.98	0.64
3:D:59:ALA:H	3:D:78:VAL:HG11	1.63	0.64
1:H:72:LYS:HB2	1:H:131:THR:HB	1.77	0.64
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.79	0.64
3:J:209:ARG:HA	3:J:347:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:838:LYS:HB3	2:I:997:LEU:HB2	1.79	0.64
2:I:1031:ARG:HA	3:J:622:ARG:HA	1.79	0.64
1:A:53:VAL:HG22	1:A:54:THR:H	1.63	0.64
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.78	0.64
3:D:34:TYR:OH	6:O:20:DT:OP2	2.14	0.64
3:D:273:ARG:HA	3:D:278:VAL:HA	1.80	0.64
3:D:1322:GLY:HA3	3:D:1339:LYS:HG3	1.78	0.64
3:J:169:TYR:HB2	3:J:393:ILE:HD12	1.79	0.64
2:I:778:PHE:HZ	5:L:434:ARG:HA	1.62	0.64
7:P:8:DT:H2"	7:P:9:DG:H5"	1.78	0.63
2:I:754:ILE:HG13	2:I:791:ARG:HG2	1.79	0.63
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.80	0.63
1:H:34:VAL:HG11	2:I:978:ARG:HB3	1.80	0.63
3:J:39:PRO:HG2	3:J:47:GLU:HG3	1.81	0.63
2:I:584:GLU:HB3	2:I:666:LEU:H	1.63	0.63
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.81	0.63
5:F:182:PRO:HD2	5:F:185:LEU:HD12	1.80	0.63
3:J:102:ILE:HD12	3:J:579:ASP:HB3	1.80	0.63
2:C:838:LYS:HB3	2:C:997:LEU:HB2	1.79	0.63
3:D:229:ALA:HB1	3:D:245:LEU:H	1.64	0.63
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.81	0.63
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.79	0.63
3:J:59:ALA:H	3:J:78:VAL:HG11	1.63	0.63
2:C:278:GLU:HG3	2:C:284:GLY:HA2	1.81	0.62
1:H:52:ALA:HB2	1:H:170:ILE:O	1.99	0.62
2:I:278:GLU:HG3	2:I:284:GLY:HA2	1.81	0.62
2:C:552:HIS:ND1	3:D:1061:PHE:O	2.32	0.62
2:I:552:HIS:ND1	3:J:1061:PHE:O	2.32	0.62
3:J:637:LEU:HD21	3:J:642:CYS:HA	1.81	0.62
3:D:39:PRO:HG2	3:D:47:GLU:HG3	1.81	0.62
1:G:53:VAL:HG22	1:G:54:THR:H	1.63	0.62
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.81	0.62
2:C:198:ARG:HG3	2:C:234:ALA:HB3	1.82	0.62
2:C:584:GLU:HB3	2:C:666:LEU:H	1.63	0.62
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.79	0.62
2:I:758:ARG:HG2	2:I:788:THR:HB	1.82	0.62
1:B:34:VAL:HG11	2:C:978:ARG:HB3	1.81	0.62
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.81	0.62
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.82	0.61
3:D:133:ILE:HD11	3:D:460:ALA:HB1	1.82	0.61
3:J:178:LEU:N	3:J:191:LEU:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ALA:HB2	1:B:170:ILE:O	2.00	0.61
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.36	0.61
1:A:48:ILE:HG23	1:A:213:GLN:HE21	1.65	0.61
3:J:162:ARG:HG3	3:J:414:ARG:HH22	1.64	0.61
5:L:182:PRO:HD2	5:L:185:LEU:HD12	1.80	0.61
3:D:411:THR:HG22	3:D:437:VAL:H	1.65	0.61
3:J:137:PRO:HA	3:J:452:ILE:HG13	1.82	0.61
3:J:133:ILE:HD11	3:J:460:ALA:HB1	1.82	0.61
2:I:72:ARG:HB3	2:I:95:TYR:HB2	1.82	0.61
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.82	0.61
2:C:174:LEU:HD13	2:C:193:LEU:HD21	1.83	0.61
3:D:759:ALA:HA	3:D:763:MET:HB3	1.83	0.61
1:G:205:VAL:HG13	1:G:209:GLU:HB2	1.82	0.61
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.81	0.61
1:H:177:VAL:HG12	1:H:199:ILE:HG12	1.81	0.61
5:L:137:LEU:HD11	5:L:177:LYS:HE3	1.83	0.61
2:I:461:VAL:HG22	2:I:467:ILE:HG12	1.83	0.61
3:J:759:ALA:HA	3:J:763:MET:HB3	1.83	0.61
2:C:72:ARG:HB3	2:C:95:TYR:HB2	1.82	0.60
2:C:758:ARG:HG2	2:C:788:THR:HB	1.82	0.60
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.82	0.60
2:I:1018:GLN:HG2	2:I:1083:GLU:HG2	1.83	0.60
1:A:205:VAL:HG13	1:A:209:GLU:HB2	1.82	0.60
3:D:213:VAL:HG12	3:D:343:LYS:HB3	1.83	0.60
3:J:908:LYS:HE3	3:J:908:LYS:O	2.00	0.60
2:C:86:LYS:HE2	2:C:813:VAL:HG23	1.82	0.60
2:C:134:ARG:NH2	7:P:18:DG:OP2	2.33	0.60
2:C:461:VAL:HG22	2:C:467:ILE:HG12	1.83	0.60
2:I:199:VAL:HA	2:I:231:PRO:HB3	1.82	0.60
3:J:1158:ARG:HH11	3:J:1158:ARG:CG	2.12	0.60
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.82	0.60
2:I:198:ARG:HG3	2:I:234:ALA:HB3	1.82	0.60
3:J:619:LEU:HD11	3:J:1439:SER:HB2	1.82	0.60
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.84	0.60
2:I:128:ILE:HA	2:I:133:ASP:HA	1.83	0.60
2:I:174:LEU:HD13	2:I:193:LEU:HD21	1.83	0.60
1:H:100:ILE:HG23	1:H:139:TYR:HE1	1.67	0.60
2:I:1063:ARG:HG3	5:L:356:PRO:HG3	1.83	0.60
3:J:184:GLU:HG2	3:J:202:VAL:HG22	1.82	0.60
3:D:557:LEU:HD12	3:D:567:ILE:HD13	1.82	0.60
2:I:64:LEU:HD11	2:I:100:LEU:HG	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:630:ARG:HG3	2:I:705:ILE:HB	1.83	0.60
3:D:1236:LEU:HD13	3:D:1256:LEU:HB2	1.83	0.60
7:P:30:DA:H2"	7:P:31:DT:H5"	1.83	0.60
3:J:521:PRO:HD2	3:J:524:LEU:HD12	1.84	0.60
3:J:1274:ILE:HD11	3:J:1334:GLN:HB3	1.83	0.60
1:B:100:ILE:HG23	1:B:139:TYR:HE1	1.67	0.59
1:G:48:ILE:HG23	1:G:213:GLN:HE21	1.66	0.59
3:J:557:LEU:HD12	3:J:567:ILE:HD13	1.82	0.59
3:J:657:LEU:HD22	3:J:691:LEU:HD13	1.84	0.59
3:D:698:LYS:HG3	4:E:59:ASN:HD21	1.68	0.59
3:D:908:LYS:HE3	3:D:908:LYS:O	2.02	0.59
7:S:30:DA:H2"	7:S:31:DT:H5"	1.83	0.59
2:C:274:ARG:HG3	2:C:285:LEU:HD23	1.84	0.59
3:D:398:ALA:HB2	3:D:447:VAL:HG12	1.85	0.59
2:I:274:ARG:HG3	2:I:285:LEU:HD23	1.84	0.59
2:I:304:LEU:HB3	2:I:305:PRO:HD3	1.84	0.59
2:I:948:GLU:OE2	2:I:962:GLN:NE2	2.35	0.59
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.84	0.59
3:J:734:GLU:OE2	3:J:780:LYS:NZ	2.28	0.59
1:B:177:VAL:HG12	1:B:199:ILE:HG12	1.84	0.59
3:D:657:LEU:HD22	3:D:691:LEU:HD13	1.85	0.59
5:F:137:LEU:HD11	5:F:177:LYS:HE3	1.83	0.59
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.84	0.59
2:C:674:VAL:HA	2:C:869:VAL:HG13	1.85	0.59
2:C:772:ARG:HG2	5:F:388:LYS:HD2	1.84	0.59
2:C:774:LEU:HD23	5:F:369:LEU:HD21	1.85	0.59
3:D:208:PRO:HA	3:D:390:PRO:HA	1.84	0.59
3:D:521:PRO:HD2	3:D:524:LEU:HD12	1.84	0.59
3:D:1108:ARG:NH1	3:D:1198:TYR:O	2.36	0.59
2:I:674:VAL:HA	2:I:869:VAL:HG13	1.85	0.59
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.84	0.59
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.84	0.59
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.84	0.59
2:I:32:ALA:HB1	2:I:73:ILE:HD13	1.85	0.59
2:I:142:ARG:HA	2:I:331:ARG:HA	1.84	0.59
2:C:839:LEU:HD23	2:C:996:LYS:HA	1.85	0.59
3:J:530:VAL:HG22	3:J:534:ARG:HB2	1.83	0.59
3:J:716:PHE:HZ	3:J:732:VAL:HG21	1.68	0.59
2:C:32:ALA:HB1	2:C:73:ILE:HD13	1.85	0.59
2:I:134:ARG:NH2	7:S:18:DG:OP2	2.36	0.58
2:I:839:LEU:HD23	2:I:996:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1236:LEU:HD13	3:J:1256:LEU:HB2	1.83	0.58
1:A:16:GLN:HB3	1:A:20:TYR:HB3	1.85	0.58
2:C:64:LEU:HD11	2:C:100:LEU:HG	1.84	0.58
1:H:51:THR:OG1	1:H:52:ALA:N	2.36	0.58
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.84	0.58
5:F:181:LEU:HD23	5:F:185:LEU:HB3	1.85	0.58
1:G:198:ARG:HH22	2:I:932:GLU:HB3	1.68	0.58
3:J:698:LYS:HG3	4:K:59:ASN:HD21	1.67	0.58
3:J:1459:LEU:HD21	3:J:1468:LEU:HG	1.84	0.58
2:C:142:ARG:HA	2:C:331:ARG:HA	1.86	0.58
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.84	0.58
2:C:128:ILE:HA	2:C:133:ASP:HA	1.86	0.58
2:C:786:LYS:NZ	5:F:438:GLU:OE1	2.36	0.58
2:I:774:LEU:HD23	5:L:369:LEU:HD21	1.85	0.58
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.85	0.58
3:J:1108:ARG:NH1	3:J:1198:TYR:O	2.37	0.58
3:D:716:PHE:HZ	3:D:732:VAL:HG21	1.69	0.58
3:J:1267:ARG:HH22	6:R:42:DC:H3'	1.69	0.58
3:D:434:ARG:HG2	3:D:447:VAL:HG22	1.86	0.58
3:D:1267:ARG:HH22	6:O:42:DC:H3'	1.68	0.58
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.39	0.58
6:O:11:DG:N2	7:P:38:DC:O2	2.36	0.58
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.86	0.58
2:I:230:ARG:HB3	2:I:231:PRO:HD2	1.86	0.58
2:I:772:ARG:HG2	5:L:388:LYS:HD2	1.84	0.58
3:J:640:HIS:O	3:J:717:GLN:N	2.32	0.58
5:L:209:LEU:HD21	5:L:255:THR:HG23	1.85	0.58
2:C:162:ILE:HD11	2:C:306:THR:HG21	1.84	0.58
2:I:162:ILE:HD11	2:I:306:THR:HG21	1.84	0.58
5:L:302:SER:H	5:L:305:GLU:HG3	1.68	0.58
2:C:576:ALA:O	2:C:671:ASN:ND2	2.37	0.57
5:F:189:LEU:HD11	5:F:193:ARG:HH21	1.69	0.57
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.86	0.57
5:L:189:LEU:HD11	5:L:193:ARG:HH21	1.68	0.57
5:L:181:LEU:HD23	5:L:185:LEU:HB3	1.85	0.57
1:A:198:ARG:HH22	2:C:932:GLU:HB3	1.68	0.57
2:C:230:ARG:HB3	2:C:231:PRO:HD2	1.86	0.57
5:F:209:LEU:HD21	5:F:255:THR:HG23	1.85	0.57
3:J:210:ARG:HH11	3:J:389:GLU:HG3	1.69	0.57
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.86	0.57
2:C:948:GLU:OE2	2:C:962:GLN:NE2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1158:ARG:HH11	3:D:1158:ARG:CG	2.15	0.57
1:G:16:GLN:HB3	1:G:20:TYR:HB3	1.85	0.57
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.86	0.57
3:J:462:GLN:HB2	3:J:513:ILE:HG21	1.86	0.57
3:J:1158:ARG:HG3	3:J:1158:ARG:NH1	2.19	0.57
2:C:41:ASN:HA	2:C:45:GLN:HB3	1.86	0.57
2:C:281:LEU:O	2:C:308:ARG:NH2	2.38	0.57
2:I:128:ILE:HG13	2:I:133:ASP:HB3	1.86	0.57
2:I:195:LEU:HD12	2:I:198:ARG:HE	1.69	0.57
3:J:205:TYR:HA	3:J:393:ILE:HG22	1.87	0.57
6:R:11:DG:N2	7:S:38:DC:O2	2.36	0.57
2:I:14:PRO:HB3	2:I:586:ARG:HH22	1.70	0.56
2:I:668:LEU:HB3	2:I:995:MET:HG2	1.87	0.56
1:B:51:THR:OG1	1:B:52:ALA:N	2.36	0.56
2:C:353:ARG:NH1	6:O:34:DA:OP1	2.36	0.56
2:C:704:HIS:HD2	2:C:831:ARG:HD2	1.70	0.56
3:D:853:VAL:HG22	3:D:858:LEU:HB3	1.88	0.56
5:F:302:SER:H	5:F:305:GLU:HG3	1.69	0.56
2:I:126:SER:HB3	2:I:407:LYS:HZ1	1.69	0.56
2:I:249:LYS:HD3	2:I:250:LYS:H	1.71	0.56
3:D:1459:LEU:HD21	3:D:1468:LEU:HG	1.86	0.56
2:I:51:THR:HG21	2:I:348:LEU:HB3	1.88	0.56
2:I:281:LEU:O	2:I:308:ARG:NH2	2.38	0.56
3:J:407:VAL:HG23	3:J:422:ALA:HB2	1.87	0.56
2:C:197:LEU:HB3	2:C:202:TYR:HD2	1.70	0.56
2:I:41:ASN:HA	2:I:45:GLN:HB3	1.86	0.56
2:I:197:LEU:HB3	2:I:202:TYR:HD2	1.70	0.56
2:I:353:ARG:NH1	6:R:34:DA:OP1	2.36	0.56
3:J:65:ARG:HG3	3:J:66:GLN:H	1.70	0.56
2:I:576:ALA:O	2:I:671:ASN:ND2	2.37	0.56
1:H:53:VAL:HB	1:H:144:VAL:HG22	1.88	0.56
3:J:1273:VAL:HG23	3:J:1325:LEU:HB2	1.88	0.56
2:C:195:LEU:HD12	2:C:198:ARG:HE	1.69	0.56
3:D:1127:GLU:HG3	3:D:1128:VAL:HG23	1.88	0.56
3:D:1264:GLU:HB3	3:D:1266:ARG:HG3	1.88	0.56
3:J:613:ARG:NH1	3:J:617:ASN:OD1	2.36	0.56
3:J:1190:SER:OG	3:J:1369:GLU:OE1	2.22	0.56
1:A:62:LEU:HD13	2:C:745:ILE:HB	1.88	0.56
1:B:53:VAL:HB	1:B:144:VAL:HG22	1.88	0.56
2:C:249:LYS:HD3	2:C:250:LYS:H	1.71	0.56
3:D:879:ARG:HH12	3:D:905:PRO:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.88	0.56
1:G:58:ILE:HB	1:G:61:VAL:HB	1.88	0.56
3:J:12:LEU:HD21	3:J:1452:ILE:HA	1.88	0.56
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.88	0.56
3:J:1267:ARG:H	3:J:1267:ARG:NE	2.02	0.56
3:D:12:LEU:HD21	3:D:1452:ILE:HA	1.88	0.55
3:J:160:GLU:HG3	3:J:165:LYS:HB2	1.88	0.55
2:C:15:LEU:O	2:C:586:ARG:NH1	2.40	0.55
3:D:1003:VAL:HG21	3:D:1041:MET:HG2	1.89	0.55
2:I:941:LYS:HE2	2:I:959:PRO:HG2	1.88	0.55
3:J:1003:VAL:HG21	3:J:1041:MET:HG2	1.89	0.55
2:C:668:LEU:HB3	2:C:995:MET:HG2	1.87	0.55
1:H:56:VAL:HG21	1:H:82:LEU:HD13	1.89	0.55
3:J:853:VAL:HG22	3:J:858:LEU:HB3	1.88	0.55
3:J:879:ARG:HH12	3:J:905:PRO:HA	1.71	0.55
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.88	0.55
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	1.88	0.55
2:C:693:GLU:HA	2:C:696:LYS:HE2	1.89	0.55
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.88	0.55
2:C:383:ARG:CZ	7:P:20:DA:H2"	2.37	0.55
2:C:941:LYS:HE2	2:C:959:PRO:HG2	1.88	0.55
2:I:15:LEU:O	2:I:586:ARG:NH1	2.40	0.55
2:I:204:GLN:HA	2:I:227:LEU:HD22	1.88	0.55
2:C:1060:ILE:HG13	2:C:1061:GLU:H	1.72	0.55
3:D:613:ARG:NH1	3:D:617:ASN:OD1	2.36	0.55
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.88	0.55
5:L:120:LYS:HD2	5:L:194:GLU:HG2	1.89	0.55
2:C:204:GLN:HA	2:C:227:LEU:HD22	1.88	0.55
3:D:97:THR:HG22	3:D:554:LEU:HD21	1.89	0.55
3:J:172:PRO:HG2	3:J:175:VAL:HB	1.89	0.55
3:J:908:LYS:HE3	3:J:908:LYS:C	2.27	0.55
3:J:1264:GLU:HB3	3:J:1266:ARG:HG3	1.88	0.55
2:C:408:ARG:NH1	2:C:455:LEU:O	2.40	0.55
3:J:3:LYS:HE3	3:J:4:GLU:H	1.71	0.55
3:J:1208:ASP:HB2	3:J:1215:VAL:HA	1.89	0.55
2:C:601:GLY:HA2	2:C:615:TYR:HA	1.89	0.54
3:D:3:LYS:HE3	3:D:4:GLU:H	1.71	0.54
5:F:252:THR:HG23	6:O:29:DC:H41	1.72	0.54
2:I:504:GLU:HB3	2:I:509:ALA:HB2	1.89	0.54
2:I:693:GLU:HA	2:I:696:LYS:HE2	1.89	0.54
2:I:762:LYS:HD3	2:I:786:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:7:LYS:CE	3:J:1456:LYS:HD2	2.35	0.54
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.88	0.54
5:F:120:LYS:HD2	5:F:194:GLU:HG2	1.89	0.54
2:I:209:ARG:HG3	2:I:210:GLU:H	1.71	0.54
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.89	0.54
2:C:1021:LEU:O	2:C:1028:GLY:HA3	2.07	0.54
3:D:1346:ARG:HH11	3:D:1346:ARG:HB3	1.72	0.54
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.88	0.54
3:J:97:THR:HG22	3:J:554:LEU:HD21	1.89	0.54
3:J:1127:GLU:HG3	3:J:1128:VAL:HG23	1.88	0.54
1:A:58:ILE:HB	1:A:61:VAL:HB	1.88	0.54
2:C:51:THR:HG21	2:C:348:LEU:HB3	1.88	0.54
2:I:601:GLY:HA2	2:I:615:TYR:HA	1.89	0.54
2:C:14:PRO:HB3	2:C:586:ARG:HH22	1.71	0.54
2:C:724:ARG:HG2	2:C:734:LEU:HD23	1.89	0.54
3:J:1486:VAL:HG11	4:K:26:ARG:HB2	1.88	0.54
2:C:126:SER:HB3	2:C:407:LYS:HZ1	1.73	0.54
2:C:209:ARG:HG3	2:C:210:GLU:H	1.72	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.90	0.54
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.89	0.54
5:F:411:ARG:NE	6:O:1:DC:H5'	2.22	0.54
2:I:277:ALA:HA	2:I:280:LYS:HG2	1.90	0.54
3:J:96:ALA:HB2	3:J:555:LYS:HG2	1.89	0.54
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.89	0.54
1:G:79:ILE:HA	1:G:82:LEU:HD12	1.90	0.54
2:I:724:ARG:HG2	2:I:734:LEU:HD23	1.89	0.54
3:J:1333:HIS:NE2	3:J:1421:LEU:O	2.40	0.54
4:K:40:LEU:HD21	4:K:67:GLU:HA	1.88	0.54
3:D:313:LEU:HG	3:D:314:PRO:HD2	1.88	0.54
3:D:553:ARG:NH2	5:F:226:ASP:OD1	2.36	0.54
2:I:836:GLY:H	2:I:849:VAL:HB	1.73	0.54
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.42	0.54
2:I:52:PHE:CG	2:I:68:PHE:HB2	2.42	0.54
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.89	0.54
3:J:777:PRO:O	3:J:912:LYS:NZ	2.40	0.54
5:L:379:ARG:NH2	5:L:411:ARG:HH21	2.06	0.54
3:D:1333:HIS:NE2	3:D:1421:LEU:O	2.40	0.53
2:I:408:ARG:NH1	2:I:455:LEU:O	2.40	0.53
2:I:1060:ILE:HG13	2:I:1061:GLU:H	1.72	0.53
3:J:169:TYR:HE1	3:J:198:ARG:HD3	1.73	0.53
4:K:41:GLU:O	4:K:45:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HA	1:A:82:LEU:HD12	1.90	0.53
2:C:277:ALA:HA	2:C:280:LYS:HG2	1.90	0.53
3:D:777:PRO:O	3:D:912:LYS:NZ	2.40	0.53
3:D:792:ILE:HG21	3:D:941:LEU:HD22	1.90	0.53
4:K:14:ASP:OD1	4:K:14:ASP:N	2.40	0.53
2:C:504:GLU:HB3	2:C:509:ALA:HB2	1.89	0.53
3:D:777:PRO:HB2	3:D:912:LYS:HE2	1.89	0.53
1:G:174:VAL:HA	1:G:201:THR:HG22	1.91	0.53
2:I:713:ARG:HA	2:I:819:VAL:HA	1.90	0.53
2:I:1021:LEU:O	2:I:1028:GLY:HA3	2.07	0.53
3:J:97:THR:HG21	3:J:571:LYS:HG2	1.90	0.53
5:L:238:ALA:HB1	5:L:254:ALA:HA	1.90	0.53
1:A:111:ALA:HB3	1:A:125:PRO:HA	1.89	0.53
2:C:836:GLY:H	2:C:849:VAL:HB	1.72	0.53
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.89	0.53
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.21	0.53
1:G:111:ALA:HB3	1:G:125:PRO:HA	1.89	0.53
3:J:770:LEU:HA	3:J:777:PRO:HA	1.91	0.53
3:J:777:PRO:HB2	3:J:912:LYS:HE2	1.89	0.53
5:L:101:HIS:CD2	6:R:31:DG:H22	2.27	0.53
2:C:91:GLN:HA	2:C:119:PRO:HA	1.91	0.53
3:D:7:LYS:CE	3:D:1456:LYS:HD2	2.37	0.53
3:D:242:LEU:HB3	3:D:312:ARG:HA	1.89	0.53
2:I:194:VAL:HG11	2:I:223:ASP:HB3	1.91	0.53
3:J:562:ALA:HB3	3:J:567:ILE:HD11	1.91	0.53
5:L:410:GLU:OE2	5:L:413:ARG:NH1	2.42	0.53
3:D:562:ALA:HB3	3:D:567:ILE:HD11	1.91	0.53
3:D:770:LEU:HA	3:D:777:PRO:HA	1.91	0.53
5:F:238:ALA:HB1	5:F:254:ALA:HA	1.90	0.53
5:F:257:TRP:O	5:F:260:GLN:HG3	2.09	0.53
2:I:91:GLN:HA	2:I:119:PRO:HA	1.91	0.53
2:I:761:PHE:HA	2:I:785:VAL:HA	1.90	0.53
1:A:53:VAL:HA	1:A:144:VAL:HG22	1.90	0.53
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.90	0.53
4:E:41:GLU:O	4:E:45:ARG:HG2	2.09	0.53
2:I:146:VAL:HG12	2:I:162:ILE:HG12	1.90	0.53
2:I:154:ARG:HG2	2:I:156:GLY:N	2.23	0.53
3:J:441:ARG:HB3	3:J:443:VAL:HG12	1.90	0.53
3:D:1078:ARG:HH11	3:D:1078:ARG:HB3	1.74	0.53
1:H:22:GLU:HG2	1:H:198:ARG:HG2	1.91	0.53
5:F:228:ILE:O	5:F:232:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:377:SER:HB3	5:F:380:GLU:HG2	1.91	0.53
1:H:27:PRO:HB3	1:H:192:LEU:HD23	1.90	0.53
5:L:228:ILE:O	5:L:232:ASN:ND2	2.42	0.53
2:I:142:ARG:HB2	2:I:142:ARG:HH11	1.74	0.53
2:I:1087:VAL:HG13	3:J:524:LEU:HD22	1.90	0.53
3:J:858:LEU:HD21	3:J:864:VAL:HG11	1.91	0.53
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.90	0.52
3:D:764:LEU:HG	3:D:766:ALA:H	1.74	0.52
1:G:174:VAL:HG21	1:G:177:VAL:HG23	1.91	0.52
3:J:625:TYR:HE2	3:J:655:PRO:HG2	1.75	0.52
3:J:1078:ARG:HH11	3:J:1078:ARG:HB3	1.74	0.52
1:A:174:VAL:HA	1:A:201:THR:HG22	1.90	0.52
2:C:194:VAL:HG11	2:C:223:ASP:HB3	1.91	0.52
1:A:174:VAL:HG21	1:A:177:VAL:HG23	1.91	0.52
2:C:20:GLU:OE1	2:C:460:ARG:NH1	2.43	0.52
2:C:154:ARG:HG2	2:C:156:GLY:N	2.23	0.52
2:C:761:PHE:HA	2:C:785:VAL:HA	1.91	0.52
5:F:379:ARG:NH2	5:F:411:ARG:HH21	2.07	0.52
5:F:410:GLU:OE2	5:F:413:ARG:NH1	2.42	0.52
1:A:53:VAL:HG23	1:A:144:VAL:HG22	1.91	0.52
1:B:20:TYR:HD1	1:B:21:GLY:N	2.07	0.52
1:B:27:PRO:HB3	1:B:192:LEU:HD23	1.90	0.52
2:C:1087:VAL:HG13	3:D:524:LEU:HD22	1.90	0.52
3:D:1267:ARG:H	3:D:1267:ARG:NE	2.02	0.52
1:G:53:VAL:HG23	1:G:144:VAL:HG22	1.92	0.52
2:I:15:LEU:HD21	2:I:457:ALA:HB1	1.90	0.52
2:I:683:ASN:HB2	2:I:872:ASN:HB2	1.91	0.52
2:I:1101:THR:HG22	3:J:8:VAL:HG22	1.91	0.52
3:J:764:LEU:HG	3:J:766:ALA:H	1.74	0.52
3:J:804:MET:H	3:J:827:ILE:HG22	1.74	0.52
5:L:252:THR:HG23	6:R:29:DC:H41	1.74	0.52
2:C:146:VAL:HG12	2:C:162:ILE:HG12	1.90	0.52
3:D:65:ARG:HG3	3:D:66:GLN:H	1.74	0.52
4:E:41:GLU:HB3	4:E:42:PRO:HD2	1.91	0.52
3:J:792:ILE:HG21	3:J:941:LEU:HD22	1.90	0.52
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.91	0.52
2:C:162:ILE:HB	2:C:172:ILE:HB	1.92	0.52
2:I:20:GLU:OE1	2:I:460:ARG:NH1	2.43	0.52
3:J:169:TYR:HB3	3:J:195:VAL:HG21	1.92	0.52
3:J:1232:PRO:HB2	3:J:1356:TYR:HE2	1.75	0.52
5:L:376:LEU:HB2	5:L:381:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:16:DG:H3'	7:S:17:DG:H8	1.74	0.52
1:B:218:LEU:O	1:B:222:LEU:HG	2.10	0.52
2:C:142:ARG:HH11	2:C:142:ARG:HB2	1.75	0.52
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.91	0.52
3:D:660:LYS:HD3	3:D:694:VAL:HG13	1.92	0.52
3:D:668:PRO:HB2	5:F:432:LYS:HD3	1.92	0.52
3:D:953:ASP:OD1	3:D:953:ASP:N	2.43	0.52
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.90	0.52
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.91	0.52
3:D:682:ASP:C	3:D:683:ILE:HG13	2.31	0.52
3:D:858:LEU:HD21	3:D:864:VAL:HG11	1.91	0.52
5:F:260:GLN:HB3	6:O:25:DT:O4	2.09	0.52
1:G:175:ARG:N	1:G:200:TRP:O	2.42	0.52
3:J:1434:TRP:HB3	3:J:1455:LYS:HD2	1.91	0.52
4:K:41:GLU:HB3	4:K:42:PRO:HD2	1.91	0.52
5:L:103:ILE:HD13	5:L:211:VAL:HG21	1.92	0.52
3:D:804:MET:H	3:D:827:ILE:HG22	1.74	0.52
1:G:13:ALA:HB3	1:H:228:PRO:HB3	1.92	0.52
1:G:90:LEU:HB2	1:G:119:ASP:HA	1.92	0.52
2:I:323:ASP:HB2	2:I:330:ASN:HD21	1.75	0.52
2:I:710:ILE:HB	2:I:790:LEU:HD22	1.91	0.52
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.92	0.52
5:L:257:TRP:O	5:L:260:GLN:HG3	2.10	0.52
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.92	0.52
2:C:1101:THR:HG22	3:D:8:VAL:HG22	1.91	0.52
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.92	0.52
1:G:53:VAL:HA	1:G:144:VAL:HG22	1.90	0.52
1:H:44:LEU:HA	1:H:48:ILE:HD13	1.91	0.52
2:I:162:ILE:HB	2:I:172:ILE:HB	1.92	0.52
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.92	0.52
7:P:16:DG:H3'	7:P:17:DG:H8	1.75	0.52
1:A:90:LEU:HB2	1:A:119:ASP:HA	1.92	0.51
3:D:272:LEU:O	3:D:279:VAL:N	2.43	0.51
5:F:385:LYS:HB2	5:F:390:LEU:HB2	1.92	0.51
1:H:218:LEU:HD23	1:H:222:LEU:HD11	1.92	0.51
2:I:711:GLU:HG2	2:I:822:VAL:HG12	1.91	0.51
3:J:67:ARG:HD3	5:L:394:ARG:HD3	1.91	0.51
3:J:371:ILE:HG12	5:L:247:ARG:HD3	1.92	0.51
5:L:228:ILE:HG22	5:L:232:ASN:HD21	1.75	0.51
5:L:377:SER:HB3	5:L:380:GLU:HG2	1.91	0.51
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:SER:HB2	1:B:158:ILE:HG23	1.92	0.51
2:C:128:ILE:HG13	2:C:133:ASP:HB3	1.92	0.51
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.91	0.51
2:C:713:ARG:HA	2:C:819:VAL:HA	1.90	0.51
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.92	0.51
1:H:20:TYR:HD1	1:H:21:GLY:N	2.08	0.51
3:J:660:LYS:HD3	3:J:694:VAL:HG13	1.91	0.51
3:J:775:GLY:HA2	3:J:1209:LEU:HB3	1.92	0.51
3:J:1379:VAL:HG21	3:J:1400:VAL:HG11	1.93	0.51
2:C:113:VAL:HG21	2:C:373:VAL:HG21	1.92	0.51
1:H:55:SER:HB2	1:H:158:ILE:HG23	1.92	0.51
3:J:210:ARG:HB2	3:J:389:GLU:HB2	1.93	0.51
1:B:218:LEU:HD23	1:B:222:LEU:HD11	1.92	0.51
2:C:36:PRO:HA	2:C:39:ARG:HD2	1.93	0.51
3:D:625:TYR:HE2	3:D:655:PRO:HG2	1.75	0.51
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.92	0.51
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.93	0.51
5:F:103:ILE:HD13	5:F:211:VAL:HG21	1.92	0.51
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.92	0.51
3:J:95:LEU:HG	3:J:574:LEU:HD21	1.92	0.51
5:F:376:LEU:HB2	5:F:381:ALA:HB2	1.92	0.51
1:G:190:THR:OG1	1:G:191:ASP:N	2.43	0.51
1:H:101:LEU:HD23	1:H:114:PHE:HA	1.93	0.51
1:H:218:LEU:O	1:H:222:LEU:HG	2.10	0.51
3:J:895:VAL:O	3:J:899:LEU:HG	2.09	0.51
3:J:1087:ARG:HH12	3:J:1236:LEU:H	1.59	0.51
4:K:79:LEU:HG	4:K:80:VAL:HG13	1.93	0.51
1:B:101:LEU:HD23	1:B:114:PHE:HA	1.93	0.51
3:D:82:ARG:HG2	3:D:84:ILE:H	1.75	0.51
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.93	0.51
3:D:868:TYR:HE2	3:D:897:GLN:HG3	1.75	0.51
2:I:197:LEU:HA	2:I:200:LEU:HB2	1.93	0.51
2:I:326:ASP:HA	2:I:331:ARG:HD2	1.93	0.51
3:J:868:TYR:HE2	3:J:897:GLN:HG3	1.75	0.51
5:L:385:LYS:HB2	5:L:390:LEU:HB2	1.92	0.51
1:A:175:ARG:N	1:A:200:TRP:O	2.42	0.51
2:C:326:ASP:HA	2:C:331:ARG:HD2	1.93	0.51
2:C:762:LYS:HD3	2:C:786:LYS:HD3	1.92	0.51
3:D:371:ILE:HG23	3:D:372:ASP:H	1.75	0.51
3:D:1117:TYR:HA	3:D:1193:THR:HG21	1.91	0.51
3:J:420:VAL:HG21	3:J:424:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:682:ASP:C	3:J:683:ILE:HG13	2.30	0.51
3:J:953:ASP:N	3:J:953:ASP:OD1	2.43	0.51
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.93	0.51
2:C:197:LEU:HA	2:C:200:LEU:HB2	1.93	0.51
3:D:95:LEU:HG	3:D:574:LEU:HD21	1.93	0.51
2:I:36:PRO:HA	2:I:39:ARG:HD2	1.93	0.51
2:I:374:ASN:OD1	2:I:375:SER:N	2.43	0.51
1:A:190:THR:OG1	1:A:191:ASP:N	2.43	0.50
3:D:1434:TRP:HB3	3:D:1455:LYS:HD2	1.91	0.50
4:E:79:LEU:HG	4:E:80:VAL:HG13	1.93	0.50
2:I:18:LEU:HD12	2:I:408:ARG:NE	2.26	0.50
2:I:113:VAL:HG21	2:I:373:VAL:HG21	1.92	0.50
2:I:168:ARG:O	2:I:267:TYR:HA	2.10	0.50
3:J:568:ARG:HA	3:J:571:LYS:HD2	1.93	0.50
3:J:900:ILE:HG12	3:J:914:LEU:HD21	1.93	0.50
1:A:13:ALA:HB3	1:B:228:PRO:HB3	1.93	0.50
3:D:1087:ARG:HH12	3:D:1236:LEU:H	1.59	0.50
3:D:1232:PRO:HB2	3:D:1356:TYR:HE2	1.75	0.50
2:I:428:ARG:O	3:J:1078:ARG:NH1	2.44	0.50
2:I:726:ILE:HG21	2:I:729:LEU:HD23	1.92	0.50
2:C:726:ILE:HG21	2:C:729:LEU:HD23	1.92	0.50
2:I:872:ASN:HD21	2:I:874:LEU:HD12	1.76	0.50
2:I:1051:GLU:HB3	2:I:1056:LYS:HD3	1.93	0.50
3:J:12:LEU:HD21	3:J:1452:ILE:HD13	1.94	0.50
3:J:99:ALA:O	3:J:514:LEU:N	2.43	0.50
3:J:970:LYS:HG2	3:J:995:LEU:HD13	1.93	0.50
2:C:627:ARG:HD3	2:C:639:GLN:O	2.12	0.50
2:C:638:ASP:H	2:C:659:PRO:HG3	1.77	0.50
2:C:872:ASN:HD21	2:C:874:LEU:HD12	1.76	0.50
2:C:1051:GLU:HB3	2:C:1056:LYS:HD3	1.93	0.50
5:F:145:VAL:HG21	5:F:174:VAL:HG11	1.94	0.50
2:I:638:ASP:H	2:I:659:PRO:HG3	1.77	0.50
3:J:553:ARG:NH2	5:L:226:ASP:OD1	2.36	0.50
3:J:628:ARG:HB3	3:J:746:ALA:HA	1.94	0.50
6:O:42:DC:H2"	6:O:43:DG:H8	1.76	0.50
6:R:42:DC:H2"	6:R:43:DG:H8	1.76	0.50
3:D:99:ALA:O	3:D:514:LEU:N	2.43	0.50
3:D:423:ASP:OD2	3:D:423:ASP:N	2.44	0.50
2:I:87:ASP:HA	2:I:131:GLY:HA3	1.92	0.50
2:I:219:GLN:HA	2:I:222:LEU:HD12	1.94	0.50
3:J:704:ARG:HD3	3:J:738:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:33:DG:H2"	6:O:34:DA:C8	2.47	0.50
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.93	0.50
1:A:111:ALA:HB1	1:A:122:ILE:HD13	1.93	0.50
2:C:97:ARG:HD2	2:C:112:GLU:HG3	1.93	0.50
1:G:83:LYS:HE3	1:G:168:ASP:HB2	1.93	0.50
6:R:33:DG:H2"	6:R:34:DA:C8	2.47	0.50
2:C:1094:ALA:HB2	3:D:520:LEU:HD13	1.93	0.50
3:D:628:ARG:HB3	3:D:746:ALA:HA	1.94	0.50
3:D:1472:ILE:HG12	3:D:1474:ALA:H	1.77	0.50
2:I:150:PRO:HD3	2:I:322:VAL:HG11	1.93	0.50
2:I:939:ARG:HB3	2:I:982:PRO:HG3	1.92	0.50
3:J:1117:TYR:HA	3:J:1193:THR:HG21	1.92	0.50
5:L:145:VAL:HG21	5:L:174:VAL:HG11	1.94	0.50
1:B:176:ARG:O	1:B:200:TRP:HE3	1.95	0.50
2:C:150:PRO:HA	2:C:158:TYR:HD2	1.77	0.50
2:C:168:ARG:O	2:C:267:TYR:HA	2.10	0.50
5:L:97:ARG:HH22	6:R:33:DG:N2	2.10	0.50
2:C:428:ARG:O	3:D:1078:ARG:NH1	2.44	0.50
2:I:1094:ALA:HB2	3:J:520:LEU:HD13	1.93	0.50
2:C:834:GLN:HG2	2:C:835:VAL:H	1.75	0.49
3:D:12:LEU:HD21	3:D:1452:ILE:HD13	1.94	0.49
3:D:640:HIS:O	3:D:717:GLN:N	2.32	0.49
3:D:900:ILE:HG12	3:D:914:LEU:HD21	1.93	0.49
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	1.94	0.49
5:F:120:LYS:HE3	5:F:198:ALA:HB2	1.94	0.49
2:I:627:ARG:HD3	2:I:639:GLN:O	2.12	0.49
3:J:572:ARG:CZ	5:L:98:GLN:HG2	2.42	0.49
3:J:697:GLY:O	3:J:760:ARG:NH1	2.45	0.49
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.28	0.49
3:D:895:VAL:O	3:D:899:LEU:HG	2.11	0.49
5:F:228:ILE:HG22	5:F:232:ASN:HD21	1.75	0.49
1:G:111:ALA:HB1	1:G:122:ILE:HD13	1.93	0.49
3:J:34:TYR:OH	6:R:20:DT:OP2	2.25	0.49
3:J:1472:ILE:HG12	3:J:1474:ALA:H	1.77	0.49
3:D:568:ARG:HA	3:D:571:LYS:HD2	1.93	0.49
4:E:30:LEU:HD23	4:E:63:TRP:HB3	1.94	0.49
1:H:99:LEU:HB2	1:H:142:VAL:HG22	1.95	0.49
3:J:185:VAL:HG12	3:J:186:VAL:H	1.77	0.49
4:K:30:LEU:HD23	4:K:63:TRP:HB3	1.93	0.49
5:L:336:ILE:HB	5:L:342:SER:HB3	1.93	0.49
2:C:18:LEU:HD12	2:C:408:ARG:NE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:950:LEU:HD11	2:C:952:LEU:HB2	1.95	0.49
3:D:970:LYS:HG2	3:D:995:LEU:HD13	1.93	0.49
5:F:336:ILE:HB	5:F:342:SER:HB3	1.93	0.49
2:I:26:TYR:HE1	2:I:340:MET:HG3	1.77	0.49
3:J:1192:LEU:HD23	3:J:1373:ARG:HB2	1.94	0.49
1:B:99:LEU:HB2	1:B:142:VAL:HG22	1.94	0.49
2:C:630:ARG:NH1	2:C:706:GLU:HA	2.27	0.49
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.94	0.49
2:I:1095:LEU:HD11	3:J:603:LEU:HB3	1.95	0.49
3:J:67:ARG:HB2	5:L:392:ASP:O	2.12	0.49
2:C:219:GLN:HA	2:C:222:LEU:HD12	1.94	0.49
2:C:261:LEU:HB3	2:C:291:VAL:HG22	1.94	0.49
3:D:1192:LEU:HD23	3:D:1373:ARG:HB2	1.94	0.49
1:G:158:ILE:HG22	1:G:160:ASP:H	1.76	0.49
3:J:1281:VAL:HG21	3:J:1313:VAL:HG11	1.95	0.49
5:L:210:VAL:HA	5:L:213:ILE:HD12	1.95	0.49
5:L:238:ALA:HB2	5:L:257:TRP:HB2	1.94	0.49
2:C:167:LYS:H	6:O:37:DT:H73	1.78	0.49
2:C:480:THR:HG22	2:C:482:GLU:H	1.77	0.49
3:D:572:ARG:CZ	5:F:98:GLN:HG2	2.42	0.49
3:D:1057:VAL:HA	3:D:1069:GLU:HG2	1.95	0.49
3:D:1281:VAL:HG21	3:D:1313:VAL:HG11	1.95	0.49
2:I:97:ARG:HD2	2:I:112:GLU:HG3	1.93	0.49
2:I:150:PRO:HA	2:I:158:TYR:HD2	1.77	0.49
2:I:950:LEU:HD11	2:I:952:LEU:HB2	1.95	0.49
3:J:1386:ASP:OD2	3:J:1413:VAL:N	2.45	0.49
2:C:605:LYS:HG2	2:C:612:ALA:HB3	1.95	0.49
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.77	0.49
2:C:1056:LYS:O	3:D:624:ASP:N	2.37	0.49
3:D:697:GLY:O	3:D:760:ARG:NH1	2.45	0.49
1:H:51:THR:HG21	1:H:86:VAL:HG23	1.94	0.49
2:C:303:PHE:HA	2:C:306:THR:HG22	1.95	0.49
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.95	0.49
3:D:351:MET:HG3	3:D:370:ALA:HB2	1.94	0.49
3:D:708:LEU:HD12	3:D:1231:GLU:HA	1.95	0.49
3:D:1106:VAL:HA	3:D:1220:ALA:HA	1.95	0.49
5:F:210:VAL:HA	5:F:213:ILE:HD12	1.94	0.49
2:I:93:PRO:HB3	2:I:114:PHE:HE2	1.78	0.49
2:I:303:PHE:HA	2:I:306:THR:HG22	1.95	0.49
2:I:420:ARG:NH2	8:T:1:U:OP2	2.46	0.49
2:I:678:PRO:HA	2:I:683:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:834:GLN:HG2	2:I:835:VAL:H	1.76	0.49
3:J:203:ALA:HA	3:J:395:VAL:HA	1.95	0.49
3:J:644:LEU:HG	3:J:649:ALA:HB2	1.95	0.49
1:B:97:THR:HG21	1:B:120:VAL:HG21	1.94	0.49
3:D:231:VAL:H	3:D:243:ALA:HA	1.78	0.49
2:I:261:LEU:HB3	2:I:291:VAL:HG22	1.95	0.49
2:I:537:LYS:NZ	2:I:904:PRO:HB3	2.28	0.49
3:D:56:TYR:O	3:D:80:VAL:HG23	2.13	0.48
3:D:417:PRO:HA	3:D:430:GLU:HA	1.95	0.48
3:D:644:LEU:HG	3:D:649:ALA:HB2	1.95	0.48
2:I:324:ASP:O	2:I:330:ASN:ND2	2.42	0.48
2:I:480:THR:HG22	2:I:482:GLU:H	1.77	0.48
3:J:108:VAL:HB	3:J:109:PRO:HD3	1.94	0.48
3:J:1020:LEU:HG	3:J:1035:ILE:HD12	1.95	0.48
3:J:1037:GLN:HG2	3:J:1042:ARG:HA	1.94	0.48
3:J:1099:VAL:O	3:J:1103:HIS:HB3	2.13	0.48
1:A:170:ILE:HG23	2:C:696:LYS:HD2	1.94	0.48
2:C:39:ARG:HD3	2:C:45:GLN:HE22	1.79	0.48
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.27	0.48
3:D:116:LEU:HD11	3:D:465:LEU:HG	1.94	0.48
3:D:596:SER:OG	3:D:598:ARG:NH1	2.47	0.48
3:D:1386:ASP:OD2	3:D:1413:VAL:N	2.45	0.48
2:I:397:GLU:HB3	2:I:631:SER:HB2	1.95	0.48
2:I:418:LEU:HA	2:I:422:ARG:HE	1.78	0.48
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.48	0.48
3:J:62:LYS:HG3	3:J:63:TYR:N	2.28	0.48
5:L:411:ARG:HD3	6:R:1:DC:C6	2.48	0.48
2:C:26:TYR:HE1	2:C:340:MET:HG3	1.78	0.48
3:D:286:ALA:O	3:D:311:LEU:HA	2.14	0.48
3:D:796:ARG:HG2	3:D:1017:PHE:CE1	2.49	0.48
4:E:14:ASP:OD1	4:E:14:ASP:N	2.40	0.48
1:H:74:ASP:O	1:H:78:ILE:HG12	2.14	0.48
2:I:259:GLY:HA2	2:I:263:ASP:HB2	1.95	0.48
2:I:605:LYS:HG2	2:I:612:ALA:HB3	1.95	0.48
2:I:607:ASP:HB3	2:I:610:ARG:O	2.13	0.48
3:J:361:VAL:HG21	3:J:367:ILE:HD11	1.96	0.48
2:C:537:LYS:NZ	2:C:904:PRO:HB3	2.28	0.48
2:C:22:GLN:HB3	2:C:121:MET:HE2	1.95	0.48
2:C:113:VAL:HB	5:F:295:GLN:HE22	1.77	0.48
2:C:607:ASP:HB3	2:C:610:ARG:O	2.13	0.48
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:222:ALA:HB1	3:D:332:HIS:HE1	1.78	0.48
5:F:238:ALA:HB2	5:F:257:TRP:HB2	1.94	0.48
1:B:161:ARG:HG3	1:B:162:ILE:H	1.78	0.48
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.94	0.48
2:C:1031:ARG:HD3	7:P:13:DC:H5'	1.96	0.48
3:D:416:ALA:HB3	3:D:419:ASP:CG	2.33	0.48
2:I:39:ARG:HD3	2:I:45:GLN:HE22	1.79	0.48
2:I:113:VAL:HB	5:L:295:GLN:HE22	1.79	0.48
3:J:116:LEU:HD11	3:J:465:LEU:HG	1.94	0.48
3:J:127:LEU:HD23	3:J:458:ALA:HA	1.95	0.48
3:J:708:LEU:HD12	3:J:1231:GLU:HA	1.95	0.48
3:J:796:ARG:HG2	3:J:1017:PHE:CE1	2.49	0.48
3:J:1057:VAL:HA	3:J:1069:GLU:HG2	1.95	0.48
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.95	0.48
2:C:418:LEU:HA	2:C:422:ARG:HE	1.79	0.48
3:D:1020:LEU:HG	3:D:1035:ILE:HD12	1.95	0.48
5:L:146:VAL:HG11	5:L:196:GLU:HG3	1.96	0.48
6:R:29:DC:H5'	6:R:30:DT:H71	1.96	0.48
1:B:51:THR:HG21	1:B:86:VAL:HG23	1.94	0.48
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.49	0.48
3:D:367:ILE:HD11	3:D:379:ALA:HB2	1.96	0.48
3:D:704:ARG:NE	3:D:705:ALA:O	2.47	0.48
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.13	0.48
1:H:97:THR:HG21	1:H:120:VAL:HG21	1.94	0.48
2:I:541:SER:O	2:I:545:ASN:HB2	2.14	0.48
3:J:56:TYR:O	3:J:80:VAL:HG23	2.13	0.48
3:J:691:LEU:HD23	3:J:720:LEU:HD11	1.96	0.48
3:J:704:ARG:NE	3:J:705:ALA:O	2.46	0.48
1:A:158:ILE:HG22	1:A:160:ASP:H	1.76	0.48
1:A:180:GLN:NE2	2:C:935:GLY:O	2.44	0.48
1:B:162:ILE:HG23	1:B:163:ASN:H	1.79	0.48
5:F:217:TYR:HB3	5:F:227:LEU:HD21	1.96	0.48
5:F:254:ALA:O	5:F:258:ILE:HG12	2.14	0.48
1:H:161:ARG:HG3	1:H:162:ILE:H	1.78	0.48
2:I:751:PRO:HB3	2:I:794:PRO:HA	1.95	0.48
2:I:874:LEU:O	2:I:877:PRO:HD2	2.14	0.48
3:J:420:VAL:HG21	3:J:425:GLY:H	1.78	0.48
3:J:1060:SER:OG	3:J:1061:PHE:N	2.47	0.48
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	1.96	0.48
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.94	0.48
1:G:170:ILE:HG23	2:I:696:LYS:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.79	0.48
3:J:165:LYS:H	3:J:397:LYS:HZ2	1.61	0.48
7:S:16:DG:H3'	7:S:17:DG:C8	2.49	0.48
1:B:25:LEU:HD23	1:B:28:LEU:HD22	1.96	0.47
2:C:630:ARG:HG2	2:C:631:SER:H	1.79	0.47
2:C:674:VAL:HG11	2:C:992:MET:HE3	1.96	0.47
4:E:85:LEU:O	4:E:89:MET:HB2	2.14	0.47
1:H:25:LEU:HD23	1:H:28:LEU:HD22	1.96	0.47
1:H:80:LEU:HD23	3:J:867:ARG:HD3	1.96	0.47
2:I:22:GLN:HB3	2:I:121:MET:HE2	1.95	0.47
2:I:136:ILE:HB	2:I:336:VAL:HG12	1.96	0.47
2:C:541:SER:O	2:C:545:ASN:HB2	2.14	0.47
2:C:952:LEU:HD21	2:C:971:LYS:HD2	1.96	0.47
3:D:639:LEU:HB3	3:D:640:HIS:H	1.55	0.47
3:D:691:LEU:HD23	3:D:720:LEU:HD11	1.96	0.47
2:I:952:LEU:HD21	2:I:971:LYS:HD2	1.97	0.47
5:L:120:LYS:HE3	5:L:198:ALA:HB2	1.94	0.47
5:L:254:ALA:O	5:L:258:ILE:HG12	2.14	0.47
1:A:74:ASP:OD2	2:C:640:ARG:NH1	2.48	0.47
1:B:52:ALA:HB3	1:B:171:PHE:CD1	2.49	0.47
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.79	0.47
3:D:127:LEU:HD23	3:D:458:ALA:HA	1.95	0.47
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.96	0.47
5:F:146:VAL:HG11	5:F:196:GLU:HG3	1.96	0.47
1:H:52:ALA:HB3	1:H:171:PHE:CD1	2.50	0.47
3:J:1106:VAL:HA	3:J:1220:ALA:HA	1.95	0.47
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.74	0.47
3:D:62:LYS:HG3	3:D:63:TYR:N	2.30	0.47
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.97	0.47
3:J:101:HIS:ND1	3:J:103:TRP:HB2	2.28	0.47
3:J:1274:ILE:HG22	3:J:1324:PRO:HA	1.97	0.47
3:D:343:LYS:HZ2	3:D:344:ASP:H	1.61	0.47
2:I:42:VAL:HA	2:I:46:ALA:HB2	1.97	0.47
7:P:16:DG:H3'	7:P:17:DG:C8	2.50	0.47
7:P:20:DA:H4'	7:P:21:DA:OP1	2.15	0.47
1:B:74:ASP:O	1:B:78:ILE:HG12	2.14	0.47
1:B:80:LEU:HD23	3:D:867:ARG:HD3	1.95	0.47
2:C:93:PRO:HB3	2:C:114:PHE:HE2	1.78	0.47
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.96	0.47
2:C:189:ARG:NH1	2:C:242:LEU:HB2	2.30	0.47
2:C:374:ASN:OD1	2:C:375:SER:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1060:SER:OG	3:D:1061:PHE:N	2.47	0.47
3:D:1492:LEU:O	3:D:1496:GLU:HB2	2.15	0.47
2:I:674:VAL:HG11	2:I:992:MET:HE3	1.95	0.47
3:J:477:LEU:HA	3:J:480:GLU:HB2	1.96	0.47
2:C:136:ILE:HB	2:C:336:VAL:HG12	1.96	0.47
2:C:689:VAL:HG23	2:C:869:VAL:O	2.15	0.47
2:C:715:THR:OG1	2:C:718:GLY:O	2.21	0.47
3:D:64:LYS:H	3:D:68:PHE:HE2	1.62	0.47
3:D:310:LEU:HD23	3:D:312:ARG:NH2	2.29	0.47
3:D:477:LEU:HA	3:D:480:GLU:HB2	1.96	0.47
3:D:860:LEU:HD12	3:D:860:LEU:H	1.79	0.47
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.15	0.47
1:G:74:ASP:OD2	2:I:640:ARG:NH1	2.48	0.47
1:H:162:ILE:HG23	1:H:163:ASN:H	1.79	0.47
2:I:189:ARG:NH1	2:I:242:LEU:HB2	2.29	0.47
3:J:351:MET:HA	3:J:370:ALA:HA	1.97	0.47
3:J:573:MET:SD	5:L:229:GLN:HG3	2.55	0.47
3:J:860:LEU:H	3:J:860:LEU:HD12	1.79	0.47
3:J:1090:ASP:O	3:J:1093:TYR:HB3	2.15	0.47
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.97	0.47
2:I:258:PHE:HB2	2:I:298:PHE:HZ	1.80	0.47
3:J:614:PHE:HA	3:J:618:LEU:HB2	1.96	0.47
2:C:258:PHE:HB2	2:C:298:PHE:HZ	1.80	0.47
3:D:238:PRO:HB3	3:D:315:ARG:O	2.14	0.47
4:E:8:LYS:O	4:E:12:MET:HG3	2.15	0.47
3:J:596:SER:OG	3:J:598:ARG:NH1	2.47	0.47
3:J:634:GLY:O	3:J:637:LEU:HB2	2.15	0.47
3:J:667:ALA:HB1	3:J:672:ALA:HB3	1.97	0.47
3:J:1087:ARG:NH1	3:J:1236:LEU:H	2.13	0.47
4:K:85:LEU:O	4:K:89:MET:HB2	2.14	0.47
5:L:154:ALA:O	5:L:158:LYS:HB2	2.15	0.47
5:L:217:TYR:HB3	5:L:227:LEU:HD21	1.95	0.47
5:L:269:GLN:HE21	5:L:269:GLN:HB2	1.50	0.47
2:C:425:PHE:O	2:C:429:ASP:HB2	2.15	0.47
3:D:838:ARG:O	3:D:865:THR:OG1	2.32	0.47
3:J:554:LEU:O	3:J:558:LEU:HB2	2.15	0.47
5:L:132:SER:OG	5:L:137:LEU:O	2.27	0.47
1:A:42:ARG:NH1	2:C:977:GLY:O	2.47	0.46
2:C:176:VAL:HA	2:C:182:VAL:HG23	1.97	0.46
2:C:806:LEU:HB2	2:C:822:VAL:HG23	1.97	0.46
3:D:667:ALA:HB1	3:D:672:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:675:ARG:HH12	5:F:437:LEU:HG	1.80	0.46
5:F:291:ARG:HD3	7:P:23:DA:N3	2.31	0.46
1:G:48:ILE:HG22	1:G:173:PRO:HD2	1.98	0.46
1:H:100:ILE:O	1:H:115:THR:HB	2.15	0.46
2:I:689:VAL:HG23	2:I:869:VAL:O	2.15	0.46
2:I:1094:ALA:HA	3:J:518:PRO:HB2	1.96	0.46
2:C:1094:ALA:HA	3:D:518:PRO:HB2	1.96	0.46
5:F:154:ALA:O	5:F:158:LYS:HB2	2.15	0.46
1:G:40:LEU:O	1:G:44:LEU:HB2	2.15	0.46
2:I:740:GLU:HG3	2:I:742:ILE:HG13	1.98	0.46
3:J:132:TYR:HA	3:J:456:MET:HB3	1.98	0.46
3:J:628:ARG:NH2	3:J:744:GLN:OE1	2.49	0.46
3:J:1335:LEU:HA	3:J:1338:ALA:HB3	1.98	0.46
4:K:8:LYS:O	4:K:12:MET:HG3	2.15	0.46
6:O:29:DC:H5'	6:O:30:DT:H71	1.96	0.46
1:A:40:LEU:O	1:A:44:LEU:HB2	2.15	0.46
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.98	0.46
3:D:122:GLU:O	3:D:126:VAL:HG23	2.15	0.46
3:D:247:GLU:O	3:D:249:TYR:N	2.47	0.46
3:D:260:GLU:HA	3:D:294:GLU:HG3	1.96	0.46
5:F:149:LYS:HD3	5:F:193:ARG:HH22	1.80	0.46
1:G:42:ARG:NH1	2:I:977:GLY:O	2.47	0.46
2:I:716:LYS:HE2	3:J:37:LEU:HD11	1.98	0.46
5:L:149:LYS:HD3	5:L:193:ARG:HH22	1.80	0.46
2:C:630:ARG:NH1	2:C:705:ILE:O	2.47	0.46
2:C:740:GLU:HG3	2:C:742:ILE:HG13	1.98	0.46
3:D:226:PRO:HA	3:D:330:SER:HA	1.98	0.46
3:D:230:TRP:CH2	3:D:333:LEU:HD21	2.50	0.46
3:D:573:MET:SD	5:F:229:GLN:HG3	2.55	0.46
1:G:180:GLN:NE2	2:I:935:GLY:O	2.44	0.46
2:I:544:THR:HA	2:I:547:ILE:HD12	1.98	0.46
3:J:573:MET:HA	3:J:576:GLU:HG2	1.97	0.46
5:L:319:VAL:O	5:L:323:LEU:HB2	2.15	0.46
6:O:39:DT:H2"	6:O:40:DC:H5'	1.97	0.46
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.96	0.46
3:D:165:LYS:H	3:D:397:LYS:HZ1	1.63	0.46
3:D:634:GLY:O	3:D:637:LEU:HB2	2.16	0.46
3:D:1087:ARG:NH1	3:D:1236:LEU:H	2.13	0.46
2:I:168:ARG:NH1	2:I:265:LYS:O	2.49	0.46
2:I:176:VAL:HA	2:I:182:VAL:HG23	1.97	0.46
2:I:238:LEU:HD23	2:I:241:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:540:LEU:HA	3:J:543:LEU:HD12	1.98	0.46
3:J:1492:LEU:O	3:J:1496:GLU:HB2	2.15	0.46
1:A:35:THR:HG23	1:B:39:PRO:HA	1.98	0.46
2:C:856:GLU:H	2:C:856:GLU:HG3	1.59	0.46
3:D:554:LEU:O	3:D:558:LEU:HB2	2.16	0.46
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.48	0.46
3:D:976:GLN:HG2	3:J:807:ALA:HA	1.97	0.46
3:D:1335:LEU:HA	3:D:1338:ALA:HB3	1.98	0.46
3:D:1435:LEU:HB3	3:D:1467:ILE:HD12	1.98	0.46
4:E:66:LYS:HA	4:E:69:LEU:HD12	1.96	0.46
5:F:166:PRO:HG2	5:F:169:LYS:HZ2	1.80	0.46
2:I:1008:ARG:NH1	2:I:1020:PRO:HB3	2.31	0.46
3:J:796:ARG:NH2	3:J:859:ASP:OD2	2.48	0.46
1:A:133:GLU:OE2	2:C:605:LYS:HB2	2.16	0.46
2:C:544:THR:HA	2:C:547:ILE:HD12	1.98	0.46
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.98	0.46
3:D:573:MET:HA	3:D:576:GLU:HG2	1.97	0.46
3:D:1158:ARG:HG3	3:D:1158:ARG:NH1	2.22	0.46
5:F:319:VAL:O	5:F:323:LEU:HB2	2.15	0.46
1:G:39:PRO:CG	1:H:39:PRO:HG3	2.46	0.46
2:I:351:LEU:HB2	2:I:377:PRO:HB2	1.98	0.46
2:I:425:PHE:O	2:I:429:ASP:HB2	2.15	0.46
3:J:1442:ASN:N	7:S:9:DG:OP1	2.43	0.46
4:K:66:LYS:HA	4:K:69:LEU:HD12	1.96	0.46
1:B:100:ILE:O	1:B:115:THR:HB	2.15	0.46
3:D:216:LEU:HD13	3:D:383:GLY:HA2	1.98	0.46
3:D:614:PHE:HA	3:D:618:LEU:HB2	1.96	0.46
1:G:35:THR:HG23	1:H:39:PRO:HA	1.98	0.46
1:G:72:LYS:HB2	2:I:606:VAL:HG11	1.97	0.46
2:I:307:LEU:HD12	2:I:307:LEU:HA	1.84	0.46
2:I:630:ARG:HG2	2:I:631:SER:H	1.81	0.46
3:J:544:TYR:O	3:J:548:ILE:HG13	2.16	0.46
5:L:266:ILE:HG13	5:L:267:ALA:N	2.31	0.46
2:I:181:VAL:HG22	2:I:182:VAL:H	1.81	0.46
3:J:353:VAL:HG21	3:J:387:LEU:HD11	1.98	0.46
3:J:371:ILE:HG23	3:J:372:ASP:H	1.81	0.46
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.46	0.46
1:B:23:PHE:HE2	1:B:199:ILE:HD12	1.80	0.46
2:C:70:GLU:HG2	2:C:97:ARG:HB3	1.98	0.46
2:C:181:VAL:HG22	2:C:182:VAL:H	1.81	0.46
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.51	0.46
2:I:856:GLU:H	2:I:856:GLU:HG3	1.59	0.46
2:I:1056:LYS:O	3:J:624:ASP:N	2.37	0.46
2:C:168:ARG:NH1	2:C:265:LYS:O	2.48	0.45
2:C:238:LEU:HD23	2:C:241:LEU:HD12	1.96	0.45
2:C:324:ASP:O	2:C:330:ASN:ND2	2.44	0.45
2:C:430:VAL:HG23	3:D:1075:HIS:HD2	1.81	0.45
5:F:266:ILE:HG13	5:F:267:ALA:N	2.31	0.45
5:F:427:GLU:OE1	5:F:433:LEU:HB2	2.16	0.45
2:I:70:GLU:HG2	2:I:97:ARG:HB3	1.98	0.45
2:I:806:LEU:HB2	2:I:822:VAL:HG23	1.97	0.45
3:J:1165:TYR:HB3	3:J:1207:TYR:HE1	1.81	0.45
3:J:1311:LEU:HD23	3:J:1311:LEU:H	1.81	0.45
2:C:126:SER:HB3	2:C:407:LYS:NZ	2.31	0.45
2:C:764:GLU:HB2	2:C:765:GLN:H	1.54	0.45
3:D:245:LEU:HD23	3:D:245:LEU:HA	1.77	0.45
3:D:1087:ARG:NH2	3:D:1237:THR:OG1	2.48	0.45
2:I:326:ASP:OD1	6:R:38:DG:N2	2.48	0.45
3:J:1344:VAL:O	3:J:1348:LEU:HG	2.15	0.45
6:R:39:DT:H2"	6:R:40:DC:H5'	1.97	0.45
2:C:431:HIS:H	2:C:434:HIS:CE1	2.34	0.45
3:D:266:GLU:HG3	3:D:286:ALA:HB2	1.98	0.45
3:D:654:LYS:O	3:D:658:LEU:HD23	2.16	0.45
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.99	0.45
3:D:1068:LEU:HD12	3:D:1068:LEU:H	1.81	0.45
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.80	0.45
1:G:111:ALA:HB1	1:G:122:ILE:HG21	1.99	0.45
2:I:660:ALA:O	2:I:667:ALA:N	2.33	0.45
3:J:34:TYR:HD1	5:L:325:ILE:HG21	1.82	0.45
3:J:192:ALA:HB3	3:J:195:VAL:HG12	1.97	0.45
3:J:1068:LEU:HD12	3:J:1068:LEU:H	1.81	0.45
1:A:72:LYS:HB2	2:C:606:VAL:HG11	1.97	0.45
3:D:221:ALA:HB3	3:D:337:LEU:HD12	1.98	0.45
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.81	0.45
5:F:132:SER:OG	5:F:137:LEU:O	2.28	0.45
1:H:23:PHE:HE2	1:H:199:ILE:HD12	1.81	0.45
1:H:176:ARG:O	1:H:200:TRP:HE3	1.98	0.45
3:J:122:GLU:O	3:J:126:VAL:HG23	2.15	0.45
3:J:128:TYR:OH	3:J:579:ASP:OD2	2.23	0.45
3:J:1364:HIS:CD2	3:J:1366:LYS:HE2	2.51	0.45
1:A:111:ALA:HB1	1:A:122:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:212:ARG:HG2	3:D:213:VAL:H	1.82	0.45
3:D:671:LYS:HG2	5:F:364:LEU:HD13	1.99	0.45
5:F:165:LYS:HA	5:F:166:PRO:HD3	1.87	0.45
3:J:1087:ARG:NH2	3:J:1237:THR:OG1	2.49	0.45
3:D:544:TYR:O	3:D:548:ILE:HG13	2.16	0.45
3:D:760:ARG:HH22	4:E:62:THR:HG23	1.81	0.45
3:D:908:LYS:HE3	3:D:908:LYS:C	2.36	0.45
3:D:916:TYR:OH	3:D:1145:TYR:OH	2.34	0.45
2:I:291:VAL:HB	2:I:299:LYS:O	2.16	0.45
2:I:764:GLU:H	2:I:764:GLU:HG2	1.33	0.45
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.99	0.45
2:C:15:LEU:HD13	2:C:16:PRO:HD2	1.99	0.45
2:C:291:VAL:HB	2:C:299:LYS:O	2.16	0.45
2:I:184:MET:N	2:I:191:PHE:O	2.48	0.45
2:I:815:LEU:HD11	2:I:822:VAL:HG22	1.98	0.45
3:J:441:ARG:HH12	3:J:445:ARG:NH1	2.15	0.45
3:J:571:LYS:NZ	5:L:155:ARG:HH22	2.15	0.45
3:J:643:GLY:HA3	3:J:727:GLN:HB2	1.97	0.45
2:C:607:ASP:O	2:C:610:ARG:N	2.50	0.45
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	2.31	0.45
5:F:209:LEU:HG	5:F:213:ILE:HD11	1.99	0.45
2:I:769:PRO:HG3	3:J:65:ARG:HH12	1.81	0.45
5:L:209:LEU:HG	5:L:213:ILE:HD11	1.99	0.45
2:C:1031:ARG:HB2	3:D:622:ARG:HG2	1.98	0.45
2:C:1063:ARG:HG3	5:F:356:PRO:HG3	1.99	0.45
3:D:1344:VAL:O	3:D:1348:LEU:HG	2.15	0.45
4:E:88:GLU:HB3	4:E:91:ARG:HH21	1.82	0.45
1:G:53:VAL:HA	1:G:144:VAL:HG13	1.98	0.45
1:G:97:THR:HG22	1:G:144:VAL:HB	1.99	0.45
1:G:133:GLU:OE2	2:I:605:LYS:HB2	2.16	0.45
2:I:430:VAL:HG23	3:J:1075:HIS:HD2	1.81	0.45
3:J:654:LYS:O	3:J:658:LEU:HD23	2.17	0.45
3:J:760:ARG:HH22	4:K:62:THR:HG23	1.81	0.45
3:D:259:VAL:HG23	3:D:294:GLU:HA	1.99	0.45
3:D:543:LEU:HG	3:D:600:LEU:HD23	1.99	0.45
5:F:214:ALA:HB1	5:F:227:LEU:HD23	1.99	0.45
5:F:229:GLN:HA	5:F:232:ASN:HD22	1.81	0.45
2:I:857:ASP:OD2	2:I:857:ASP:N	2.47	0.45
3:J:64:LYS:H	3:J:68:PHE:HE2	1.63	0.45
3:J:1435:LEU:HB3	3:J:1467:ILE:HD12	1.99	0.45
1:B:75:VAL:O	1:B:79:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ALA:O	1:B:220:GLU:HB2	2.17	0.44
2:C:688:ILE:HD12	2:C:839:LEU:HB2	1.99	0.44
5:F:291:ARG:HD3	7:P:23:DA:C2	2.52	0.44
1:G:186:LEU:HD23	1:G:187:GLY:H	1.82	0.44
2:I:710:ILE:HD11	2:I:758:ARG:HE	1.82	0.44
2:I:1031:ARG:HB2	3:J:622:ARG:HG2	1.98	0.44
2:I:1059:ASP:O	2:I:1063:ARG:NH1	2.47	0.44
3:J:543:LEU:HG	3:J:600:LEU:HD23	1.99	0.44
5:L:160:PRO:HB2	5:L:164:GLU:HB2	1.99	0.44
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.99	0.44
2:C:470:PRO:HG3	2:C:485:TYR:CZ	2.52	0.44
2:C:607:ASP:O	2:C:609:THR:N	2.50	0.44
3:D:769:LEU:O	3:D:778:LEU:HB3	2.17	0.44
5:F:428:SER:HA	5:F:434:ARG:HH21	1.83	0.44
1:G:32:PHE:CZ	1:H:43:ILE:HG12	2.52	0.44
1:G:39:PRO:HG2	1:H:39:PRO:HG3	1.98	0.44
1:G:54:THR:O	1:G:167:VAL:HG22	2.18	0.44
1:H:77:GLU:O	1:H:81:ASN:ND2	2.48	0.44
2:I:15:LEU:HD13	2:I:16:PRO:HD2	1.99	0.44
2:I:207:LEU:HD22	2:I:221:LEU:HD21	1.99	0.44
2:I:604:VAL:HG23	2:I:605:LYS:HG2	1.99	0.44
3:J:62:LYS:HE2	3:J:62:LYS:HB2	1.85	0.44
6:R:4:DG:H1	7:S:45:DC:H42	1.65	0.44
1:A:54:THR:O	1:A:167:VAL:HG22	2.18	0.44
2:C:196:LEU:O	2:C:198:ARG:NH1	2.49	0.44
2:C:673:LEU:HG	2:C:867:VAL:HG12	1.99	0.44
2:C:874:LEU:O	2:C:877:PRO:HD2	2.18	0.44
3:D:628:ARG:NH2	3:D:744:GLN:OE1	2.50	0.44
5:F:160:PRO:HB2	5:F:164:GLU:HB2	1.99	0.44
2:I:45:GLN:HE21	2:I:45:GLN:HB2	1.59	0.44
2:I:102:HIS:HB2	2:I:107:LEU:H	1.82	0.44
2:I:399:ASN:ND2	2:I:402:SER:HB2	2.32	0.44
2:I:431:HIS:H	2:I:434:HIS:CE1	2.34	0.44
2:I:607:ASP:O	2:I:609:THR:N	2.50	0.44
3:J:838:ARG:O	3:J:865:THR:OG1	2.32	0.44
3:J:1459:LEU:HA	3:J:1464:GLU:HG3	1.99	0.44
5:L:214:ALA:HB3	5:L:228:ILE:HG12	1.99	0.44
1:A:186:LEU:HD23	1:A:187:GLY:H	1.82	0.44
1:B:77:GLU:O	1:B:81:ASN:ND2	2.48	0.44
2:C:207:LEU:HD22	2:C:221:LEU:HD21	2.00	0.44
2:C:351:LEU:HB2	2:C:377:PRO:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:604:VAL:HG23	2:C:605:LYS:HG2	1.99	0.44
2:C:710:ILE:HD11	2:C:758:ARG:HE	1.82	0.44
3:D:34:TYR:HD1	5:F:325:ILE:HG21	1.82	0.44
3:D:132:TYR:HA	3:D:456:MET:HB3	2.00	0.44
3:D:415:VAL:HG11	3:D:433:GLY:H	1.82	0.44
3:D:667:ALA:HB1	3:D:672:ALA:CB	2.47	0.44
5:F:368:GLU:HB3	5:F:433:LEU:HD21	1.98	0.44
5:F:372:ALA:HA	5:F:375:LYS:HE3	2.00	0.44
2:I:688:ILE:HD12	2:I:839:LEU:HB2	1.99	0.44
2:I:832:LYS:HB2	2:I:832:LYS:HE3	1.83	0.44
2:I:999:HIS:CD2	2:I:1004:LYS:HE3	2.53	0.44
5:L:229:GLN:HA	5:L:232:ASN:HD22	1.81	0.44
5:L:372:ALA:HA	5:L:375:LYS:HE3	1.99	0.44
2:C:498:GLN:HG3	3:D:1068:LEU:HD11	1.99	0.44
3:D:433:GLY:HA3	3:D:447:VAL:O	2.18	0.44
3:D:1137:ARG:HE	3:D:1137:ARG:HB3	1.35	0.44
1:H:216:ALA:O	1:H:220:GLU:HB2	2.17	0.44
2:I:607:ASP:O	2:I:610:ARG:N	2.50	0.44
2:I:889:HIS:CE1	2:I:970:GLY:HA3	2.53	0.44
2:I:1066:ALA:O	2:I:1070:ILE:HG13	2.18	0.44
3:J:671:LYS:HG3	5:L:436:PHE:CE2	2.52	0.44
5:L:166:PRO:HG2	5:L:169:LYS:HZ2	1.82	0.44
5:L:214:ALA:HB1	5:L:227:LEU:HD23	2.00	0.44
1:A:53:VAL:HA	1:A:144:VAL:HG13	1.98	0.44
2:C:564:MET:SD	2:C:846:LYS:HG2	2.58	0.44
3:D:571:LYS:NZ	5:F:155:ARG:HH22	2.15	0.44
3:D:1459:LEU:HB3	3:D:1465:ASN:HD21	1.82	0.44
2:I:12:VAL:HG22	2:I:534:VAL:HG13	1.99	0.44
2:I:86:LYS:HE2	2:I:813:VAL:HG23	2.00	0.44
2:I:704:HIS:HB2	2:I:831:ARG:NH1	2.32	0.44
3:J:1144:LEU:HB3	3:J:1171:VAL:HG22	1.99	0.44
4:K:88:GLU:HB3	4:K:91:ARG:HH21	1.82	0.44
1:A:39:PRO:HG2	1:B:39:PRO:HG3	1.98	0.44
2:C:399:ASN:ND2	2:C:402:SER:HB2	2.32	0.44
2:C:815:LEU:HD11	2:C:822:VAL:HG22	1.98	0.44
2:C:889:HIS:CE1	2:C:970:GLY:HA3	2.53	0.44
3:J:347:VAL:HG22	3:J:348:ALA:H	1.81	0.44
2:C:731:GLU:H	2:C:731:GLU:HG3	1.58	0.44
5:F:214:ALA:HB3	5:F:228:ILE:HG12	1.99	0.44
2:I:669:GLY:HA3	2:I:995:MET:HA	2.00	0.44
2:I:769:PRO:HG3	3:J:65:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:773:LEU:HD13	5:L:388:LYS:HG3	2.00	0.44
2:C:594:ALA:HB1	2:C:654:LEU:HD11	1.99	0.44
2:C:999:HIS:CD2	2:C:1004:LYS:HE3	2.53	0.44
3:D:224:ARG:NH2	3:D:254:GLU:OE2	2.43	0.44
3:D:242:LEU:H	3:D:312:ARG:HA	1.83	0.44
3:D:701:LEU:HD22	3:D:763:MET:HG2	2.00	0.44
3:D:780:LYS:HD2	3:D:912:LYS:HZ1	1.82	0.44
5:F:167:ASP:O	5:F:171:VAL:HB	2.18	0.44
1:H:75:VAL:O	1:H:79:ILE:HG13	2.17	0.44
2:I:90:TYR:CB	2:I:128:ILE:HB	2.48	0.44
2:I:564:MET:SD	2:I:846:LYS:HG2	2.58	0.44
3:J:167:GLU:OE2	3:J:198:ARG:NH2	2.51	0.44
1:A:32:PHE:CZ	1:B:43:ILE:HG12	2.52	0.43
2:C:326:ASP:HB2	2:C:431:HIS:HD2	1.83	0.43
2:C:641:PRO:HA	2:C:656:ALA:HA	2.00	0.43
2:C:669:GLY:HA3	2:C:995:MET:HA	2.00	0.43
2:C:876:VAL:HG11	2:C:885:ILE:HD11	2.00	0.43
2:C:1067:TYR:CZ	5:F:357:VAL:HG12	2.53	0.43
3:D:268:HIS:HB2	3:D:284:LEU:HB2	2.00	0.43
3:D:639:LEU:H	3:D:729:HIS:CD2	2.36	0.43
5:F:150:ILE:HD11	5:F:193:ARG:HH11	1.83	0.43
5:F:375:LYS:HD3	5:F:426:HIS:CG	2.53	0.43
1:G:101:LEU:HD21	1:G:109:VAL:HG11	1.99	0.43
2:I:470:PRO:HG3	2:I:485:TYR:CZ	2.52	0.43
3:J:639:LEU:H	3:J:729:HIS:CD2	2.36	0.43
3:J:784:ASP:HB2	3:J:939:PHE:HE2	1.83	0.43
3:J:947:ILE:HG23	3:J:1019:PRO:HB3	2.00	0.43
3:J:1426:LYS:HE2	3:J:1426:LYS:HB3	1.82	0.43
2:C:90:TYR:CB	2:C:128:ILE:HB	2.49	0.43
2:C:425:PHE:HE1	3:D:1086:LEU:HD12	1.83	0.43
2:C:853:LEU:HD23	2:C:853:LEU:H	1.82	0.43
3:D:217:ARG:O	3:D:338:GLU:HA	2.18	0.43
3:D:1144:LEU:HB3	3:D:1171:VAL:HG22	1.99	0.43
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.99	0.43
5:F:101:HIS:CD2	6:O:31:DG:H22	2.35	0.43
1:G:15:THR:O	1:H:232:LEU:HD22	2.18	0.43
2:I:326:ASP:HB2	2:I:431:HIS:HD2	1.83	0.43
2:I:498:GLN:HG3	3:J:1068:LEU:HD11	1.99	0.43
2:I:673:LEU:HG	2:I:867:VAL:HG12	2.00	0.43
2:I:778:PHE:CZ	5:L:434:ARG:HA	2.49	0.43
3:J:7:LYS:HE3	3:J:1458:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:166:GLN:HE21	3:J:396:VAL:HG22	1.83	0.43
3:J:834:THR:OG1	3:J:835:SER:N	2.51	0.43
3:J:1122:LEU:HD11	3:J:1186:VAL:HG23	2.00	0.43
1:A:97:THR:HG22	1:A:144:VAL:HB	1.99	0.43
2:C:937:ASP:HB3	2:C:940:GLU:HG3	2.00	0.43
3:D:834:THR:OG1	3:D:835:SER:N	2.51	0.43
3:D:947:ILE:HG23	3:D:1019:PRO:HB3	2.00	0.43
5:F:427:GLU:OE2	5:F:434:ARG:N	2.51	0.43
2:I:18:LEU:HB3	2:I:408:ARG:HD2	2.00	0.43
2:I:594:ALA:HB1	2:I:654:LEU:HD11	1.99	0.43
3:J:642:CYS:HB3	3:J:716:PHE:HB3	2.01	0.43
3:J:701:LEU:HD22	3:J:763:MET:HG2	2.00	0.43
5:L:369:LEU:HD23	5:L:433:LEU:HD13	1.99	0.43
1:A:15:THR:O	1:B:232:LEU:HD22	2.18	0.43
2:C:102:HIS:HB2	2:C:107:LEU:H	1.82	0.43
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.18	0.43
2:C:1073:GLY:HA3	3:D:659:LYS:HE2	2.00	0.43
3:D:260:GLU:OE1	3:D:273:ARG:NH2	2.52	0.43
2:I:89:THR:HG23	2:I:129:ILE:HA	2.00	0.43
2:I:148:PHE:HE2	2:I:280:LYS:HE3	1.84	0.43
3:J:894:LYS:HG3	3:J:895:VAL:H	1.83	0.43
3:J:965:GLU:HA	3:J:968:ASP:HB2	1.99	0.43
3:J:1293:PHE:CD2	3:J:1302:GLU:HB3	2.54	0.43
5:L:303:TYR:HA	5:L:306:ILE:HG22	2.00	0.43
6:O:4:DG:H1	7:P:45:DC:H42	1.65	0.43
2:C:184:MET:N	2:C:191:PHE:O	2.48	0.43
2:C:773:LEU:HD13	5:F:388:LYS:HG3	2.00	0.43
2:C:1102:LEU:HB3	2:C:1106:ASP:HA	2.00	0.43
3:D:7:LYS:HE3	3:D:1458:GLU:OE1	2.19	0.43
3:D:409:VAL:HG21	3:D:421:LEU:HD23	2.00	0.43
1:G:63:HIS:CE1	2:I:801:VAL:HG13	2.53	0.43
2:I:31:GLN:HB3	2:I:34:VAL:HB	2.01	0.43
3:J:634:GLY:O	3:J:637:LEU:N	2.52	0.43
3:J:1145:TYR:O	3:J:1364:HIS:NE2	2.52	0.43
5:L:150:ILE:HD11	5:L:193:ARG:HH11	1.83	0.43
2:C:1017:THR:OG1	2:C:1084:SER:HB3	2.18	0.43
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.54	0.43
3:D:31:THR:OG1	3:D:32:ILE:N	2.50	0.43
3:D:1060:SER:HB3	3:D:1063:GLU:HG3	2.01	0.43
3:D:1293:PHE:CD2	3:D:1302:GLU:HB3	2.54	0.43
5:F:269:GLN:HE21	5:F:269:GLN:HB2	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:ILE:HA	1:H:49:PRO:HD2	1.76	0.43
1:H:149:GLY:O	1:H:171:PHE:HB2	2.18	0.43
2:I:853:LEU:H	2:I:853:LEU:HD23	1.82	0.43
2:C:18:LEU:HB3	2:C:408:ARG:HD2	2.01	0.43
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.19	0.43
3:D:708:LEU:HD12	3:D:1231:GLU:HG2	2.01	0.43
5:F:202:LEU:HD22	5:F:239:VAL:HG22	2.01	0.43
2:I:738:ASP:OD2	2:I:744:ARG:HB3	2.19	0.43
2:I:876:VAL:HG11	2:I:885:ILE:HD11	2.01	0.43
3:J:769:LEU:O	3:J:778:LEU:HB3	2.18	0.43
3:J:796:ARG:HG3	3:J:861:GLN:HB2	2.00	0.43
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.99	0.43
2:C:252:LYS:HE3	2:C:252:LYS:HB2	1.87	0.43
2:C:836:GLY:N	2:C:849:VAL:O	2.52	0.43
3:D:1072:ILE:O	3:D:1075:HIS:HB2	2.19	0.43
5:F:244:TYR:H	5:F:244:TYR:HD2	1.65	0.43
5:F:411:ARG:HG2	6:O:1:DC:H3'	2.01	0.43
1:G:104:GLU:HB3	1:G:137:LYS:HG2	2.01	0.43
1:G:199:ILE:HB	1:G:207:PRO:HB3	2.00	0.43
3:J:31:THR:OG1	3:J:32:ILE:N	2.50	0.43
3:J:708:LEU:HD12	3:J:1231:GLU:HG2	2.01	0.43
3:J:1060:SER:HB3	3:J:1063:GLU:HG3	2.01	0.43
2:C:1042:ALA:HB1	3:D:1224:VAL:HG22	2.01	0.43
3:D:169:TYR:OH	3:D:198:ARG:N	2.36	0.43
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.82	0.43
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	2.00	0.43
2:I:750:LYS:HG2	2:I:751:PRO:HD2	2.01	0.43
2:I:937:ASP:HB3	2:I:940:GLU:HG3	2.00	0.43
5:L:167:ASP:O	5:L:171:VAL:HB	2.18	0.43
5:L:220:ARG:CZ	5:L:266:ILE:HD13	2.49	0.43
1:A:104:GLU:HB3	1:A:137:LYS:HG2	2.01	0.43
3:D:237:ARG:HG2	3:D:240:GLU:HB2	2.00	0.43
5:F:203:ILE:HD13	5:F:236:ILE:HG12	2.00	0.43
2:I:92:ALA:HA	2:I:93:PRO:HD3	1.88	0.43
2:I:425:PHE:HE1	3:J:1086:LEU:HD12	1.83	0.43
2:I:1106:ASP:OD1	3:J:7:LYS:NZ	2.37	0.43
3:J:411:THR:HG23	3:J:437:VAL:H	1.84	0.43
5:L:203:ILE:HD13	5:L:236:ILE:HG12	2.00	0.43
1:B:123:MET:O	1:B:125:PRO:HD3	2.19	0.42
2:C:12:VAL:HG22	2:C:534:VAL:HG13	2.00	0.42
2:C:89:THR:HG23	2:C:129:ILE:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:642:CYS:HB3	3:D:716:PHE:HB3	2.01	0.42
3:D:760:ARG:NH1	4:E:61:VAL:HB	2.34	0.42
5:F:96:VAL:HA	5:F:225:LEU:HD11	2.01	0.42
1:G:24:VAL:HG22	1:G:196:THR:HG23	2.01	0.42
3:J:397:LYS:NZ	3:J:448:GLU:O	2.50	0.42
3:J:671:LYS:HG3	5:L:436:PHE:CZ	2.54	0.42
3:J:1072:ILE:O	3:J:1075:HIS:HB2	2.19	0.42
5:L:244:TYR:HD2	5:L:244:TYR:H	1.65	0.42
1:B:149:GLY:O	1:B:171:PHE:HB2	2.18	0.42
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.53	0.42
3:D:628:ARG:HB2	3:D:745:MET:O	2.19	0.42
2:I:126:SER:HB3	2:I:407:LYS:NZ	2.33	0.42
2:I:641:PRO:HA	2:I:656:ALA:HA	2.00	0.42
2:I:836:GLY:N	2:I:849:VAL:O	2.52	0.42
2:I:1017:THR:OG1	2:I:1084:SER:HB3	2.18	0.42
5:L:409:ARG:NH2	7:S:43:DG:N7	2.66	0.42
2:C:954:SER:HA	2:C:955:PRO:HD3	1.89	0.42
3:D:258:VAL:HG12	3:D:259:VAL:H	1.83	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.91	0.42
3:D:796:ARG:HG3	3:D:861:GLN:HB2	2.00	0.42
3:D:1145:TYR:O	3:D:1364:HIS:NE2	2.52	0.42
5:F:303:TYR:HA	5:F:306:ILE:HG22	2.00	0.42
2:I:139:GLN:HB2	2:I:391:LEU:HD21	2.01	0.42
2:I:1038:TRP:CE2	3:J:1099:VAL:HG11	2.54	0.42
3:J:130:ASN:HA	5:L:98:GLN:HE22	1.85	0.42
3:J:437:VAL:HA	3:J:444:VAL:HG12	2.00	0.42
3:J:760:ARG:NH1	4:K:61:VAL:HB	2.35	0.42
5:L:166:PRO:HB2	5:L:169:LYS:HB3	2.02	0.42
1:A:63:HIS:CE1	1:A:66:SER:H	2.38	0.42
1:A:199:ILE:HB	1:A:207:PRO:HB3	2.00	0.42
2:C:139:GLN:HB2	2:C:391:LEU:HD21	2.00	0.42
2:C:448:ASN:HA	2:C:451:LEU:HD22	2.01	0.42
2:C:937:ASP:OD2	2:C:939:ARG:NE	2.50	0.42
3:D:397:LYS:NZ	3:D:397:LYS:HB3	2.35	0.42
3:D:894:LYS:HE3	3:D:894:LYS:HB2	1.85	0.42
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.99	0.42
1:H:122:ILE:HG22	1:H:124:ASN:H	1.84	0.42
2:I:11:GLU:HG3	2:I:535:SER:HB2	2.01	0.42
2:I:918:LEU:HD13	2:I:918:LEU:HA	1.92	0.42
3:J:667:ALA:HB1	3:J:672:ALA:CB	2.49	0.42
5:L:418:LYS:O	5:L:422:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:O	1:A:115:THR:N	2.53	0.42
2:C:436:GLY:HA3	2:C:469:THR:HG21	2.01	0.42
5:F:355:SER:HB3	5:F:358:GLU:HG3	2.01	0.42
5:F:418:LYS:O	5:F:422:LYS:HG3	2.20	0.42
1:H:123:MET:O	1:H:125:PRO:HD3	2.19	0.42
2:I:252:LYS:HB2	2:I:252:LYS:HE3	1.87	0.42
2:I:1020:PRO:HD2	3:J:622:ARG:O	2.19	0.42
3:J:124:GLU:OE2	3:J:587:ARG:NH2	2.53	0.42
3:J:633:VAL:C	3:J:635:PRO:HD3	2.40	0.42
3:J:1093:TYR:CD1	7:S:10:DA:H5"	2.55	0.42
5:L:124:GLY:O	5:L:128:ILE:HG13	2.19	0.42
1:B:54:THR:OG1	1:B:158:ILE:HG21	2.20	0.42
2:C:207:LEU:HD13	2:C:221:LEU:HD21	2.01	0.42
2:C:660:ALA:O	2:C:667:ALA:N	2.33	0.42
2:C:750:LYS:HG2	2:C:751:PRO:HD2	2.01	0.42
3:D:714:GLN:HB3	3:D:765:SER:HB3	2.02	0.42
3:D:894:LYS:HG3	3:D:895:VAL:H	1.83	0.42
3:D:896:ALA:O	3:D:900:ILE:HG13	2.20	0.42
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.20	0.42
5:F:166:PRO:HB2	5:F:169:LYS:HB3	2.02	0.42
2:I:1037:VAL:O	2:I:1041:GLU:HG3	2.19	0.42
3:J:714:GLN:HB3	3:J:765:SER:HB3	2.02	0.42
1:A:24:VAL:HG22	1:A:196:THR:HG23	2.01	0.42
1:B:161:ARG:HG3	1:B:162:ILE:N	2.35	0.42
2:C:9:ILE:H	2:C:9:ILE:HG13	1.68	0.42
2:C:1021:LEU:HD22	5:F:346:ASP:O	2.18	0.42
3:D:1439:SER:OG	3:D:1463:LYS:NZ	2.50	0.42
5:F:260:GLN:HE21	5:F:260:GLN:HB2	1.67	0.42
2:I:196:LEU:O	2:I:198:ARG:NH1	2.49	0.42
2:I:505:GLY:O	2:I:506:ASP:HB3	2.20	0.42
2:I:966:LEU:HD21	2:I:986:PRO:HB3	2.01	0.42
2:I:1013:TYR:O	5:L:350:ASP:N	2.48	0.42
3:J:166:GLN:HB3	3:J:396:VAL:HG13	2.02	0.42
5:L:301:PRO:HG3	5:L:306:ILE:HD13	2.01	0.42
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.55	0.42
1:B:211:LEU:O	1:B:215:VAL:HG13	2.20	0.42
2:C:1007:ALA:HB2	3:D:648:MET:HG3	2.02	0.42
3:D:172:PRO:HG2	3:D:175:VAL:HG21	2.02	0.42
3:D:224:ARG:HB3	3:D:251:PHE:HE1	1.84	0.42
3:D:735:ALA:HB2	3:D:778:LEU:HD21	2.02	0.42
3:D:1370:ILE:O	3:D:1374:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:THR:HG22	1:G:158:ILE:HD11	2.01	0.42
1:H:54:THR:OG1	1:H:158:ILE:HG21	2.20	0.42
2:I:100:LEU:HD21	2:I:102:HIS:HE1	1.85	0.42
3:J:660:LYS:HD2	3:J:660:LYS:HA	1.87	0.42
3:J:894:LYS:HB2	3:J:894:LYS:HE3	1.85	0.42
5:L:96:VAL:HA	5:L:225:LEU:HD11	2.01	0.42
6:O:42:DC:H2"	6:O:43:DG:C8	2.55	0.42
2:C:31:GLN:HB3	2:C:34:VAL:HB	2.01	0.42
2:C:191:PHE:HA	2:C:192:PRO:HD3	1.93	0.42
2:C:1020:PRO:HD2	3:D:622:ARG:O	2.19	0.42
2:C:1106:ASP:OD1	3:D:7:LYS:NZ	2.37	0.42
3:D:633:VAL:C	3:D:635:PRO:HD3	2.40	0.42
3:D:714:GLN:HB2	3:D:716:PHE:HE1	1.85	0.42
3:D:956:ILE:HG13	3:D:1062:ARG:HD3	2.01	0.42
3:D:1093:TYR:CD1	7:P:10:DA:H5"	2.55	0.42
1:H:184:THR:HG23	1:H:192:LEU:HB2	2.02	0.42
2:I:726:ILE:HG23	2:I:787:ASP:HB2	2.02	0.42
2:I:1042:ALA:HB1	3:J:1224:VAL:HG22	2.01	0.42
3:J:735:ALA:HB2	3:J:778:LEU:HD21	2.02	0.42
3:J:970:LYS:O	3:J:974:ILE:HG13	2.19	0.42
3:J:1351:GLU:O	3:J:1354:LYS:HB3	2.20	0.42
4:K:22:VAL:HG11	4:K:68:LEU:HD22	2.02	0.42
2:C:11:GLU:HG3	2:C:535:SER:HB2	2.01	0.42
2:C:148:PHE:HE2	2:C:280:LYS:HE3	1.84	0.42
2:C:530:GLU:H	2:C:530:GLU:HG2	1.58	0.42
3:D:634:GLY:O	3:D:637:LEU:N	2.52	0.42
3:D:638:LYS:HG2	3:D:932:ASP:CG	2.41	0.42
3:D:1006:ALA:O	3:D:1010:ASN:HB2	2.20	0.42
3:D:1459:LEU:HB3	3:D:1465:ASN:ND2	2.35	0.42
5:F:111:LEU:O	5:F:115:ILE:HG12	2.19	0.42
5:F:124:GLY:O	5:F:128:ILE:HG13	2.19	0.42
5:F:220:ARG:CZ	5:F:266:ILE:HD13	2.49	0.42
1:G:63:HIS:CE1	1:G:66:SER:H	2.38	0.42
2:I:250:LYS:HE2	2:I:250:LYS:HB3	1.92	0.42
2:I:676:ILE:HD13	2:I:988:VAL:HG23	2.02	0.42
2:I:1007:ALA:HB2	3:J:648:MET:HG3	2.02	0.42
3:J:31:THR:HG21	5:L:272:THR:HG22	2.02	0.42
3:J:638:LYS:HG2	3:J:932:ASP:CG	2.41	0.42
3:J:956:ILE:HG13	3:J:1062:ARG:HD3	2.01	0.42
3:J:1098:LEU:HD12	3:J:1424:VAL:HG11	2.02	0.42
3:J:1370:ILE:O	3:J:1374:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.20	0.42
1:B:122:ILE:HG22	1:B:124:ASN:H	1.84	0.41
2:C:327:HIS:NE2	2:C:492:ASP:OD1	2.53	0.41
2:C:603:VAL:HG21	2:C:643:VAL:HB	2.02	0.41
3:D:674:ARG:HH21	5:F:357:VAL:HG11	1.85	0.41
3:D:937:TYR:O	3:D:941:LEU:HG	2.19	0.41
3:D:970:LYS:O	3:D:974:ILE:HG13	2.20	0.41
1:H:132:LEU:HD12	1:H:136:GLY:HA3	2.02	0.41
2:I:1102:LEU:HB3	2:I:1106:ASP:HA	2.00	0.41
3:J:115:LEU:HD12	3:J:468:LEU:HD13	2.02	0.41
5:L:217:TYR:HD1	5:L:217:TYR:HA	1.77	0.41
5:L:379:ARG:HG3	5:L:405:PHE:CE2	2.55	0.41
1:B:48:ILE:HA	1:B:213:GLN:HE22	1.85	0.41
2:C:242:LEU:HD13	2:C:243:ARG:N	2.35	0.41
3:D:314:PRO:HG2	3:D:317:MET:HB3	2.01	0.41
3:D:1149:LEU:HD23	3:D:1149:LEU:HA	1.89	0.41
3:D:1426:LYS:HE2	3:D:1426:LYS:HB3	1.82	0.41
1:G:63:HIS:CE1	1:G:65:PHE:HB2	2.55	0.41
1:H:226:ALA:O	1:H:228:PRO:HD3	2.20	0.41
2:I:640:ARG:O	2:I:657:ASP:HB2	2.20	0.41
2:I:937:ASP:OD2	2:I:939:ARG:NE	2.50	0.41
3:J:22:SER:HA	3:J:90:MET:O	2.20	0.41
3:J:618:LEU:HD13	3:J:618:LEU:HA	1.86	0.41
3:J:937:TYR:O	3:J:941:LEU:HG	2.19	0.41
3:J:1006:ALA:O	3:J:1010:ASN:HB2	2.20	0.41
3:J:1149:LEU:HD23	3:J:1149:LEU:HA	1.88	0.41
4:K:49:ARG:HA	4:K:54:LEU:HG	2.02	0.41
5:L:111:LEU:O	5:L:115:ILE:HG12	2.20	0.41
5:L:355:SER:HB3	5:L:358:GLU:HG3	2.01	0.41
1:B:132:LEU:HD12	1:B:136:GLY:HA3	2.02	0.41
2:C:726:ILE:HG23	2:C:787:ASP:HB2	2.02	0.41
3:D:696:HIS:HB3	4:E:48:MET:HE1	2.02	0.41
3:D:1098:LEU:HD12	3:D:1424:VAL:HG11	2.02	0.41
4:E:3:GLU:HG2	4:E:65:MET:SD	2.61	0.41
4:E:49:ARG:HA	4:E:54:LEU:HG	2.02	0.41
5:F:379:ARG:HG3	5:F:405:PHE:CE2	2.55	0.41
1:H:48:ILE:HA	1:H:213:GLN:HE22	1.85	0.41
1:H:106:PRO:HA	1:H:132:LEU:O	2.21	0.41
2:I:708:TYR:HE1	2:I:827:VAL:HB	1.85	0.41
3:J:132:TYR:HB3	3:J:454:ALA:O	2.21	0.41
3:J:214:ASP:O	3:J:383:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:597:GLU:OE1	3:J:597:GLU:N	2.54	0.41
3:J:714:GLN:HB2	3:J:716:PHE:HE1	1.85	0.41
4:K:3:GLU:HG2	4:K:65:MET:SD	2.60	0.41
5:L:202:LEU:HD22	5:L:239:VAL:HG22	2.01	0.41
2:C:859:PRO:HG2	2:C:867:VAL:HG21	2.01	0.41
3:D:130:ASN:HA	5:F:98:GLN:HE22	1.85	0.41
3:D:156:GLU:H	3:D:156:GLU:HG3	1.70	0.41
3:D:212:ARG:HG2	3:D:213:VAL:N	2.34	0.41
3:D:402:PRO:HA	3:D:443:VAL:HA	2.01	0.41
3:D:660:LYS:HD2	3:D:660:LYS:HA	1.87	0.41
3:D:1093:TYR:HD1	7:P:10:DA:H5"	1.85	0.41
3:D:1351:GLU:O	3:D:1354:LYS:HB3	2.20	0.41
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.21	0.41
2:I:872:ASN:ND2	2:I:874:LEU:HB2	2.36	0.41
3:J:684:LYS:O	3:J:687:VAL:HG22	2.21	0.41
3:J:688:TRP:CE3	3:J:688:TRP:HA	2.55	0.41
7:S:33:DT:H2"	7:S:34:DA:C8	2.56	0.41
1:A:55:SER:HB2	1:A:158:ILE:HG13	2.02	0.41
2:C:411:SER:HB2	2:C:413:LEU:HG	2.03	0.41
2:C:640:ARG:O	2:C:657:ASP:HB2	2.20	0.41
2:C:832:LYS:HE3	2:C:832:LYS:HB2	1.83	0.41
2:C:918:LEU:HD13	2:C:918:LEU:HA	1.92	0.41
3:D:31:THR:HG21	5:F:272:THR:HG22	2.03	0.41
3:D:955:VAL:HA	3:D:1062:ARG:NH1	2.35	0.41
3:D:1196:THR:OG1	3:D:1201:CYS:HB3	2.20	0.41
2:I:328:LEU:HD11	2:I:434:HIS:ND1	2.35	0.41
2:I:491:GLU:OE1	2:I:516:ARG:NH2	2.53	0.41
3:J:696:HIS:HB3	4:K:48:MET:HE1	2.02	0.41
3:J:792:ILE:HG13	3:J:793:THR:N	2.36	0.41
3:J:896:ALA:O	3:J:900:ILE:HG13	2.20	0.41
1:B:106:PRO:HA	1:B:132:LEU:O	2.20	0.41
2:C:491:GLU:OE1	2:C:516:ARG:NH2	2.53	0.41
2:C:738:ASP:OD2	2:C:744:ARG:HB3	2.20	0.41
3:D:792:ILE:HG13	3:D:793:THR:N	2.35	0.41
3:D:970:LYS:O	3:D:973:GLN:HB3	2.21	0.41
4:E:22:VAL:HG11	4:E:68:LEU:HD22	2.02	0.41
5:F:252:THR:HA	6:O:29:DC:C5	2.55	0.41
2:I:207:LEU:HD13	2:I:221:LEU:HD21	2.01	0.41
2:I:436:GLY:HA3	2:I:469:THR:HG21	2.01	0.41
2:I:498:GLN:O	2:I:501:THR:OG1	2.30	0.41
2:I:859:PRO:HG2	2:I:867:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1020:PRO:O	3:J:622:ARG:HD2	2.21	0.41
3:J:698:LYS:HG3	4:K:59:ASN:ND2	2.35	0.41
3:J:1123:PHE:HB3	3:J:1132:LEU:HD22	2.03	0.41
2:C:90:TYR:HB3	2:C:128:ILE:HB	2.02	0.41
2:C:328:LEU:HD11	2:C:434:HIS:ND1	2.35	0.41
2:C:505:GLY:O	2:C:506:ASP:HB3	2.19	0.41
2:C:676:ILE:HD13	2:C:988:VAL:HG23	2.02	0.41
3:D:716:PHE:CZ	3:D:732:VAL:HG21	2.52	0.41
2:I:45:GLN:HA	2:I:48:PHE:HB2	2.03	0.41
2:I:151:ASP:HB2	2:I:157:ARG:O	2.21	0.41
2:I:603:VAL:HG21	2:I:643:VAL:HB	2.01	0.41
3:J:553:ARG:HD2	3:J:570:GLU:OE1	2.21	0.41
3:J:955:VAL:HA	3:J:1062:ARG:NH1	2.35	0.41
7:P:33:DT:H2"	7:P:34:DA:C8	2.56	0.41
1:A:54:THR:HG22	1:A:158:ILE:HD11	2.01	0.41
1:A:59:GLU:HG3	1:A:139:TYR:HD2	1.86	0.41
1:A:227:ASN:HA	1:A:228:PRO:HD2	1.85	0.41
1:B:184:THR:HG23	1:B:192:LEU:HB2	2.02	0.41
3:D:115:LEU:HD12	3:D:468:LEU:HD13	2.02	0.41
5:F:301:PRO:HG3	5:F:306:ILE:HD13	2.01	0.41
3:J:597:GLU:OE1	3:J:597:GLU:CA	2.68	0.41
3:J:628:ARG:HB2	3:J:745:MET:O	2.21	0.41
1:B:226:ALA:O	1:B:228:PRO:HD3	2.20	0.41
2:C:100:LEU:HD21	2:C:102:HIS:CE1	2.56	0.41
2:C:100:LEU:HD21	2:C:102:HIS:HE1	1.85	0.41
2:C:1020:PRO:O	3:D:622:ARG:HD2	2.21	0.41
3:D:291:LEU:HB2	3:D:304:LEU:O	2.21	0.41
3:D:353:VAL:HA	3:D:368:VAL:HG22	2.03	0.41
3:D:432:TYR:O	3:D:448:GLU:HA	2.20	0.41
3:D:670:VAL:HB	5:F:364:LEU:HD11	2.02	0.41
3:D:895:VAL:O	3:D:898:GLU:HB3	2.21	0.41
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.94	0.41
1:G:40:LEU:HD23	1:G:40:LEU:HA	1.97	0.41
1:G:223:ASN:HD22	1:G:223:ASN:HA	1.74	0.41
1:H:89:PHE:HB2	1:H:146:ARG:NH2	2.36	0.41
1:H:161:ARG:HG3	1:H:162:ILE:N	2.35	0.41
1:H:211:LEU:O	1:H:215:VAL:HG13	2.20	0.41
2:I:242:LEU:HD13	2:I:243:ARG:N	2.35	0.41
2:I:446:GLY:O	2:I:449:ILE:HG13	2.21	0.41
2:I:448:ASN:HA	2:I:451:LEU:HD22	2.02	0.41
2:I:537:LYS:O	2:I:545:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1107:ASN:HA	2:I:1108:PRO:HD3	1.87	0.41
3:J:22:SER:HG	3:J:92:HIS:CE1	2.36	0.41
3:J:56:TYR:CE2	3:J:82:ARG:HB3	2.56	0.41
3:J:348:ALA:HB1	3:J:350:HIS:CE1	2.55	0.41
3:J:441:ARG:HH12	3:J:445:ARG:HH11	1.68	0.41
3:J:970:LYS:O	3:J:973:GLN:HB3	2.21	0.41
3:J:1353:GLN:HG2	3:J:1368:ILE:HD12	2.03	0.41
3:J:1500:LYS:O	3:J:1503:VAL:HG22	2.21	0.41
1:B:28:LEU:HD21	1:B:36:LEU:HD13	2.03	0.41
2:C:45:GLN:HA	2:C:48:PHE:HB2	2.03	0.41
2:C:198:ARG:HG2	2:C:199:VAL:HG23	2.03	0.41
2:C:446:GLY:O	2:C:449:ILE:HG13	2.21	0.41
2:C:718:GLY:HA3	2:C:761:PHE:CD2	2.56	0.41
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.94	0.41
3:D:203:ALA:HA	3:D:395:VAL:HA	2.03	0.41
3:D:520:LEU:O	3:D:525:ARG:NE	2.54	0.41
3:D:569:ASN:OD1	3:D:572:ARG:NH2	2.48	0.41
3:D:596:SER:OG	3:D:598:ARG:HG2	2.21	0.41
3:D:625:TYR:CE2	3:D:655:PRO:HG2	2.54	0.41
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.03	0.41
3:D:1353:GLN:HG2	3:D:1368:ILE:HD12	2.03	0.41
1:G:100:ILE:O	1:G:115:THR:N	2.52	0.41
1:G:109:VAL:HG12	1:G:110:ARG:H	1.86	0.41
2:I:194:VAL:HG11	2:I:223:ASP:CB	2.51	0.41
2:I:411:SER:HB2	2:I:413:LEU:HG	2.02	0.41
3:J:657:LEU:HG	3:J:661:MET:SD	2.61	0.41
3:J:1462:LEU:O	3:J:1466:VAL:HG23	2.21	0.41
5:L:427:GLU:HA	5:L:430:THR:OG1	2.21	0.41
6:R:42:DC:H2"	6:R:43:DG:C8	2.55	0.41
1:A:72:LYS:HE3	2:C:641:PRO:O	2.21	0.40
1:A:109:VAL:HG12	1:A:110:ARG:H	1.86	0.40
2:C:151:ASP:HB2	2:C:157:ARG:O	2.21	0.40
2:C:441:VAL:O	2:C:443:THR:HG22	2.21	0.40
3:D:140:ALA:HA	3:D:450:TYR:CG	2.56	0.40
3:D:210:ARG:HD2	3:D:388:HIS:HB2	2.03	0.40
3:D:233:LYS:HZ2	3:D:235:ALA:H	1.68	0.40
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.55	0.40
3:D:908:LYS:HB2	3:D:1026:SER:O	2.21	0.40
1:G:72:LYS:HE3	2:I:641:PRO:O	2.21	0.40
3:J:209:ARG:HB3	3:J:347:VAL:HG11	2.03	0.40
3:J:565:ILE:HD12	3:J:565:ILE:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:675:ARG:HD2	3:J:679:ARG:CZ	2.51	0.40
3:J:749:VAL:HA	3:J:750:PRO:HD2	1.95	0.40
3:J:1093:TYR:HD1	7:S:10:DA:H5"	1.86	0.40
3:J:1153:VAL:HB	3:J:1160:LEU:HB2	2.03	0.40
2:C:92:ALA:HA	2:C:93:PRO:HD3	1.89	0.40
2:C:290:LEU:HD22	2:C:302:VAL:HG11	2.03	0.40
2:C:966:LEU:HD21	2:C:986:PRO:HB3	2.02	0.40
2:C:1050:GLN:HG3	3:D:1471:LEU:HA	2.03	0.40
3:D:556:LYS:HD2	3:D:556:LYS:HA	1.97	0.40
1:G:55:SER:HB2	1:G:158:ILE:HG13	2.02	0.40
1:G:182:GLU:O	1:G:193:ASP:HA	2.21	0.40
3:J:843:PHE:HB2	3:J:866:VAL:HG23	2.04	0.40
4:K:57:ASP:HA	4:K:58:PRO:HD2	1.94	0.40
1:B:32:PHE:HD2	1:B:32:PHE:HA	1.75	0.40
2:C:45:GLN:HE21	2:C:45:GLN:HB2	1.59	0.40
2:C:307:LEU:HD12	2:C:307:LEU:HA	1.84	0.40
2:C:430:VAL:HG11	2:C:440:PRO:HA	2.04	0.40
2:C:708:TYR:HE1	2:C:827:VAL:HB	1.85	0.40
3:D:230:TRP:HA	3:D:243:ALA:CB	2.51	0.40
3:D:231:VAL:O	3:D:236:TYR:OH	2.39	0.40
3:D:995:LEU:O	3:D:998:GLU:HG2	2.22	0.40
3:D:1470:ARG:HG2	3:D:1471:LEU:H	1.86	0.40
1:H:143:ARG:HD2	1:H:160:ASP:OD2	2.20	0.40
2:I:327:HIS:NE2	2:I:433:THR:HG21	2.36	0.40
2:I:718:GLY:HA3	2:I:761:PHE:CD2	2.56	0.40
2:I:874:LEU:O	3:J:1029:ARG:HG2	2.22	0.40
5:L:375:LYS:HE2	5:L:375:LYS:HB3	1.83	0.40
2:C:65:VAL:HG13	2:C:101:ILE:HB	2.03	0.40
2:C:327:HIS:NE2	2:C:433:THR:HG21	2.37	0.40
2:C:537:LYS:O	2:C:545:ASN:ND2	2.54	0.40
2:C:627:ARG:HD2	2:C:639:GLN:H	1.87	0.40
2:C:872:ASN:ND2	2:C:874:LEU:HB2	2.36	0.40
3:D:218:LYS:HZ2	3:D:338:GLU:HB2	1.87	0.40
3:D:553:ARG:HD2	3:D:570:GLU:OE1	2.21	0.40
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.36	0.40
3:D:911:LEU:O	3:D:915:VAL:HG23	2.22	0.40
5:F:375:LYS:HE2	5:F:375:LYS:HB3	1.83	0.40
2:I:100:LEU:HD21	2:I:102:HIS:CE1	2.56	0.40
3:J:671:LYS:HE3	3:J:671:LYS:HB3	1.94	0.40
3:J:1479:ASP:HA	3:J:1482:ARG:HG2	2.04	0.40
6:R:12:DT:H3	7:S:37:DA:H61	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:HD2	1:B:160:ASP:OD2	2.21	0.40
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.57	0.40
2:C:675:ALA:O	2:C:870:ILE:HA	2.21	0.40
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.56	0.40
1:G:27:PRO:HD3	1:G:186:LEU:HD22	2.04	0.40
2:I:90:TYR:HB3	2:I:128:ILE:HB	2.02	0.40
2:I:598:GLU:HG2	2:I:615:TYR:CZ	2.57	0.40
3:J:65:ARG:HG2	5:L:393:GLY:O	2.22	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	225/314 (72%)	206 (92%)	18 (8%)	1 (0%)	34	71
1	B	225/314 (72%)	205 (91%)	17 (8%)	3 (1%)	12	48
1	G	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	34	71
1	H	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	34	71
2	C	1108/1119 (99%)	1011 (91%)	94 (8%)	3 (0%)	41	75
2	I	1108/1119 (99%)	1012 (91%)	94 (8%)	2 (0%)	47	79
3	D	1486/1524 (98%)	1340 (90%)	141 (10%)	5 (0%)	41	75
3	J	1361/1524 (89%)	1235 (91%)	123 (9%)	3 (0%)	47	79
4	E	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
5	F	345/347 (99%)	316 (92%)	29 (8%)	0	100	100
5	L	345/347 (99%)	314 (91%)	31 (9%)	0	100	100
All	All	6835/7434 (92%)	6214 (91%)	602 (9%)	19 (0%)	41	75

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	765	GLN
3	D	1128	VAL
3	J	1128	VAL
1	A	53	VAL
1	B	178	ALA
3	D	415	VAL
3	D	431	ILE
3	D	666	PHE
1	G	53	VAL
3	J	179	VAL
1	B	51	THR
1	H	51	THR
2	I	1084	SER
1	B	177	VAL
2	C	1084	SER
3	D	667	ALA
3	J	667	ALA
2	C	870	ILE
2	I	870	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	194/270 (72%)	186 (96%)	8 (4%)	30 57
1	B	194/270 (72%)	179 (92%)	15 (8%)	13 40
1	G	194/270 (72%)	186 (96%)	8 (4%)	30 57
1	H	194/270 (72%)	179 (92%)	15 (8%)	13 40
2	C	931/936 (100%)	837 (90%)	94 (10%)	7 29
2	I	931/936 (100%)	838 (90%)	93 (10%)	7 29
3	D	1252/1281 (98%)	1128 (90%)	124 (10%)	8 29
3	J	1150/1281 (90%)	1048 (91%)	102 (9%)	9 34
4	E	83/88 (94%)	77 (93%)	6 (7%)	14 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	83/88 (94%)	77 (93%)	6 (7%)	14 42
5	F	297/299 (99%)	269 (91%)	28 (9%)	8 31
5	L	297/299 (99%)	269 (91%)	28 (9%)	8 31
All	All	5800/6288 (92%)	5273 (91%)	527 (9%)	9 33

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	44	LEU
1	A	59	GLU
1	A	86	VAL
1	A	98	THR
1	A	109	VAL
1	A	172	SER
1	A	186	LEU
1	B	7	LYS
1	B	20	TYR
1	B	30	ARG
1	B	53	VAL
1	B	54	THR
1	B	58	ILE
1	B	75	VAL
1	B	114	PHE
1	B	115	THR
1	B	145	ASP
1	B	170	ILE
1	B	176	ARG
1	B	177	VAL
1	B	184	THR
1	B	218	LEU
2	C	15	LEU
2	C	30	LEU
2	C	41	ASN
2	C	45	GLN
2	C	48	PHE
2	C	56	GLU
2	C	73	ILE
2	C	75	ASP
2	C	80	GLN
2	C	81	ASP

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Mol	Chain	Res	Type
2	C	87	ASP
2	C	98	LEU
2	C	100	LEU
2	C	104	ASP
2	C	111	ASP
2	C	112	GLU
2	C	120	LEU
2	C	122	THR
2	C	142	ARG
2	C	151	ASP
2	C	159	ILE
2	C	163	ILE
2	C	174	LEU
2	C	179	SER
2	C	197	LEU
2	C	198	ARG
2	C	199	VAL
2	C	211	LEU
2	C	217	LEU
2	C	222	LEU
2	C	237	ARG
2	C	242	LEU
2	C	251	ASP
2	C	258	PHE
2	C	260	LEU
2	C	280	LYS
2	C	301	GLU
2	C	323	ASP
2	C	340	MET
2	C	365	ASP
2	C	393	GLN
2	C	394	PHE
2	C	396	ASP
2	C	398	THR
2	C	421	GLU
2	C	427	VAL
2	C	429	ASP
2	C	430	VAL
2	C	453	THR
2	C	469	THR
2	C	474	VAL
2	C	495	THR

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Mol	Chain	Res	Type
2	C	503	LEU
2	C	523	ILE
2	C	528	GLU
2	C	530	GLU
2	C	533	ASP
2	C	543	ASN
2	C	545	ASN
2	C	553	ASP
2	C	600	ASP
2	C	609	THR
2	C	616	GLU
2	C	679	PHE
2	C	680	ASP
2	C	685	GLU
2	C	703	ILE
2	C	707	ARG
2	C	729	LEU
2	C	738	ASP
2	C	745	ILE
2	C	764	GLU
2	C	766	GLU
2	C	788	THR
2	C	796	GLU
2	C	808	ARG
2	C	814	GLU
2	C	815	LEU
2	C	829	GLN
2	C	857	ASP
2	C	861	LEU
2	C	869	VAL
2	C	946	ARG
2	C	960	GLU
2	C	963	LEU
2	C	966	LEU
2	C	995	MET
2	C	1050	GLN
2	C	1056	LYS
2	C	1058	ASP
2	C	1061	GLU
2	C	1081	VAL
2	C	1099	VAL
2	C	1106	ASP

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Mol	Chain	Res	Type
3	D	3	LYS
3	D	26	VAL
3	D	35	ARG
3	D	38	LYS
3	D	58	CYS
3	D	66	GLN
3	D	68	PHE
3	D	73	CYS
3	D	92	HIS
3	D	97	THR
3	D	112	ILE
3	D	115	LEU
3	D	135	LEU
3	D	142	LEU
3	D	156	GLU
3	D	165	LYS
3	D	166	GLN
3	D	199	MET
3	D	213	VAL
3	D	261	LEU
3	D	277	GLU
3	D	281	ARG
3	D	283	PHE
3	D	297	ILE
3	D	299	GLU
3	D	304	LEU
3	D	306	GLU
3	D	315	ARG
3	D	316	HIS
3	D	333	LEU
3	D	334	THR
3	D	347	VAL
3	D	371	ILE
3	D	372	ASP
3	D	387	LEU
3	D	389	GLU
3	D	395	VAL
3	D	397	LYS
3	D	414	ARG
3	D	421	LEU
3	D	423	ASP
3	D	430	GLU

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Mol	Chain	Res	Type
3	D	434	ARG
3	D	440	VAL
3	D	445	ARG
3	D	448	GLU
3	D	450	TYR
3	D	464	LEU
3	D	472	LYS
3	D	480	GLU
3	D	523	ASP
3	D	534	ARG
3	D	535	PHE
3	D	557	LEU
3	D	558	LEU
3	D	597	GLU
3	D	618	LEU
3	D	636	GLN
3	D	637	LEU
3	D	639	LEU
3	D	682	ASP
3	D	683	ILE
3	D	685	ASP
3	D	694	VAL
3	D	704	ARG
3	D	708	LEU
3	D	709	HIS
3	D	741	ASP
3	D	749	VAL
3	D	776	GLU
3	D	778	LEU
3	D	780	LYS
3	D	794	GLN
3	D	795	VAL
3	D	804	MET
3	D	817	GLU
3	D	845	ASN
3	D	865	THR
3	D	884	ARG
3	D	888	GLU
3	D	901	GLN
3	D	903	ASP
3	D	908	LYS
3	D	914	LEU

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Mol	Chain	Res	Type
3	D	927	THR
3	D	932	ASP
3	D	953	ASP
3	D	959	GLU
3	D	968	ASP
3	D	971	LEU
3	D	976	GLN
3	D	1017	PHE
3	D	1052	THR
3	D	1053	PHE
3	D	1070	TYR
3	D	1078	ARG
3	D	1083	ASP
3	D	1098	LEU
3	D	1132	LEU
3	D	1134	LEU
3	D	1137	ARG
3	D	1158	ARG
3	D	1159	ARG
3	D	1161	GLU
3	D	1234	THR
3	D	1235	GLN
3	D	1237	THR
3	D	1267	ARG
3	D	1269	LYS
3	D	1278	ASP
3	D	1285	GLU
3	D	1297	GLU
3	D	1307	LYS
3	D	1311	LEU
3	D	1312	LEU
3	D	1335	LEU
3	D	1346	ARG
3	D	1364	HIS
3	D	1397	LYS
3	D	1398	TRP
3	D	1443	THR
3	D	1448	THR
3	D	1462	LEU
3	D	1499	ARG
4	E	3	GLU
4	E	39	VAL

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Mol	Chain	Res	Type
4	E	56	ASP
4	E	59	ASN
4	E	62	THR
4	E	65	MET
5	F	101	HIS
5	F	105	GLN
5	F	151	LEU
5	F	159	ILE
5	F	189	LEU
5	F	217	TYR
5	F	224	PHE
5	F	226	ASP
5	F	227	LEU
5	F	244	TYR
5	F	255	THR
5	F	259	ARG
5	F	260	GLN
5	F	268	ASP
5	F	269	GLN
5	F	274	ARG
5	F	293	LEU
5	F	294	GLN
5	F	305	GLU
5	F	323	LEU
5	F	328	GLU
5	F	346	ASP
5	F	352	ASN
5	F	362	GLN
5	F	404	TYR
5	F	405	PHE
5	F	409	ARG
5	F	435	ASP
1	G	32	PHE
1	G	44	LEU
1	G	59	GLU
1	G	86	VAL
1	G	98	THR
1	G	109	VAL
1	G	172	SER
1	G	186	LEU
1	H	7	LYS
1	H	20	TYR

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Mol	Chain	Res	Type
1	H	30	ARG
1	H	53	VAL
1	H	54	THR
1	H	58	ILE
1	H	75	VAL
1	H	114	PHE
1	H	115	THR
1	H	145	ASP
1	H	170	ILE
1	H	176	ARG
1	H	177	VAL
1	H	184	THR
1	H	218	LEU
2	I	15	LEU
2	I	30	LEU
2	I	41	ASN
2	I	45	GLN
2	I	48	PHE
2	I	56	GLU
2	I	73	ILE
2	I	75	ASP
2	I	80	GLN
2	I	81	ASP
2	I	87	ASP
2	I	98	LEU
2	I	100	LEU
2	I	104	ASP
2	I	111	ASP
2	I	112	GLU
2	I	120	LEU
2	I	122	THR
2	I	142	ARG
2	I	151	ASP
2	I	159	ILE
2	I	163	ILE
2	I	174	LEU
2	I	179	SER
2	I	197	LEU
2	I	198	ARG
2	I	199	VAL
2	I	211	LEU
2	I	217	LEU

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Mol	Chain	Res	Type
2	I	222	LEU
2	I	237	ARG
2	I	242	LEU
2	I	251	ASP
2	I	258	PHE
2	I	260	LEU
2	I	280	LYS
2	I	301	GLU
2	I	323	ASP
2	I	340	MET
2	I	365	ASP
2	I	393	GLN
2	I	394	PHE
2	I	396	ASP
2	I	398	THR
2	I	421	GLU
2	I	427	VAL
2	I	429	ASP
2	I	430	VAL
2	I	453	THR
2	I	469	THR
2	I	474	VAL
2	I	495	THR
2	I	503	LEU
2	I	523	ILE
2	I	528	GLU
2	I	530	GLU
2	I	533	ASP
2	I	543	ASN
2	I	545	ASN
2	I	553	ASP
2	I	600	ASP
2	I	609	THR
2	I	616	GLU
2	I	679	PHE
2	I	680	ASP
2	I	685	GLU
2	I	703	ILE
2	I	707	ARG
2	I	729	LEU
2	I	738	ASP
2	I	764	GLU

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Mol	Chain	Res	Type
2	I	766	GLU
2	I	788	THR
2	I	796	GLU
2	I	808	ARG
2	I	814	GLU
2	I	815	LEU
2	I	829	GLN
2	I	857	ASP
2	I	861	LEU
2	I	869	VAL
2	I	946	ARG
2	I	960	GLU
2	I	963	LEU
2	I	966	LEU
2	I	995	MET
2	I	1050	GLN
2	I	1056	LYS
2	I	1058	ASP
2	I	1061	GLU
2	I	1081	VAL
2	I	1099	VAL
2	I	1106	ASP
3	J	3	LYS
3	J	26	VAL
3	J	35	ARG
3	J	38	LYS
3	J	58	CYS
3	J	66	GLN
3	J	68	PHE
3	J	73	CYS
3	J	92	HIS
3	J	97	THR
3	J	112	ILE
3	J	115	LEU
3	J	135	LEU
3	J	142	LEU
3	J	156	GLU
3	J	178	LEU
3	J	187	LYS
3	J	200	ASP
3	J	344	ASP
3	J	350	HIS

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Mol	Chain	Res	Type
3	J	372	ASP
3	J	393	ILE
3	J	397	LYS
3	J	404	GLU
3	J	443	VAL
3	J	445	ARG
3	J	464	LEU
3	J	472	LYS
3	J	480	GLU
3	J	523	ASP
3	J	535	PHE
3	J	557	LEU
3	J	558	LEU
3	J	597	GLU
3	J	618	LEU
3	J	636	GLN
3	J	637	LEU
3	J	639	LEU
3	J	682	ASP
3	J	683	ILE
3	J	685	ASP
3	J	694	VAL
3	J	704	ARG
3	J	708	LEU
3	J	709	HIS
3	J	741	ASP
3	J	749	VAL
3	J	776	GLU
3	J	778	LEU
3	J	780	LYS
3	J	794	GLN
3	J	795	VAL
3	J	804	MET
3	J	817	GLU
3	J	845	ASN
3	J	865	THR
3	J	884	ARG
3	J	888	GLU
3	J	901	GLN
3	J	903	ASP
3	J	908	LYS
3	J	914	LEU

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Mol	Chain	Res	Type
3	J	927	THR
3	J	932	ASP
3	J	953	ASP
3	J	959	GLU
3	J	968	ASP
3	J	971	LEU
3	J	976	GLN
3	J	1017	PHE
3	J	1052	THR
3	J	1053	PHE
3	J	1070	TYR
3	J	1078	ARG
3	J	1083	ASP
3	J	1098	LEU
3	J	1132	LEU
3	J	1134	LEU
3	J	1137	ARG
3	J	1158	ARG
3	J	1159	ARG
3	J	1161	GLU
3	J	1234	THR
3	J	1235	GLN
3	J	1237	THR
3	J	1267	ARG
3	J	1269	LYS
3	J	1278	ASP
3	J	1285	GLU
3	J	1297	GLU
3	J	1307	LYS
3	J	1311	LEU
3	J	1312	LEU
3	J	1335	LEU
3	J	1346	ARG
3	J	1364	HIS
3	J	1397	LYS
3	J	1398	TRP
3	J	1443	THR
3	J	1448	THR
3	J	1462	LEU
3	J	1499	ARG
4	K	3	GLU
4	K	39	VAL

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Mol	Chain	Res	Type
4	K	56	ASP
4	K	59	ASN
4	K	62	THR
4	K	65	MET
5	L	101	HIS
5	L	105	GLN
5	L	151	LEU
5	L	159	ILE
5	L	189	LEU
5	L	217	TYR
5	L	224	PHE
5	L	226	ASP
5	L	227	LEU
5	L	244	TYR
5	L	255	THR
5	L	259	ARG
5	L	260	GLN
5	L	268	ASP
5	L	269	GLN
5	L	274	ARG
5	L	293	LEU
5	L	294	GLN
5	L	305	GLU
5	L	323	LEU
5	L	328	GLU
5	L	346	ASP
5	L	352	ASN
5	L	362	GLN
5	L	404	TYR
5	L	405	PHE
5	L	409	ARG
5	L	426	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	212	ASN
1	A	213	GLN
1	A	223	ASN
1	B	156	HIS
1	B	213	GLN

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Mol	Chain	Res	Type
1	B	227	ASN
2	C	41	ASN
2	C	45	GLN
2	C	80	GLN
2	C	390	GLN
2	C	829	GLN
2	C	899	GLN
2	C	1050	GLN
2	C	1068	GLN
2	C	1107	ASN
3	D	66	GLN
3	D	166	GLN
3	D	332	HIS
3	D	507	ASN
3	D	549	ASN
3	D	703	ASN
3	D	762	GLN
3	D	794	GLN
3	D	991	GLN
3	D	1046	GLN
3	D	1075	HIS
3	D	1235	GLN
5	F	98	GLN
5	F	101	HIS
5	F	229	GLN
5	F	232	ASN
5	F	260	GLN
5	F	269	GLN
5	F	295	GLN
1	G	81	ASN
1	G	212	ASN
1	G	213	GLN
1	G	223	ASN
1	H	156	HIS
1	H	213	GLN
1	H	227	ASN
2	I	41	ASN
2	I	45	GLN
2	I	80	GLN
2	I	765	GLN
2	I	829	GLN
2	I	899	GLN

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Mol	Chain	Res	Type
2	I	1050	GLN
2	I	1068	GLN
2	I	1107	ASN
3	J	66	GLN
3	J	166	GLN
3	J	350	HIS
3	J	507	ASN
3	J	549	ASN
3	J	703	ASN
3	J	762	GLN
3	J	794	GLN
3	J	991	GLN
3	J	1046	GLN
3	J	1075	HIS
3	J	1235	GLN
5	L	98	GLN
5	L	101	HIS
5	L	229	GLN
5	L	232	ASN
5	L	260	GLN
5	L	269	GLN
5	L	295	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Q	3/4 (75%)	1 (33%)	0
8	T	3/4 (75%)	1 (33%)	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	Q	2	C
8	T	2	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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	227/314 (72%)	-0.33	0 100 100	68, 121, 176, 228	0
1	B	227/314 (72%)	-0.49	0 100 100	42, 95, 150, 180	0
1	G	227/314 (72%)	-0.01	2 (0%) 84 77	96, 156, 194, 223	0
1	H	227/314 (72%)	-0.29	0 100 100	80, 131, 171, 192	0
2	C	1112/1119 (99%)	-0.30	6 (0%) 91 85	30, 123, 203, 260	0
2	I	1112/1119 (99%)	-0.17	15 (1%) 77 68	60, 146, 214, 259	0
3	D	1490/1524 (97%)	-0.42	1 (0%) 95 94	22, 88, 155, 231	0
3	J	1367/1524 (89%)	-0.33	1 (0%) 95 94	29, 112, 177, 240	0
4	E	93/99 (93%)	-0.41	0 100 100	23, 89, 154, 187	0
4	K	93/99 (93%)	-0.24	0 100 100	67, 126, 181, 236	0
5	F	347/347 (100%)	-0.20	6 (1%) 70 60	52, 131, 221, 275	0
5	L	347/347 (100%)	-0.12	5 (1%) 75 65	81, 151, 225, 270	0
6	O	48/48 (100%)	0.40	4 (8%) 11 10	86, 193, 267, 293	0
6	R	48/48 (100%)	0.08	1 (2%) 63 54	109, 184, 277, 300	0
7	P	48/48 (100%)	0.61	4 (8%) 11 10	77, 199, 251, 283	0
7	S	43/48 (89%)	0.14	1 (2%) 60 51	100, 195, 234, 248	0
8	Q	4/4 (100%)	0.06	0 100 100	116, 124, 128, 150	0
8	T	4/4 (100%)	0.05	0 100 100	122, 130, 143, 154	0
All	All	7064/7634 (92%)	-0.28	46 (0%) 87 82	22, 120, 200, 300	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	GLY	5.3
5	L	177	LYS	4.4
2	I	246	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	1253	THR	3.6
7	P	48	DG	3.2
2	I	64	LEU	3.2
2	C	292	ARG	3.2
6	O	1	DC	3.1
7	P	47	DA	3.0
5	L	157	GLN	3.0
6	O	2	DT	3.0
6	O	48	DC	3.0
2	I	296	GLY	2.9
2	I	248	PRO	2.9
2	I	247	PRO	2.8
2	C	251	ASP	2.7
2	I	255	ALA	2.7
2	I	649	VAL	2.6
7	S	1	DG	2.6
3	J	406	ASP	2.5
2	I	295	ASP	2.5
2	C	252	LYS	2.4
7	P	1	DG	2.4
2	C	250	LYS	2.4
2	I	252	LYS	2.4
2	I	63	GLY	2.4
2	I	784	ASP	2.3
5	L	174	VAL	2.3
2	C	249	LYS	2.3
6	R	48	DC	2.3
2	I	362	GLY	2.2
6	O	8	DA	2.2
2	I	254	LEU	2.1
2	I	245	GLY	2.1
1	G	186	LEU	2.1
5	F	167	ASP	2.1
5	F	157	GLN	2.1
2	C	102	HIS	2.1
2	I	621	VAL	2.1
7	P	45	DC	2.1
5	F	154	ALA	2.1
5	F	155	ARG	2.0
5	L	135	THR	2.0
5	L	178	LEU	2.0
5	F	168	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	171	VAL	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
10	MG	D	2003	1/1	0.94	0.07	180,180,180,180	0
9	ZN	J	2002	1/1	0.95	0.07	166,166,166,166	0
10	MG	J	2003	1/1	0.95	0.25	188,188,188,188	0
9	ZN	D	2002	1/1	0.96	0.07	79,79,79,79	0
9	ZN	D	2001	1/1	0.97	0.12	79,79,79,79	0
9	ZN	J	2001	1/1	0.99	0.12	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.