Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 01:10 PM EDT

PDB ID	:	3SIV
Title	:	Structure of a hPrp31-15.5K-U4atac 5' stem loop complex, dimeric form
Authors	:	Liu, S.; Ghalei, H.; Luhrmann, R.; Wahl, M.C.
Deposited on	:	2011-06-20
Resolution	:	3.30 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 (i) 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 (1)) were used in the production of this report:

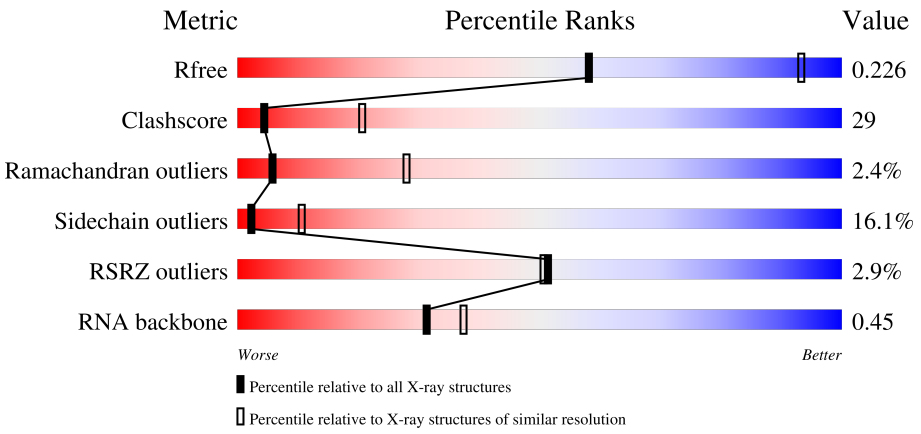
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	130	40% 49% 9% •
1	D	130	4% 40% 45% 11% •
1	G	130	% 48% 42% 8% •
1	J	130	2% 45% 41% 12% •

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Mol	Chain	Length	Quality of chain
2	B	254	%, 36%, 46%, 11%, 7%
2	E	254	%, 47%, 35%, 10%, 7%
2	H	254	10%, 46%, 39%, 7%, 7%
2	K	254	3%, 51%, 37%, 6%, 5%
3	C	32	50%, 41%, 9%
3	F	32	38%, 41%, 19%
3	I	32	50%, 41%, 9%
3	L	32	38%, 41%, 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14114 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 NHP2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	128	991	625	175	185	6	0	0	0
1	D	125	968	611	172	180	5	0	0	0
1	G	128	992	625	175	186	6	0	0	0
1	J	126	976	616	173	182	5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P55769
A	0	SER	-	expression tag	UNP P55769
D	-1	GLY	-	expression tag	UNP P55769
D	0	SER	-	expression tag	UNP P55769
G	-1	GLY	-	expression tag	UNP P55769
G	0	SER	-	expression tag	UNP P55769
J	-1	GLY	-	expression tag	UNP P55769
J	0	SER	-	expression tag	UNP P55769

- Molecule 2 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	237	1860	1168	321	361	10	1	0	0
2	E	236	1851	1163	320	358	10	0	0	0
2	H	235	1844	1158	319	357	10	3	0	0
2	K	241	1892	1188	329	365	10	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	80	GLY	-	expression tag	UNP Q8WWY3
B	81	PRO	-	expression tag	UNP Q8WWY3
B	82	LEU	-	expression tag	UNP Q8WWY3
B	83	GLY	-	expression tag	UNP Q8WWY3
B	84	SER	-	expression tag	UNP Q8WWY3
E	80	GLY	-	expression tag	UNP Q8WWY3
E	81	PRO	-	expression tag	UNP Q8WWY3
E	82	LEU	-	expression tag	UNP Q8WWY3
E	83	GLY	-	expression tag	UNP Q8WWY3
E	84	SER	-	expression tag	UNP Q8WWY3
H	80	GLY	-	expression tag	UNP Q8WWY3
H	81	PRO	-	expression tag	UNP Q8WWY3
H	82	LEU	-	expression tag	UNP Q8WWY3
H	83	GLY	-	expression tag	UNP Q8WWY3
H	84	SER	-	expression tag	UNP Q8WWY3
K	80	GLY	-	expression tag	UNP Q8WWY3
K	81	PRO	-	expression tag	UNP Q8WWY3
K	82	LEU	-	expression tag	UNP Q8WWY3
K	83	GLY	-	expression tag	UNP Q8WWY3
K	84	SER	-	expression tag	UNP Q8WWY3

- Molecule 3 is a RNA chain called U4atac snRNA.

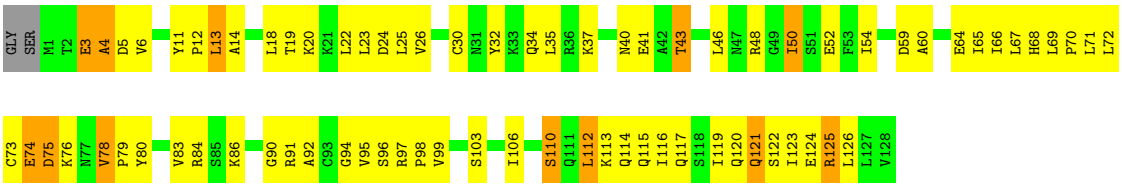
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	32	685	307	127	220	31	0	0	0
3	F	32	685	307	127	220	31	0	0	0
3	I	32	685	307	127	220	31	0	0	0
3	L	32	685	307	127	220	31	0	0	0

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.

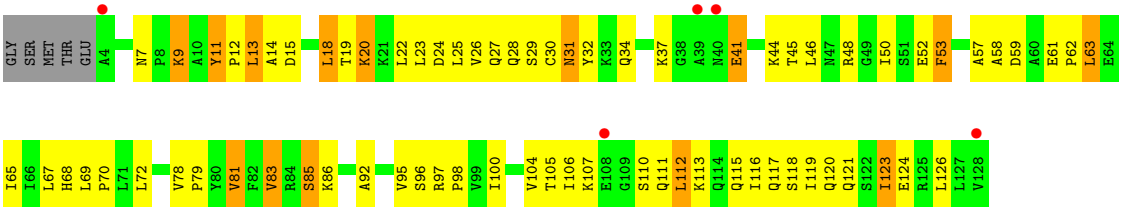
• Molecule 1: NHP2-like protein 1

Chain A:



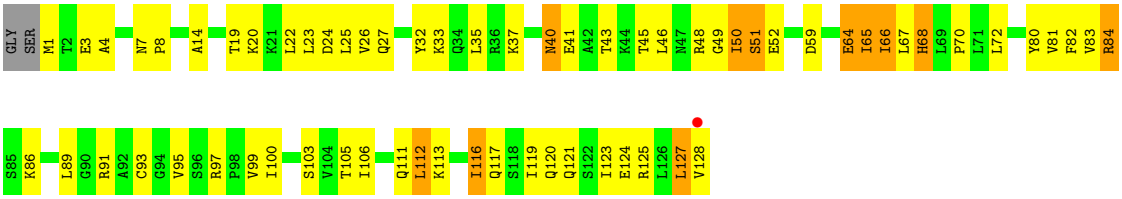
• Molecule 1: NHP2-like protein 1

Chain D:



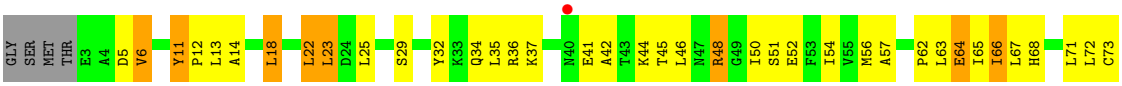
• Molecule 1: NHP2-like protein 1

Chain G:



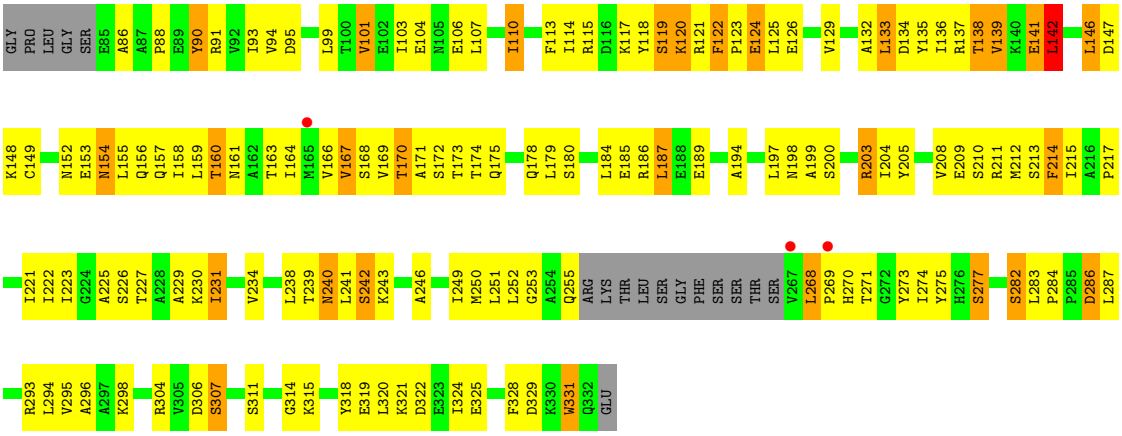
• Molecule 1: NHP2-like protein 1

Chain J:



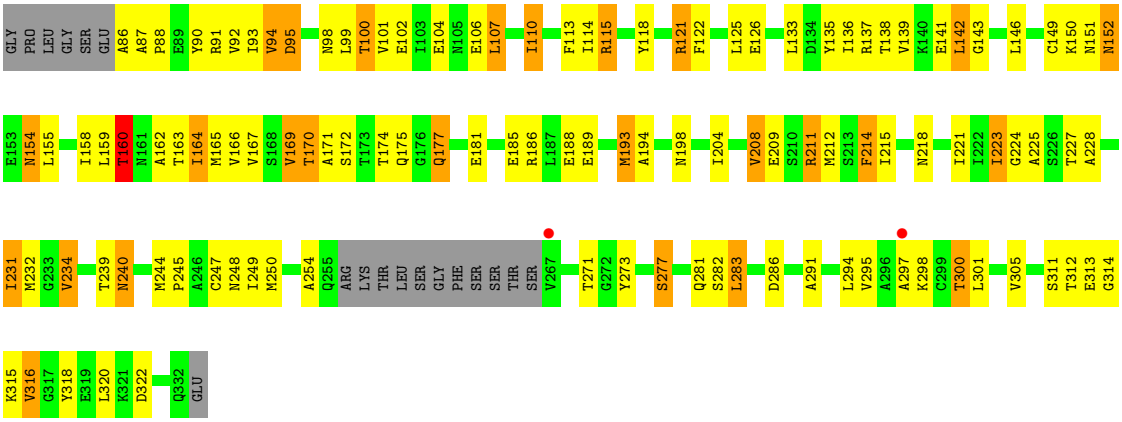
• Molecule 2: U4/U6 small nuclear ribonucleoprotein Prp31

Chain B:



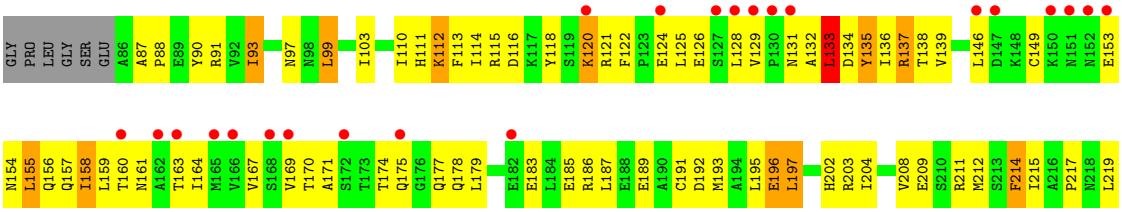
• Molecule 2: U4/U6 small nuclear ribonucleoprotein Prp31

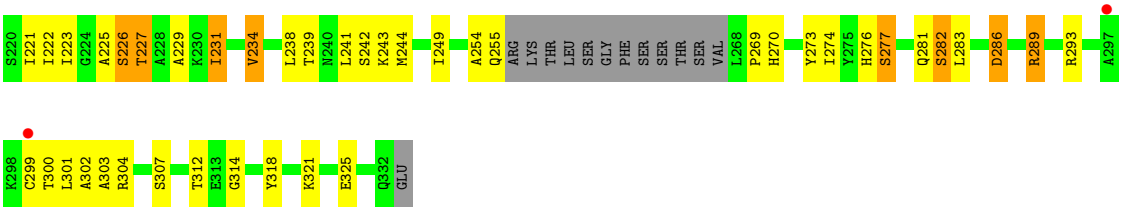
Chain E:



• Molecule 2: U4/U6 small nuclear ribonucleoprotein Prp31

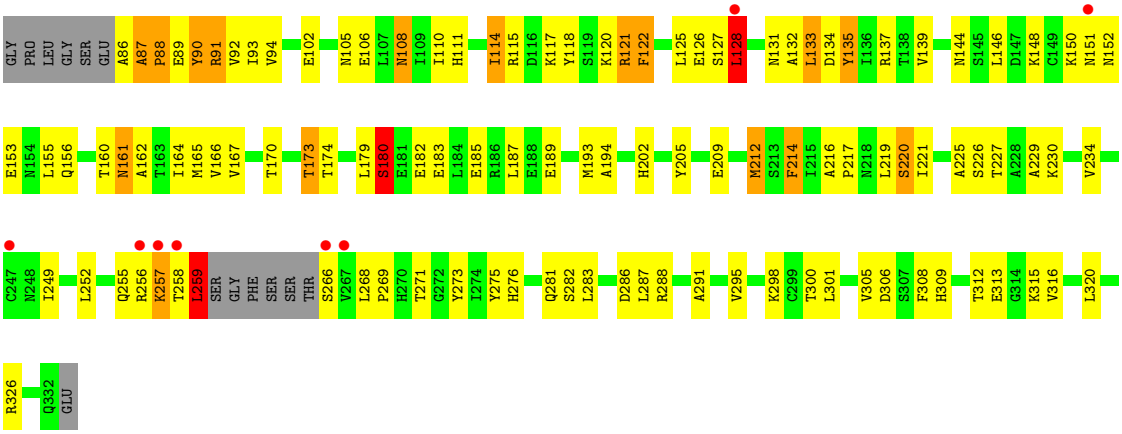
Chain H:





• Molecule 2: U4/U6 small nuclear ribonucleoprotein Prp31

Chain K:

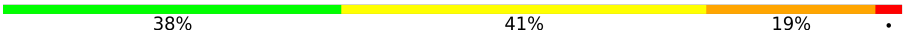


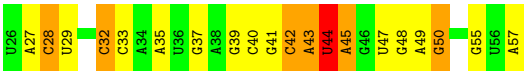
• Molecule 3: U4atac snRNA

Chain C:

• Molecule 3: U4atac snRNA

Chain F:



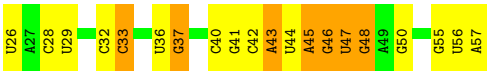


• Molecule 3: U4atac snRNA

Chain I:

• Molecule 3: U4atac snRNA

Chain L:


U26
A27
C28
U29
C32
C33
U36
G37
C40
G41
C42
A43
U44
A45
G46
U47
G48
A49
G50
G55
U56
A57

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	255.41Å 105.33Å 188.64Å 90.00° 127.52° 90.00°	Depositor
Resolution (Å)	29.92 – 3.30 29.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.92-3.30) 99.3 (29.92-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.198 , 0.239 0.177 , 0.226	Depositor DCC
R_{free} test set	2991 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	119.0	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 76.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14114	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 (i)

5.1 Standard geometry (i)

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	0.52	0/1003	0.70	0/1355
1	D	0.43	0/980	0.65	0/1323
1	G	0.56	0/1004	0.68	0/1355
1	J	0.44	0/988	0.65	0/1335
2	B	0.50	0/1886	0.65	0/2548
2	E	0.49	0/1877	0.68	0/2536
2	H	0.46	0/1870	0.65	1/2526 (0.0%)
2	K	0.45	0/1918	0.63	1/2590 (0.0%)
3	C	0.76	0/767	1.09	0/1195
3	F	0.82	0/767	1.24	7/1195 (0.6%)
3	I	0.76	0/767	1.12	0/1195
3	L	0.75	0/767	1.26	6/1195 (0.5%)
All	All	0.55	0/14594	0.81	15/20348 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	55	G	C2-N3-C4	8.44	116.12	111.90
3	L	33	C	C6-N1-C2	7.46	123.28	120.30
3	L	33	C	C5-C6-N1	-7.43	117.28	121.00
3	F	55	G	C5-C6-N1	7.29	115.15	111.50
3	F	33	C	C6-N1-C2	7.11	123.14	120.30
3	L	37	G	N3-C4-N9	6.20	129.72	126.00
3	F	37	G	N3-C4-N9	6.01	129.61	126.00
2	K	259	LEU	CA-CB-CG	5.90	128.87	115.30
3	F	33	C	C5-C6-N1	-5.73	118.13	121.00
3	F	44	U	N3-C2-O2	-5.64	118.25	122.20
3	L	33	C	C2-N1-C1'	-5.57	112.68	118.80
3	F	28	C	C5-C6-N1	-5.32	118.34	121.00
2	H	133	LEU	CA-CB-CG	5.10	127.04	115.30
3	L	33	C	N1-C2-O2	-5.07	115.86	118.90
3	L	46	G	C8-N9-C4	5.07	108.43	106.40

There are no chirality outliers.

There are no planarity outliers.

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	991	0	1042	80	0
1	D	968	0	1017	66	0
1	G	992	0	1042	64	0
1	J	976	0	1023	60	0
2	B	1860	0	1879	144	0
2	E	1851	0	1873	106	0
2	H	1844	0	1864	125	0
2	K	1892	0	1922	87	0
3	C	685	0	347	18	0
3	F	685	0	347	24	0
3	I	685	0	347	18	0
3	L	685	0	347	23	0
All	All	14114	0	13050	782	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 29.

All (782) 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:D:14:ALA:HB1	1:D:18:LEU:HB3	1.34	1.07
2:H:134:ASP:HA	2:H:137:ARG:NH2	1.75	1.00
2:E:240:ASN:HD22	2:E:240:ASN:H	1.10	0.99
2:K:276:HIS:HA	2:K:281:GLN:HE21	1.24	0.99
1:G:95:VAL:HG12	1:G:97:ARG:H	1.26	0.98
2:H:289:ARG:HB3	2:H:289:ARG:HH11	1.29	0.97
2:B:268:LEU:HD12	2:B:269:PRO:CD	1.94	0.96
2:E:218:ASN:HA	2:E:221:ILE:HD12	1.45	0.96
2:B:133:LEU:H	2:B:133:LEU:HD22	1.30	0.96
2:H:293:ARG:HD3	3:L:41:G:O6	1.69	0.93
2:B:154:ASN:HA	2:B:157:GLN:HG2	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:G:H1	2:E:250:MET:HE1	1.32	0.91
1:J:46:LEU:HD23	1:J:72:LEU:HB2	1.53	0.90
1:D:95:VAL:HG12	1:D:97:ARG:H	1.34	0.89
2:K:170:THR:HA	2:K:173:THR:HG23	1.54	0.89
2:E:142:LEU:HD23	2:E:143:GLY:H	1.33	0.89
2:H:88:PRO:HD2	2:H:91:ARG:HE	1.37	0.88
1:A:59:ASP:HB3	1:A:86:LYS:HE2	1.56	0.88
2:E:166:VAL:O	2:E:170:THR:HG23	1.72	0.87
2:E:115:ARG:HD3	2:E:126:GLU:HG2	1.56	0.87
1:A:120:GLN:O	1:A:124:GLU:HG2	1.75	0.86
2:B:268:LEU:HD12	2:B:269:PRO:HD3	1.55	0.86
2:E:93:ILE:HG21	2:E:212:MET:CE	2.04	0.86
2:E:162:ALA:O	2:E:166:VAL:HG23	1.75	0.86
2:H:110:ILE:O	2:H:114:ILE:HG13	1.76	0.85
2:E:142:LEU:HD23	2:E:143:GLY:N	1.92	0.84
2:B:126:GLU:HA	2:B:135:TYR:HE1	1.43	0.84
2:H:137:ARG:HH11	2:H:158:ILE:HB	1.42	0.84
2:H:234:VAL:HG11	2:H:273:TYR:HE1	1.39	0.84
1:J:45:THR:HG22	1:J:51:SER:HB2	1.58	0.83
2:B:135:TYR:CE2	2:B:139:VAL:HG11	2.14	0.82
2:K:152:ASN:HB3	2:K:155:LEU:HB3	1.61	0.81
2:B:147:ASP:O	2:B:148:LYS:HG2	1.81	0.80
2:E:240:ASN:HD22	2:E:240:ASN:N	1.77	0.80
1:G:64:GLU:HA	1:G:67:LEU:HD12	1.61	0.80
2:H:122:PHE:CE1	2:H:125:LEU:HB2	2.16	0.80
1:D:63:LEU:HD22	1:D:67:LEU:HD11	1.62	0.79
2:E:165:MET:O	2:E:169:VAL:HG13	1.83	0.79
1:A:59:ASP:HB3	1:A:86:LYS:CE	2.12	0.79
2:B:268:LEU:HD12	2:B:269:PRO:HD2	1.64	0.79
2:E:249:ILE:HD12	2:E:300:THR:HG23	1.65	0.79
2:H:118:TYR:HD2	2:H:187:LEU:HD13	1.47	0.78
2:K:234:VAL:HG11	2:K:273:TYR:HE1	1.49	0.78
2:E:152:ASN:ND2	2:E:155:LEU:H	1.82	0.78
2:K:87:ALA:N	2:K:88:PRO:HD3	1.98	0.78
2:H:289:ARG:HH11	2:H:289:ARG:CB	1.98	0.77
1:G:1:MET:HE2	1:G:3:GLU:H	1.49	0.77
3:F:44:U:H4'	3:F:44:U:OP1	1.84	0.77
1:A:19:THR:HG23	1:A:83:VAL:HG12	1.68	0.76
2:K:90:TYR:O	2:K:94:VAL:HG23	1.85	0.76
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.48	0.76
1:G:22:LEU:O	1:G:26:VAL:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ARG:HG2	2:B:158:ILE:HG21	1.68	0.76
2:H:131:ASN:HB3	2:H:134:ASP:HB2	1.67	0.76
2:H:155:LEU:O	2:H:158:ILE:HG12	1.86	0.76
2:B:133:LEU:HD22	2:B:133:LEU:N	2.02	0.75
2:E:283:LEU:HD12	2:E:283:LEU:N	2.02	0.75
2:K:268:LEU:HD23	2:K:269:PRO:HD3	1.67	0.75
1:A:22:LEU:H	1:A:22:LEU:HD12	1.51	0.75
1:J:95:VAL:HG12	1:J:97:ARG:H	1.52	0.74
1:G:40:ASN:H	1:G:40:ASN:HD22	1.34	0.74
1:J:32:TYR:HD1	1:J:112:LEU:HD11	1.51	0.74
1:A:19:THR:HG23	1:A:83:VAL:CG1	2.17	0.74
2:H:88:PRO:HD2	2:H:91:ARG:NE	2.03	0.73
1:D:86:LYS:HG3	1:D:98:PRO:HB3	1.70	0.73
2:K:128:LEU:HD12	2:K:167:VAL:HG12	1.69	0.73
1:A:34:GLN:HE22	1:A:110:SER:CB	2.01	0.73
1:D:52:GLU:OE1	1:D:106:ILE:HG12	1.89	0.73
2:B:156:GLN:HE22	2:B:161:ASN:HD22	1.36	0.72
1:A:34:GLN:HE22	1:A:110:SER:HB2	1.54	0.72
1:D:79:PRO:HB2	1:D:123:ILE:HD12	1.72	0.72
2:H:124:GLU:OE1	2:H:170:THR:HG22	1.90	0.72
2:H:136:ILE:HD12	2:H:136:ILE:H	1.54	0.72
2:E:177:GLN:H	2:E:177:GLN:HE21	1.36	0.71
2:E:93:ILE:HG21	2:E:212:MET:HE3	1.73	0.71
1:G:37:LYS:HD3	1:G:93:CYS:HB3	1.72	0.70
2:B:121:ARG:O	2:B:122:PHE:HB2	1.91	0.70
2:K:131:ASN:HB3	2:K:134:ASP:OD2	1.90	0.70
2:B:200:SER:O	2:B:204:ILE:HG13	1.90	0.70
1:D:46:LEU:HD12	1:D:69:LEU:HD23	1.74	0.70
2:H:153:GLU:O	2:H:157:GLN:HG3	1.92	0.69
3:C:44:U:H4'	3:C:45:A:H5"	1.74	0.69
1:G:19:THR:HG23	1:G:83:VAL:HG12	1.74	0.69
1:A:119:ILE:O	1:A:123:ILE:HG13	1.92	0.69
2:E:152:ASN:C	2:E:152:ASN:HD22	1.95	0.69
2:H:111:HIS:ND1	2:H:136:ILE:HD11	2.07	0.69
1:J:117:GLN:O	1:J:121:GLN:HG3	1.92	0.69
2:B:135:TYR:O	2:B:139:VAL:HG13	1.92	0.69
3:I:44:U:H4'	3:I:45:A:C5'	2.23	0.69
3:L:28:C:N3	3:L:29:U:C5	2.61	0.69
2:B:217:PRO:O	2:B:221:ILE:HG12	1.93	0.68
1:D:62:PRO:O	1:D:65:ILE:HG23	1.93	0.68
1:G:113:LYS:O	1:G:117:GLN:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:TYR:HE2	2:B:139:VAL:HG11	1.59	0.68
2:E:218:ASN:HA	2:E:221:ILE:CD1	2.24	0.68
1:G:20:LYS:HG2	1:G:24:ASP:OD2	1.93	0.68
2:H:115:ARG:HG3	2:H:116:ASP:N	2.08	0.68
1:D:53:PHE:HB3	1:D:79:PRO:HG2	1.74	0.68
1:G:70:PRO:HB3	1:G:80:TYR:CE2	2.27	0.68
2:B:315:LYS:HE2	2:B:319:GLU:OE2	1.94	0.67
2:H:234:VAL:HG11	2:H:273:TYR:CE1	2.28	0.67
2:K:135:TYR:HE2	2:K:139:VAL:CG1	2.08	0.67
2:B:101:VAL:HA	2:B:104:GLU:HG3	1.76	0.67
1:D:25:LEU:CD2	1:D:119:ILE:HG13	2.24	0.67
2:H:133:LEU:O	2:H:133:LEU:HD12	1.95	0.67
1:D:63:LEU:HD22	1:D:67:LEU:CD1	2.24	0.67
2:H:135:TYR:HE1	2:H:139:VAL:HG11	1.60	0.67
1:J:115:GLN:O	1:J:118:SER:HB3	1.95	0.67
2:E:91:ARG:HE	2:E:91:ARG:HA	1.59	0.67
2:H:217:PRO:O	2:H:221:ILE:HG13	1.94	0.67
1:G:48:ARG:HB2	1:G:50:ILE:HD13	1.75	0.66
2:B:255:GLN:NE2	2:B:255:GLN:HA	2.10	0.66
1:D:19:THR:O	1:D:23:LEU:HD12	1.96	0.66
1:A:34:GLN:NE2	1:A:110:SER:HB2	2.09	0.66
3:C:57:A:H2'	3:F:57:A:O2'	1.95	0.66
1:A:48:ARG:HB2	1:A:50:ILE:HD12	1.78	0.66
1:A:18:LEU:O	1:A:22:LEU:HD12	1.96	0.66
1:A:30:CYS:HB2	1:A:35:LEU:HD22	1.78	0.66
2:K:135:TYR:HE2	2:K:139:VAL:HG11	1.61	0.65
2:E:245:PRO:HB2	2:E:247:CYS:SG	2.36	0.65
2:H:241:LEU:HA	2:H:244:MET:HE3	1.78	0.65
2:K:313:GLU:OE1	2:K:315:LYS:HE3	1.96	0.65
3:I:44:U:H4'	3:I:45:A:H5"	1.77	0.65
1:D:41:GLU:O	1:D:45:THR:HG23	1.97	0.65
1:G:25:LEU:HD23	1:G:119:ILE:HG13	1.78	0.65
2:H:202:HIS:O	2:H:204:ILE:N	2.29	0.65
2:H:241:LEU:HA	2:H:244:MET:CE	2.27	0.65
1:A:74:GLU:OE2	1:A:74:GLU:HA	1.96	0.65
2:E:240:ASN:N	2:E:240:ASN:ND2	2.45	0.65
1:D:57:ALA:O	1:D:59:ASP:N	2.30	0.65
1:G:48:ARG:HB2	1:G:50:ILE:CD1	2.26	0.65
2:H:87:ALA:HA	2:H:91:ARG:HH21	1.61	0.65
3:L:43:A:H8	3:L:46:G:HO2'	1.41	0.65
2:E:240:ASN:H	2:E:240:ASN:ND2	1.89	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:GLU:HG3	2:B:225:ALA:HB2	1.79	0.64
2:K:106:GLU:O	2:K:110:ILE:HG13	1.97	0.64
1:J:68:HIS:HA	1:J:71:LEU:HD23	1.78	0.64
2:H:136:ILE:HD12	2:H:136:ILE:N	2.12	0.64
2:K:121:ARG:HG3	2:K:179:LEU:HG	1.79	0.64
2:E:305:VAL:HG11	2:E:316:VAL:HG21	1.78	0.64
2:H:138:THR:HG22	2:H:158:ILE:HD12	1.80	0.64
1:J:41:GLU:HA	1:J:44:LYS:HD3	1.80	0.64
1:D:44:LYS:NZ	3:F:48:G:N7	2.46	0.64
2:H:211:ARG:O	2:H:215:ILE:HG13	1.97	0.64
2:E:91:ARG:HD3	2:E:91:ARG:O	1.98	0.63
1:A:48:ARG:O	1:A:50:ILE:HG23	1.97	0.63
2:B:118:TYR:C	2:B:120:LYS:H	2.02	0.63
1:D:52:GLU:HG3	1:D:120:GLN:HE21	1.64	0.63
1:A:25:LEU:HD22	1:A:119:ILE:HG13	1.81	0.63
1:D:110:SER:O	1:D:113:LYS:HB2	1.99	0.63
1:J:14:ALA:HB1	1:J:18:LEU:HB3	1.81	0.63
2:K:125:LEU:HD12	2:K:125:LEU:O	1.99	0.62
3:C:43:A:H5'	3:C:44:U:OP2	1.99	0.62
2:E:223:ILE:HD13	2:E:228:ALA:HB2	1.81	0.62
2:H:122:PHE:HE1	2:H:125:LEU:HB2	1.64	0.62
1:A:73:CYS:HB3	1:A:78:VAL:O	1.99	0.62
2:B:110:ILE:O	2:B:114:ILE:HG13	2.00	0.62
2:K:214:PHE:CD1	2:K:214:PHE:C	2.73	0.62
2:B:121:ARG:HD3	2:B:146:LEU:CD1	2.29	0.62
2:K:305:VAL:HG11	2:K:316:VAL:HG21	1.81	0.62
2:E:91:ARG:HA	2:E:94:VAL:CG1	2.29	0.62
2:B:134:ASP:O	2:B:138:THR:HG22	2.00	0.61
3:L:43:A:H8	3:L:46:G:O2'	1.83	0.61
2:B:223:ILE:HD12	2:B:231:ILE:HD11	1.81	0.61
1:D:34:GLN:CD	1:D:107:LYS:HB3	2.20	0.61
2:K:170:THR:HA	2:K:173:THR:CG2	2.30	0.61
2:B:121:ARG:HD3	2:B:146:LEU:HD11	1.80	0.61
2:B:155:LEU:O	2:B:159:LEU:HD13	2.00	0.61
2:K:135:TYR:CE2	2:K:139:VAL:CG1	2.84	0.61
2:B:152:ASN:HB3	2:B:155:LEU:HD13	1.82	0.61
1:D:44:LYS:HE2	3:F:47:U:OP2	2.01	0.61
1:G:52:GLU:OE2	1:G:106:ILE:HG23	2.01	0.61
1:G:80:TYR:CE1	1:G:127:LEU:HD21	2.35	0.60
1:D:95:VAL:HG12	1:D:97:ARG:N	2.12	0.60
2:H:135:TYR:HB3	2:H:136:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG21	1:A:13:LEU:HD23	1.82	0.60
1:A:18:LEU:HG	1:A:22:LEU:HD11	1.82	0.60
1:A:79:PRO:HG3	1:A:120:GLN:HG2	1.82	0.60
2:E:99:LEU:O	2:E:102:GLU:N	2.35	0.60
1:A:11:TYR:HD1	1:A:12:PRO:HA	1.66	0.60
2:K:86:ALA:HB1	2:K:88:PRO:HD3	1.82	0.60
2:K:249:ILE:HD12	2:K:300:THR:HG23	1.83	0.60
1:G:46:LEU:HB3	1:G:72:LEU:CD2	2.32	0.60
2:B:141:GLU:HA	2:B:141:GLU:OE1	2.02	0.60
1:G:40:ASN:H	1:G:40:ASN:ND2	2.00	0.60
1:A:22:LEU:HD12	1:A:22:LEU:N	2.16	0.59
2:B:122:PHE:N	2:B:123:PRO:CD	2.65	0.59
2:E:100:THR:O	2:E:104:GLU:HB2	2.01	0.59
2:K:217:PRO:O	2:K:221:ILE:HG13	2.03	0.59
1:A:114:GLN:O	1:A:117:GLN:HB2	2.02	0.59
2:B:208:VAL:O	2:B:212:MET:HB2	2.01	0.59
2:E:208:VAL:O	2:E:212:MET:HB2	2.02	0.59
2:H:196:GLU:OE1	2:H:196:GLU:HA	2.01	0.59
1:J:44:LYS:NZ	3:L:48:G:N7	2.50	0.59
1:J:123:ILE:O	1:J:126:LEU:HB2	2.02	0.59
2:K:92:VAL:HG12	2:K:93:ILE:HD13	1.82	0.59
1:A:91:ARG:HG3	1:A:91:ARG:NH1	2.15	0.59
1:A:112:LEU:O	1:A:116:ILE:HG13	2.02	0.59
1:D:50:ILE:O	1:D:50:ILE:HG13	2.02	0.59
3:I:34:A:N1	1:J:96:SER:HB2	2.17	0.59
2:B:90:TYR:O	2:B:94:VAL:HG23	2.02	0.59
2:B:117:LYS:HD2	2:B:186:ARG:NH2	2.17	0.59
1:G:4:ALA:HB1	1:G:84:ARG:NH2	2.18	0.59
1:J:25:LEU:HD12	1:J:25:LEU:O	2.03	0.59
2:H:223:ILE:HG23	2:H:299:CYS:SG	2.43	0.59
2:B:135:TYR:O	2:B:138:THR:HG23	2.03	0.58
2:E:291:ALA:O	2:E:295:VAL:HG23	2.03	0.58
2:H:131:ASN:HD22	2:H:134:ASP:CG	2.06	0.58
2:E:305:VAL:HG21	2:E:316:VAL:HG11	1.84	0.58
1:J:45:THR:HG21	1:J:103:SER:OG	2.03	0.58
2:B:124:GLU:OE2	2:B:175:GLN:HB2	2.04	0.58
2:B:154:ASN:HD22	2:B:155:LEU:HD12	1.68	0.58
3:I:43:A:C8	3:I:46:G:O2'	2.54	0.58
2:E:214:PHE:C	2:E:214:PHE:HD1	2.07	0.58
2:B:154:ASN:O	2:B:158:ILE:HG12	2.03	0.58
2:H:156:GLN:HA	2:H:159:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:177:GLN:H	2:E:177:GLN:NE2	2.02	0.58
1:G:51:SER:HB2	1:G:103:SER:OG	2.04	0.57
1:A:113:LYS:O	1:A:117:GLN:HG2	2.05	0.57
1:J:44:LYS:O	1:J:48:ARG:HG3	2.04	0.57
2:B:99:LEU:O	2:B:103:ILE:HG13	2.05	0.57
1:J:89:LEU:HD12	1:J:89:LEU:O	2.04	0.57
1:J:108:GLU:OE2	1:J:108:GLU:HA	2.04	0.57
2:K:230:LYS:O	2:K:234:VAL:HG12	2.04	0.57
2:H:121:ARG:NH1	2:H:178:GLN:HG2	2.19	0.57
2:H:137:ARG:O	2:H:137:ARG:HG2	2.04	0.57
2:H:174:THR:HG23	2:H:175:GLN:N	2.20	0.57
1:D:116:ILE:HG22	1:D:117:GLN:N	2.19	0.57
1:G:14:ALA:HB2	1:G:81:VAL:HG21	1.86	0.57
2:H:293:ARG:NH1	3:L:40:C:C5	2.73	0.57
2:B:106:GLU:O	2:B:110:ILE:HG13	2.04	0.57
2:E:152:ASN:ND2	2:E:152:ASN:C	2.58	0.57
2:B:126:GLU:HA	2:B:135:TYR:CE1	2.33	0.57
1:D:53:PHE:CB	1:D:79:PRO:HG2	2.34	0.57
2:B:93:ILE:HG23	2:B:208:VAL:HG12	1.87	0.56
2:B:249:ILE:HA	2:B:252:LEU:HD12	1.87	0.56
2:E:115:ARG:HD3	2:E:126:GLU:CG	2.31	0.56
2:E:163:THR:O	2:E:167:VAL:HG13	2.05	0.56
2:E:214:PHE:C	2:E:214:PHE:CD1	2.79	0.56
1:D:95:VAL:CG1	1:D:97:ARG:H	2.10	0.56
3:F:43:A:C4'	3:F:43:A:OP1	2.54	0.56
2:B:154:ASN:ND2	2:B:155:LEU:HD12	2.20	0.56
2:B:250:MET:HE1	3:F:41:G:H1	1.69	0.56
3:C:42:C:H5"	3:C:43:A:OP2	2.05	0.56
1:J:83:VAL:HG23	1:J:85:SER:H	1.70	0.56
2:K:126:GLU:HA	2:K:135:TYR:CE1	2.40	0.56
2:B:118:TYR:C	2:B:120:LYS:N	2.59	0.56
1:G:46:LEU:HD13	1:G:72:LEU:HD22	1.88	0.56
2:H:289:ARG:HB3	2:H:289:ARG:NH1	2.11	0.56
2:B:158:ILE:HB	2:B:159:LEU:HD12	1.87	0.56
2:H:118:TYR:HD2	2:H:187:LEU:CD1	2.18	0.56
2:K:276:HIS:HA	2:K:281:GLN:NE2	2.08	0.56
2:H:114:ILE:O	2:H:118:TYR:HB2	2.06	0.56
3:F:40:C:O2'	3:F:41:G:H5'	2.06	0.56
1:A:86:LYS:HG3	1:A:98:PRO:HB3	1.87	0.56
1:J:48:ARG:O	1:J:50:ILE:HG23	2.05	0.56
1:G:67:LEU:O	1:G:70:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:SER:O	2:B:283:LEU:HD12	2.06	0.55
3:I:32:C:H5'	3:I:33:C:OP2	2.06	0.55
2:B:223:ILE:CD1	2:B:231:ILE:HD11	2.36	0.55
2:E:90:TYR:O	2:E:94:VAL:HG12	2.05	0.55
3:C:39:G:O2'	3:C:40:C:H5'	2.07	0.55
2:H:227:THR:O	2:H:231:ILE:HG23	2.05	0.55
1:J:11:TYR:C	1:J:11:TYR:CD2	2.80	0.55
1:J:32:TYR:CD1	1:J:112:LEU:HD11	2.37	0.55
1:A:11:TYR:CD1	1:A:12:PRO:HA	2.40	0.55
1:G:19:THR:HG23	1:G:83:VAL:CG1	2.36	0.55
1:A:6:VAL:HG21	1:A:13:LEU:CD2	2.37	0.55
1:G:95:VAL:HG12	1:G:97:ARG:N	2.09	0.55
2:K:173:THR:O	2:K:173:THR:OG1	2.25	0.55
1:D:52:GLU:HB2	1:D:104:VAL:O	2.07	0.55
2:E:100:THR:HG22	2:E:204:ILE:HG21	1.89	0.55
2:E:277:SER:O	2:E:281:GLN:HB2	2.07	0.55
3:F:42:C:H4'	3:F:42:C:OP1	2.06	0.55
1:G:66:ILE:HG21	1:G:100:ILE:HG13	1.89	0.54
2:K:135:TYR:CE2	2:K:139:VAL:HG11	2.42	0.54
1:G:59:ASP:O	1:G:86:LYS:HE2	2.07	0.54
2:K:114:ILE:HG23	2:K:187:LEU:HD22	1.87	0.54
1:A:67:LEU:O	1:A:70:PRO:HD2	2.07	0.54
2:B:152:ASN:O	2:B:156:GLN:HB2	2.06	0.54
1:D:7:ASN:ND2	1:D:9:LYS:H	2.06	0.54
2:H:122:PHE:HE1	2:H:125:LEU:N	2.04	0.54
1:A:26:VAL:HG13	1:A:35:LEU:CD1	2.37	0.54
2:B:284:PRO:O	2:B:287:LEU:HB2	2.08	0.54
1:D:44:LYS:O	1:D:48:ARG:HG3	2.06	0.54
1:J:25:LEU:HD23	1:J:119:ILE:HG13	1.89	0.54
1:J:63:LEU:HD12	1:J:66:ILE:HD11	1.89	0.54
2:K:122:PHE:CD2	2:K:146:LEU:HD13	2.43	0.54
2:B:118:TYR:O	2:B:120:LYS:N	2.41	0.54
1:J:45:THR:CG2	1:J:51:SER:HB2	2.35	0.54
2:H:136:ILE:H	2:H:136:ILE:CD1	2.18	0.54
2:B:93:ILE:HD12	2:B:215:ILE:CD1	2.38	0.54
2:B:93:ILE:HG21	2:B:212:MET:HE2	1.89	0.54
2:K:87:ALA:N	2:K:88:PRO:CD	2.69	0.54
2:H:254:ALA:O	2:H:255:GLN:HB3	2.07	0.53
1:J:12:PRO:HB2	1:J:126:LEU:HD22	1.89	0.53
2:B:135:TYR:CE2	2:B:139:VAL:CG1	2.90	0.53
3:F:39:G:C2'	3:F:40:C:H5'	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:46:G:C6	3:L:41:G:N2	2.76	0.53
2:K:286:ASP:OD1	2:K:286:ASP:N	2.35	0.53
1:A:99:VAL:HG13	3:F:35:A:O2'	2.08	0.53
1:D:20:LYS:NZ	3:I:27:A:O3'	2.41	0.53
2:K:185:GLU:O	2:K:189:GLU:HB2	2.09	0.53
1:A:18:LEU:CD1	1:A:22:LEU:HD11	2.39	0.53
2:B:314:GLY:O	2:B:318:TYR:HD1	1.92	0.53
1:D:25:LEU:HD23	1:D:119:ILE:HG13	1.90	0.53
2:H:103:ILE:HG23	2:H:197:LEU:HD13	1.89	0.53
2:K:115:ARG:HG3	2:K:126:GLU:OE1	2.09	0.53
1:D:22:LEU:CD2	1:D:53:PHE:HE1	2.21	0.53
1:D:41:GLU:HA	1:D:44:LYS:HD3	1.91	0.53
2:H:115:ARG:CG	2:H:116:ASP:N	2.71	0.53
2:H:191:CYS:C	2:H:193:MET:N	2.59	0.53
2:H:249:ILE:HD12	2:H:300:THR:HG23	1.89	0.53
1:A:90:GLY:HA2	1:A:99:VAL:HG23	1.90	0.53
1:G:25:LEU:CD2	1:G:119:ILE:HG13	2.38	0.53
1:J:23:LEU:N	1:J:23:LEU:HD23	2.23	0.53
2:K:298:LYS:HA	2:K:301:LEU:HD12	1.91	0.53
1:D:23:LEU:HD23	1:D:92:ALA:CB	2.38	0.53
1:D:52:GLU:HG3	1:D:120:GLN:NE2	2.24	0.53
2:B:125:LEU:HD12	2:B:125:LEU:O	2.08	0.53
2:E:118:TYR:CE1	2:E:122:PHE:HB3	2.44	0.53
2:H:115:ARG:HB2	2:H:135:TYR:CE2	2.44	0.53
3:C:43:A:C5'	3:C:44:U:OP2	2.57	0.52
2:E:86:ALA:HB1	2:E:88:PRO:HD3	1.91	0.52
2:E:177:GLN:HE21	2:E:177:GLN:N	2.05	0.52
1:A:13:LEU:C	1:A:13:LEU:HD12	2.30	0.52
1:A:95:VAL:HG12	1:A:97:ARG:H	1.74	0.52
2:B:118:TYR:CE2	2:B:139:VAL:HB	2.44	0.52
2:E:283:LEU:N	2:E:283:LEU:CD1	2.71	0.52
2:B:133:LEU:H	2:B:133:LEU:CD2	2.00	0.52
2:E:231:ILE:HG12	2:E:232:MET:N	2.25	0.52
2:E:311:SER:CB	2:E:316:VAL:HG23	2.40	0.52
1:G:67:LEU:C	1:G:70:PRO:HD2	2.30	0.52
2:K:305:VAL:HG21	2:K:316:VAL:HG11	1.92	0.52
2:B:122:PHE:N	2:B:123:PRO:HD2	2.25	0.52
2:B:325:GLU:O	2:B:328:PHE:HB2	2.09	0.52
3:L:28:C:C2	3:L:29:U:C5	2.98	0.52
1:D:11:TYR:C	1:D:11:TYR:CD2	2.83	0.52
2:E:91:ARG:O	2:E:94:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:ILE:O	1:J:120:GLN:C	2.47	0.52
2:K:287:LEU:N	2:K:287:LEU:HD23	2.25	0.52
1:A:59:ASP:OD2	1:A:86:LYS:HG2	2.10	0.52
1:D:68:HIS:O	1:D:72:LEU:HD12	2.09	0.52
2:H:286:ASP:OD1	2:H:286:ASP:N	2.43	0.52
1:A:18:LEU:O	1:A:22:LEU:CD1	2.57	0.52
2:B:295:VAL:O	2:B:296:ALA:C	2.48	0.52
1:A:54:ILE:CD1	1:A:103:SER:HB2	2.40	0.52
2:B:93:ILE:HD12	2:B:215:ILE:HD11	1.91	0.52
2:B:141:GLU:O	2:B:142:LEU:C	2.48	0.52
2:H:97:ASN:HD22	2:H:229:ALA:HB3	1.75	0.52
2:H:154:ASN:O	2:H:157:GLN:HB2	2.10	0.52
1:G:32:TYR:HE1	1:G:111:GLN:HB2	1.76	0.51
2:H:114:ILE:HD12	2:H:115:ARG:N	2.25	0.51
1:J:62:PRO:HB2	1:J:64:GLU:HG2	1.92	0.51
2:B:178:GLN:HG2	2:B:179:LEU:N	2.26	0.51
2:E:214:PHE:HD1	2:E:214:PHE:O	1.93	0.51
2:E:298:LYS:HB3	2:E:320:LEU:HD22	1.92	0.51
2:H:174:THR:CG2	2:H:175:GLN:N	2.74	0.51
2:K:316:VAL:HG12	2:K:320:LEU:HD12	1.91	0.51
2:E:282:SER:C	2:E:283:LEU:HD12	2.31	0.51
1:A:112:LEU:HA	1:A:115:GLN:HG3	1.93	0.51
2:B:86:ALA:O	2:B:88:PRO:HD3	2.11	0.51
1:G:19:THR:O	1:G:23:LEU:CD2	2.59	0.51
2:B:136:ILE:HG21	2:B:194:ALA:CB	2.41	0.51
2:E:159:LEU:HB2	2:E:164:ILE:HG12	1.93	0.51
1:G:41:GLU:O	1:G:45:THR:HG23	2.10	0.51
3:I:57:A:C2	3:L:57:A:C2	2.99	0.51
1:J:95:VAL:HG12	1:J:97:ARG:N	2.24	0.51
1:G:65:ILE:HB	2:H:301:LEU:HD23	1.93	0.51
1:J:42:ALA:O	1:J:45:THR:HB	2.10	0.51
1:J:115:GLN:HA	1:J:118:SER:HB3	1.92	0.51
2:K:259:LEU:C	2:K:259:LEU:HD23	2.31	0.51
1:G:81:VAL:HG12	1:G:123:ILE:HD13	1.93	0.51
3:I:29:U:H2'	3:I:30:G:O4'	2.11	0.51
2:B:119:SER:O	2:B:123:PRO:HB3	2.11	0.51
2:E:104:GLU:OE1	2:E:104:GLU:HA	2.10	0.51
1:G:72:LEU:HD23	1:G:72:LEU:O	2.10	0.51
2:B:113:PHE:CE2	2:B:117:LYS:HG3	2.46	0.50
2:H:146:LEU:HD13	2:H:171:ALA:O	2.11	0.50
2:B:214:PHE:CD1	2:B:214:PHE:C	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HD13	1:D:14:ALA:N	2.27	0.50
2:H:174:THR:CG2	2:H:175:GLN:H	2.25	0.50
1:J:123:ILE:O	1:J:126:LEU:CB	2.59	0.50
3:C:36:U:P	1:D:100:ILE:HG12	2.51	0.50
2:B:135:TYR:CD2	2:B:139:VAL:HG11	2.45	0.50
2:B:154:ASN:HD22	2:B:155:LEU:N	2.09	0.50
2:B:160:THR:HG23	2:B:163:THR:OG1	2.11	0.50
2:E:133:LEU:HD23	2:E:137:ARG:HG3	1.93	0.50
2:E:185:GLU:O	2:E:189:GLU:HB2	2.12	0.50
2:H:115:ARG:HD2	2:H:126:GLU:HG3	1.93	0.50
2:H:175:GLN:HG3	2:H:175:GLN:O	2.12	0.50
3:C:39:G:C2'	3:C:40:C:H5'	2.42	0.50
1:G:112:LEU:O	1:G:116:ILE:HG13	2.11	0.50
2:H:202:HIS:C	2:H:204:ILE:N	2.65	0.50
2:K:301:LEU:O	2:K:305:VAL:HG23	2.11	0.50
2:B:158:ILE:C	2:B:159:LEU:HD12	2.32	0.50
2:B:320:LEU:O	2:B:324:ILE:HG13	2.12	0.50
2:E:152:ASN:ND2	2:E:154:ASN:N	2.59	0.50
2:E:316:VAL:HG12	2:E:320:LEU:HD12	1.92	0.50
2:K:135:TYR:HD2	2:K:135:TYR:C	2.14	0.50
2:E:121:ARG:O	2:E:121:ARG:HD3	2.10	0.50
2:H:129:VAL:HG11	2:H:159:LEU:HD21	1.93	0.50
2:K:114:ILE:HG23	2:K:187:LEU:CD2	2.42	0.50
2:K:118:TYR:C	2:K:120:LYS:H	2.14	0.50
1:D:78:VAL:HG13	1:D:79:PRO:HD2	1.94	0.50
2:H:138:THR:HG22	2:H:158:ILE:CD1	2.42	0.50
2:K:180:SER:OG	2:K:183:GLU:HB3	2.12	0.50
2:B:135:TYR:CD2	2:B:139:VAL:CG1	2.95	0.49
2:B:164:ILE:O	2:B:167:VAL:HG13	2.12	0.49
2:B:178:GLN:HG2	2:B:179:LEU:H	1.77	0.49
2:B:293:ARG:NH1	3:F:40:C:C5	2.80	0.49
1:D:32:TYR:HE1	1:D:111:GLN:CG	2.24	0.49
1:G:65:ILE:HB	2:H:301:LEU:CD2	2.42	0.49
2:B:199:ALA:O	2:B:203:ARG:HG3	2.12	0.49
2:E:98:ASN:O	2:E:101:VAL:HG22	2.12	0.49
2:E:114:ILE:HD12	2:E:136:ILE:HG12	1.94	0.49
1:J:46:LEU:HD21	1:J:73:CYS:SG	2.51	0.49
1:J:62:PRO:O	1:J:65:ILE:HG23	2.11	0.49
2:K:212:MET:SD	2:K:229:ALA:HB2	2.52	0.49
2:B:269:PRO:O	2:B:270:HIS:HB2	2.11	0.49
2:E:93:ILE:HG22	2:E:208:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:275:TYR:CE2	2:K:288:ARG:HB3	2.48	0.49
2:H:114:ILE:O	2:H:118:TYR:CB	2.61	0.49
2:K:89:GLU:O	2:K:93:ILE:HG12	2.12	0.49
2:B:286:ASP:OD1	2:B:286:ASP:N	2.43	0.49
2:E:209:GLU:HG2	2:E:225:ALA:HB3	1.95	0.49
2:H:169:VAL:HG12	2:H:169:VAL:O	2.12	0.49
2:H:226:SER:O	2:H:229:ALA:N	2.45	0.49
2:K:121:ARG:HD2	2:K:144:ASN:HA	1.95	0.49
1:A:114:GLN:HA	1:A:117:GLN:CG	2.42	0.49
2:E:254:ALA:HB2	2:E:271:THR:O	2.13	0.49
1:J:6:VAL:HG11	1:J:13:LEU:HD22	1.95	0.49
2:K:120:LYS:HB3	2:K:179:LEU:HD21	1.94	0.49
2:B:240:ASN:O	2:B:241:LEU:C	2.50	0.49
2:E:158:ILE:C	2:E:159:LEU:HD23	2.33	0.49
2:H:321:LYS:O	2:H:325:GLU:HG3	2.12	0.49
1:A:114:GLN:HA	1:A:117:GLN:HG3	1.94	0.49
1:D:32:TYR:HE1	1:D:111:GLN:HG2	1.77	0.49
2:K:255:GLN:NE2	2:K:266:SER:HB3	2.28	0.49
2:B:121:ARG:HD3	2:B:146:LEU:CD2	2.43	0.49
2:B:205:TYR:HA	2:B:208:VAL:HG22	1.95	0.49
2:K:86:ALA:O	2:K:87:ALA:HB3	2.12	0.49
2:K:308:PHE:O	2:K:309:HIS:C	2.50	0.49
1:D:25:LEU:HD12	1:D:25:LEU:O	2.13	0.49
1:D:41:GLU:OE2	3:F:48:G:C8	2.66	0.49
2:E:88:PRO:HG2	2:E:91:ARG:HB3	1.94	0.49
3:F:28:C:N3	3:F:29:U:C5	2.81	0.49
1:G:64:GLU:CD	1:G:64:GLU:H	2.14	0.49
2:H:227:THR:O	2:H:231:ILE:CG2	2.61	0.49
1:J:22:LEU:HD13	1:J:119:ILE:HD12	1.95	0.49
2:B:156:GLN:HE22	2:B:161:ASN:ND2	2.07	0.48
2:E:118:TYR:HE1	2:E:122:PHE:HB3	1.78	0.48
2:H:87:ALA:CA	2:H:91:ARG:HH21	2.26	0.48
2:B:238:LEU:HD23	2:B:307:SER:HA	1.95	0.48
2:E:223:ILE:CD1	2:E:228:ALA:HB2	2.41	0.48
2:K:135:TYR:C	2:K:135:TYR:CD2	2.86	0.48
3:C:47:U:C2'	3:C:48:G:H5'	2.42	0.48
2:E:150:LYS:O	2:E:151:ASN:CB	2.61	0.48
1:D:25:LEU:HD22	1:D:119:ILE:HG13	1.95	0.48
2:H:293:ARG:NH2	3:L:40:C:OP2	2.41	0.48
2:K:102:GLU:O	2:K:105:ASN:HB2	2.14	0.48
2:B:93:ILE:HG21	2:B:212:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:LEU:HD23	2:E:133:LEU:O	2.14	0.48
2:K:209:GLU:O	2:K:209:GLU:HG2	2.12	0.48
2:H:134:ASP:O	2:H:135:TYR:C	2.52	0.48
1:J:62:PRO:HD2	1:J:65:ILE:CG2	2.43	0.48
2:B:221:ILE:HD12	2:B:318:TYR:CE1	2.49	0.48
2:E:244:MET:HE1	3:F:45:A:C2	2.49	0.48
1:G:121:GLN:HB3	1:G:125:ARG:HH12	1.79	0.48
2:H:88:PRO:HG2	2:H:91:ARG:HG2	1.95	0.48
2:H:111:HIS:O	2:H:113:PHE:N	2.46	0.48
1:J:36:ARG:HG2	1:J:105:THR:HG22	1.95	0.48
3:L:55:G:C6	3:L:56:U:C4	3.01	0.48
2:E:211:ARG:HD2	2:E:211:ARG:HA	1.51	0.48
2:H:155:LEU:C	2:H:158:ILE:HG12	2.33	0.48
3:C:35:A:H8	1:D:37:LYS:O	1.97	0.47
1:D:27:GLN:O	1:D:30:CYS:HB3	2.14	0.47
2:H:164:ILE:HA	2:H:167:VAL:HG22	1.96	0.47
1:J:35:LEU:HD21	1:J:93:CYS:SG	2.54	0.47
1:A:20:LYS:HG2	1:A:24:ASP:OD2	2.14	0.47
1:G:33:LYS:HA	1:G:33:LYS:HE2	1.96	0.47
2:H:156:GLN:C	2:H:158:ILE:H	2.16	0.47
2:H:202:HIS:C	2:H:204:ILE:H	2.17	0.47
2:K:160:THR:HG22	2:K:162:ALA:H	1.78	0.47
2:K:291:ALA:O	2:K:295:VAL:HG23	2.14	0.47
1:A:50:ILE:HD13	1:A:50:ILE:H	1.80	0.47
2:E:152:ASN:HB3	2:E:155:LEU:HB2	1.96	0.47
1:G:68:HIS:CD2	1:G:68:HIS:C	2.88	0.47
2:H:154:ASN:O	2:H:158:ILE:HG23	2.14	0.47
2:K:156:GLN:HG2	2:K:161:ASN:OD1	2.13	0.47
1:A:70:PRO:HB3	1:A:80:TYR:CE2	2.49	0.47
2:B:238:LEU:HD21	2:B:306:ASP:HB3	1.96	0.47
1:A:23:LEU:CD1	1:A:92:ALA:HB2	2.45	0.47
1:D:31:ASN:H	1:D:31:ASN:ND2	2.12	0.47
1:D:11:TYR:C	1:D:11:TYR:HD2	2.18	0.47
1:A:13:LEU:HD11	1:A:84:ARG:HG3	1.97	0.47
2:B:121:ARG:HD3	2:B:146:LEU:HD21	1.96	0.47
2:B:148:LYS:CG	2:B:148:LYS:O	2.62	0.47
3:C:47:U:H2'	3:C:48:G:H5'	1.97	0.47
2:E:110:ILE:O	2:E:113:PHE:HB3	2.14	0.47
1:G:80:TYR:CE1	1:G:127:LEU:CD2	2.98	0.47
1:G:89:LEU:HD23	1:G:99:VAL:O	2.14	0.47
2:H:111:HIS:HA	2:H:114:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:276:HIS:O	2:H:277:SER:C	2.53	0.47
1:J:106:ILE:HG22	1:J:106:ILE:O	2.13	0.47
2:K:316:VAL:HG12	2:K:320:LEU:CD1	2.44	0.47
3:L:43:A:H2'	3:L:46:G:HO2'	1.78	0.47
1:D:32:TYR:CD1	1:D:112:LEU:HD12	2.50	0.47
2:E:92:VAL:HG12	2:E:93:ILE:N	2.30	0.47
2:H:93:ILE:HD12	2:H:211:ARG:CB	2.44	0.47
2:H:191:CYS:C	2:H:193:MET:H	2.19	0.47
1:J:111:GLN:HG3	1:J:112:LEU:HD12	1.97	0.47
3:F:49:A:O3'	3:F:50:G:H4'	2.15	0.47
1:G:100:ILE:HG21	3:L:36:U:C5	2.50	0.47
2:B:227:THR:O	2:B:231:ILE:CD1	2.63	0.47
1:G:1:MET:CE	1:G:3:GLU:H	2.23	0.47
2:H:118:TYR:CD2	2:H:187:LEU:HD13	2.38	0.47
1:J:83:VAL:HG23	1:J:84:ARG:N	2.29	0.47
1:A:68:HIS:CD2	1:A:69:LEU:HD23	2.50	0.46
2:B:154:ASN:HD22	2:B:155:LEU:H	1.64	0.46
2:K:216:ALA:O	2:K:220:SER:OG	2.31	0.46
2:B:117:LYS:HD2	2:B:186:ARG:HH21	1.79	0.46
2:B:137:ARG:HG2	2:B:158:ILE:CG2	2.40	0.46
2:B:239:THR:HG22	2:B:243:LYS:HE2	1.97	0.46
2:E:223:ILE:HD12	2:E:224:GLY:H	1.80	0.46
1:A:50:ILE:HG12	1:A:50:ILE:O	2.16	0.46
2:B:121:ARG:HH11	2:B:146:LEU:HD11	1.80	0.46
1:G:19:THR:O	1:G:23:LEU:HD23	2.16	0.46
3:C:44:U:H4'	3:C:45:A:C5'	2.43	0.46
1:D:81:VAL:HG22	1:D:123:ILE:HD13	1.96	0.46
1:D:115:GLN:O	1:D:118:SER:OG	2.32	0.46
2:E:244:MET:CE	3:F:45:A:C2	2.99	0.46
3:I:49:A:O3'	3:I:50:G:H4'	2.15	0.46
2:K:91:ARG:HE	2:K:91:ARG:HA	1.80	0.46
2:K:205:TYR:C	2:K:205:TYR:CD2	2.89	0.46
1:A:113:LYS:HE3	1:A:117:GLN:OE1	2.15	0.46
2:B:115:ARG:O	2:B:119:SER:HB3	2.15	0.46
2:E:86:ALA:O	2:E:87:ALA:HB3	2.16	0.46
2:E:93:ILE:CG2	2:E:208:VAL:HG22	2.45	0.46
2:E:133:LEU:HD21	2:E:137:ARG:CZ	2.45	0.46
2:H:125:LEU:HD13	2:H:128:LEU:HD13	1.98	0.46
2:K:162:ALA:O	2:K:166:VAL:HG23	2.14	0.46
3:L:26:U:HO5'	3:L:26:U:H6	1.63	0.46
3:L:28:C:C2	3:L:29:U:C6	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ILE:HB	2:E:301:LEU:HD22	1.96	0.46
1:D:83:VAL:HG23	1:D:85:SER:H	1.79	0.46
2:H:87:ALA:CB	2:H:91:ARG:HH21	2.29	0.46
2:H:120:LYS:HG3	2:H:177:GLN:HE22	1.80	0.46
3:L:28:C:C4	3:L:29:U:C5	3.04	0.46
2:B:120:LYS:HD2	2:B:179:LEU:CD2	2.46	0.46
2:B:153:GLU:O	2:B:156:GLN:HB3	2.16	0.46
1:G:51:SER:HB2	1:G:103:SER:HG	1.80	0.46
1:J:57:ALA:HB2	1:J:86:LYS:HA	1.98	0.46
2:B:121:ARG:NH1	2:B:146:LEU:HD21	2.30	0.46
3:F:43:A:OP1	3:F:43:A:O4'	2.34	0.46
1:G:119:ILE:O	1:G:123:ILE:HG13	2.15	0.46
1:J:56:MET:HE3	1:J:82:PHE:CE1	2.51	0.46
1:A:52:GLU:HG2	1:A:106:ILE:HG12	1.96	0.46
1:A:90:GLY:HA2	1:A:99:VAL:CG2	2.45	0.46
2:B:136:ILE:HG21	2:B:194:ALA:HB3	1.98	0.46
2:B:185:GLU:O	2:B:189:GLU:HG3	2.15	0.46
1:D:28:GLN:HA	1:D:31:ASN:HD21	1.81	0.46
2:E:231:ILE:HG12	2:E:232:MET:H	1.79	0.46
2:H:111:HIS:C	2:H:113:PHE:N	2.68	0.46
2:B:170:THR:HA	2:B:173:THR:OG1	2.15	0.45
2:K:133:LEU:O	2:K:137:ARG:HB2	2.16	0.45
2:B:152:ASN:HB2	2:B:155:LEU:HD22	1.98	0.45
2:B:221:ILE:O	2:B:321:LYS:HE2	2.16	0.45
2:B:329:ASP:C	2:B:331:TRP:N	2.70	0.45
1:A:13:LEU:HD12	1:A:14:ALA:N	2.31	0.45
1:D:69:LEU:HB2	1:D:70:PRO:HD3	1.96	0.45
2:E:91:ARG:HA	2:E:91:ARG:NE	2.30	0.45
2:E:209:GLU:HG2	2:E:225:ALA:CB	2.47	0.45
1:G:46:LEU:HB3	1:G:72:LEU:HD22	1.97	0.45
1:G:50:ILE:H	1:G:50:ILE:HG12	1.52	0.45
2:K:271:THR:HB	2:K:275:TYR:CD1	2.52	0.45
2:B:274:ILE:O	2:B:277:SER:HB3	2.16	0.45
2:E:133:LEU:HD23	2:E:133:LEU:C	2.36	0.45
1:G:81:VAL:CG2	1:G:82:PHE:N	2.79	0.45
2:H:149:CYS:SG	2:H:171:ALA:CB	3.05	0.45
2:H:132:ALA:O	2:H:136:ILE:HD13	2.16	0.45
2:B:120:LYS:HE3	2:B:120:LYS:HB2	1.75	0.45
2:B:133:LEU:HD12	2:B:198:ASN:ND2	2.32	0.45
2:E:150:LYS:O	2:E:151:ASN:HB3	2.16	0.45
3:F:32:C:O2	3:F:32:C:H2'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:234:VAL:HG22	2:K:252:LEU:HD22	1.97	0.45
3:L:43:A:H2'	3:L:46:G:O2'	2.17	0.45
2:B:160:THR:O	2:B:164:ILE:HG13	2.17	0.45
2:B:184:LEU:C	2:B:184:LEU:HD23	2.37	0.45
3:C:46:G:C6	3:F:41:G:N2	2.84	0.45
2:E:106:GLU:HA	2:E:106:GLU:OE1	2.16	0.45
1:G:65:ILE:O	1:G:66:ILE:CG2	2.65	0.45
3:I:44:U:H4'	3:I:45:A:H5'	1.99	0.45
2:K:150:LYS:NZ	2:K:164:ILE:HG22	2.32	0.45
2:K:150:LYS:HZ2	2:K:165:MET:HB3	1.82	0.45
2:E:122:PHE:CZ	2:E:171:ALA:HB2	2.52	0.45
2:H:314:GLY:O	2:H:318:TYR:CD1	2.69	0.45
1:J:54:ILE:HG22	1:J:56:MET:HG3	1.99	0.45
2:B:253:GLY:HA3	2:B:273:TYR:CE1	2.51	0.45
1:D:41:GLU:HA	1:D:44:LYS:CD	2.47	0.45
2:K:108:ASN:HA	2:K:111:HIS:HB3	1.99	0.45
2:K:164:ILE:O	2:K:167:VAL:HG22	2.16	0.45
2:E:136:ILE:HG22	2:E:137:ARG:N	2.31	0.45
2:E:107:LEU:HD12	2:E:107:LEU:HA	1.81	0.44
2:H:221:ILE:HD13	2:H:318:TYR:CE1	2.52	0.44
2:K:234:VAL:HG11	2:K:273:TYR:CE1	2.40	0.44
1:A:50:ILE:C	1:A:106:ILE:HG13	2.37	0.44
2:B:222:ILE:HA	2:B:321:LYS:HG3	2.00	0.44
2:B:230:LYS:HD3	2:B:273:TYR:CE2	2.52	0.44
2:H:238:LEU:HD21	2:H:307:SER:HA	1.98	0.44
2:K:268:LEU:HD23	2:K:269:PRO:CD	2.41	0.44
3:L:43:A:H62	3:L:46:G:H21	1.65	0.44
1:A:25:LEU:CD2	1:A:119:ILE:HG13	2.47	0.44
1:D:29:SER:O	1:D:32:TYR:O	2.36	0.44
2:E:87:ALA:N	2:E:88:PRO:HD3	2.32	0.44
2:H:87:ALA:HA	2:H:91:ARG:HE	1.82	0.44
2:H:88:PRO:O	2:H:91:ARG:HG2	2.17	0.44
2:H:238:LEU:O	2:H:242:SER:HB3	2.17	0.44
2:H:302:ALA:O	2:H:303:ALA:C	2.56	0.44
1:A:59:ASP:HB2	1:A:86:LYS:HB3	2.00	0.44
2:B:107:LEU:HD21	2:B:194:ALA:O	2.18	0.44
2:B:167:VAL:O	2:B:171:ALA:N	2.51	0.44
2:H:111:HIS:O	2:H:112:LYS:C	2.56	0.44
2:H:137:ARG:HE	2:H:137:ARG:HB3	1.28	0.44
2:K:150:LYS:NZ	2:K:165:MET:HB3	2.32	0.44
2:K:220:SER:HB3	2:K:225:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LYS:HD3	2:B:298:LYS:N	2.33	0.44
1:J:23:LEU:HD23	1:J:23:LEU:H	1.83	0.44
2:K:152:ASN:CB	2:K:155:LEU:HB3	2.41	0.44
1:A:40:ASN:OD1	2:B:246:ALA:N	2.45	0.44
2:B:271:THR:HB	2:B:275:TYR:CG	2.53	0.44
1:D:23:LEU:HD23	1:D:92:ALA:HB2	2.00	0.44
2:H:185:GLU:O	2:H:189:GLU:HB2	2.18	0.44
2:H:191:CYS:O	2:H:193:MET:N	2.51	0.44
2:K:89:GLU:O	2:K:92:VAL:HB	2.18	0.44
1:D:53:PHE:N	1:D:53:PHE:CD2	2.86	0.44
2:E:100:THR:HG22	2:E:204:ILE:CG2	2.48	0.44
1:J:50:ILE:O	1:J:50:ILE:HG13	2.18	0.44
2:E:110:ILE:O	2:E:114:ILE:HG13	2.18	0.43
2:K:298:LYS:HB3	2:K:320:LEU:HD22	2.00	0.43
1:G:33:LYS:HD2	1:G:33:LYS:N	2.33	0.43
3:I:57:A:H2	3:L:57:A:C2	2.36	0.43
1:J:22:LEU:HD21	1:J:81:VAL:HG21	2.01	0.43
2:B:135:TYR:CD2	2:B:135:TYR:C	2.92	0.43
2:B:148:LYS:O	2:B:148:LYS:HG3	2.18	0.43
2:B:226:SER:O	2:B:229:ALA:N	2.51	0.43
2:E:138:THR:O	2:E:141:GLU:N	2.52	0.43
2:E:175:GLN:HA	2:E:175:GLN:OE1	2.19	0.43
2:E:214:PHE:CD1	2:E:214:PHE:O	2.70	0.43
1:A:43:THR:HG23	1:A:68:HIS:NE2	2.33	0.43
2:K:258:THR:O	2:K:259:LEU:HD22	2.18	0.43
1:A:59:ASP:HB3	1:A:86:LYS:HE3	1.95	0.43
1:A:59:ASP:CG	1:A:86:LYS:H	2.21	0.43
1:A:65:ILE:HG13	1:A:66:ILE:HG23	1.99	0.43
2:B:120:LYS:HG2	2:B:179:LEU:HD21	2.00	0.43
3:C:40:C:O2'	3:C:41:G:H5'	2.19	0.43
2:H:90:TYR:CD2	2:H:91:ARG:N	2.86	0.43
1:A:69:LEU:HB2	1:A:70:PRO:HD3	2.00	0.43
2:H:114:ILE:HD11	2:H:136:ILE:HG13	2.00	0.43
2:H:137:ARG:HH11	2:H:158:ILE:CB	2.22	0.43
3:I:56:U:H2'	3:I:57:A:H8	1.83	0.43
1:J:11:TYR:N	1:J:82:PHE:CE2	2.86	0.43
1:A:22:LEU:H	1:A:22:LEU:CD1	2.28	0.43
1:A:26:VAL:HG13	1:A:35:LEU:HD13	2.01	0.43
3:I:33:C:O2	3:I:33:C:H2'	2.17	0.43
2:B:135:TYR:HA	2:B:138:THR:HG23	2.00	0.43
3:F:27:A:H2'	3:F:28:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ILE:CG2	2:B:208:VAL:HG12	2.49	0.43
2:B:275:TYR:CD1	2:B:275:TYR:C	2.92	0.43
3:F:42:C:H2'	3:F:43:A:C8	2.54	0.43
1:G:45:THR:O	1:G:50:ILE:HG12	2.19	0.43
1:G:52:GLU:O	1:G:120:GLN:NE2	2.50	0.43
2:B:121:ARG:CZ	2:B:146:LEU:HD21	2.49	0.42
3:C:29:U:C2'	3:C:30:G:H5'	2.48	0.42
3:F:43:A:OP1	3:F:43:A:H4'	2.19	0.42
1:G:68:HIS:HE1	2:H:304:ARG:CZ	2.32	0.42
2:H:135:TYR:CE1	2:H:139:VAL:HG11	2.48	0.42
2:E:135:TYR:C	2:E:135:TYR:CD2	2.91	0.42
1:J:22:LEU:CD1	1:J:119:ILE:HD12	2.49	0.42
1:J:36:ARG:HG3	1:J:45:THR:OG1	2.19	0.42
3:L:47:U:C2'	3:L:48:G:H5'	2.49	0.42
2:B:158:ILE:HB	2:B:159:LEU:CD1	2.49	0.42
2:B:329:ASP:C	2:B:331:TRP:H	2.22	0.42
1:D:7:ASN:ND2	1:D:9:LYS:HB2	2.34	0.42
2:K:219:LEU:N	2:K:306:ASP:OD2	2.49	0.42
1:G:121:GLN:HB3	1:G:125:ARG:NH1	2.35	0.42
2:E:193:MET:O	2:E:194:ALA:C	2.57	0.42
2:K:193:MET:O	2:K:194:ALA:C	2.57	0.42
1:A:3:GLU:C	1:A:5:ASP:H	2.22	0.42
2:B:251:LEU:HD21	3:F:41:G:N2	2.35	0.42
2:B:304:ARG:O	2:B:307:SER:HB3	2.20	0.42
3:F:28:C:C4	3:F:29:U:C5	3.07	0.42
3:L:44:U:H4'	3:L:45:A:H5"	2.02	0.42
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.84	0.42
2:B:294:LEU:CD2	2:B:324:ILE:HG23	2.50	0.42
1:D:12:PRO:HB2	1:D:126:LEU:HG	2.01	0.42
2:H:269:PRO:O	2:H:270:HIS:C	2.58	0.42
3:I:31:U:H2'	3:I:32:C:C6	2.55	0.42
1:J:95:VAL:CG1	1:J:97:ARG:H	2.27	0.42
1:A:18:LEU:CG	1:A:22:LEU:HD11	2.47	0.42
1:A:19:THR:HA	1:A:22:LEU:HD13	2.01	0.42
2:B:91:ARG:HD3	2:B:95:ASP:OD1	2.18	0.42
2:B:255:GLN:NE2	2:B:255:GLN:CA	2.79	0.42
2:E:91:ARG:O	2:E:95:ASP:HB2	2.20	0.42
1:G:7:ASN:OD1	1:G:8:PRO:HD2	2.20	0.42
1:G:50:ILE:O	1:G:105:THR:HA	2.20	0.42
2:H:121:ARG:HB2	2:H:179:LEU:HG	2.02	0.42
2:H:242:SER:OG	2:H:243:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:150:LYS:HA	2:K:150:LYS:HD3	1.60	0.42
1:A:4:ALA:HA	1:A:84:ARG:HH22	1.83	0.42
1:A:121:GLN:HB3	1:A:125:ARG:HH21	1.85	0.42
1:G:65:ILE:HG13	1:G:66:ILE:HG23	2.02	0.42
2:H:214:PHE:O	2:H:214:PHE:CD1	2.73	0.42
2:K:110:ILE:O	2:K:114:ILE:CG1	2.68	0.42
2:E:125:LEU:O	2:E:126:GLU:C	2.58	0.42
2:E:160:THR:OG1	2:E:162:ALA:HB3	2.20	0.42
3:I:55:G:H2'	3:I:56:U:O5'	2.20	0.42
1:J:97:ARG:HB3	1:J:98:PRO:CD	2.50	0.42
1:G:40:ASN:ND2	1:G:40:ASN:N	2.65	0.41
1:G:41:GLU:HG3	3:L:37:G:H1	1.85	0.41
2:H:270:HIS:CE1	3:I:44:U:N3	2.88	0.41
1:J:51:SER:OG	1:J:103:SER:OG	2.32	0.41
2:E:294:LEU:O	2:E:297:ALA:HB3	2.20	0.41
1:G:123:ILE:O	1:G:127:LEU:HD12	2.21	0.41
2:H:208:VAL:O	2:H:212:MET:HB2	2.20	0.41
1:A:74:GLU:O	1:A:75:ASP:C	2.58	0.41
2:B:119:SER:HA	2:B:123:PRO:HA	2.02	0.41
1:D:57:ALA:HB1	1:D:86:LYS:HB3	2.03	0.41
1:D:120:GLN:O	1:D:124:GLU:HG2	2.20	0.41
2:H:209:GLU:HA	2:H:225:ALA:HB1	2.03	0.41
1:A:97:ARG:HA	1:A:97:ARG:HD2	1.93	0.41
3:C:29:U:O2'	3:C:30:G:H5'	2.20	0.41
1:J:34:GLN:O	1:J:105:THR:HG23	2.20	0.41
2:B:239:THR:O	2:B:242:SER:HB3	2.21	0.41
3:C:41:G:H1	2:E:250:MET:CE	2.17	0.41
1:D:34:GLN:HE22	1:D:107:LYS:N	2.18	0.41
1:J:86:LYS:HG3	1:J:98:PRO:HB3	2.02	0.41
2:K:326:ARG:HE	2:K:326:ARG:HB2	1.71	0.41
1:A:110:SER:OG	1:A:112:LEU:HD12	2.20	0.41
2:B:268:LEU:HG	2:B:271:THR:HG21	2.01	0.41
2:H:99:LEU:HD22	2:H:99:LEU:HA	1.90	0.41
2:H:121:ARG:HH12	2:H:178:GLN:HG2	1.86	0.41
1:J:18:LEU:HD12	1:J:18:LEU:O	2.20	0.41
1:J:121:GLN:O	1:J:125:ARG:HG3	2.21	0.41
1:G:116:ILE:O	1:G:120:GLN:HB2	2.20	0.41
2:H:135:TYR:C	2:H:135:TYR:CD1	2.94	0.41
2:H:160:THR:HG22	2:H:161:ASN:H	1.86	0.41
2:H:183:GLU:HG2	2:H:186:ARG:NH1	2.36	0.41
2:K:91:ARG:HA	2:K:91:ARG:NE	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ALA:C	1:A:94:GLY:H	2.24	0.41
2:B:114:ILE:HD12	2:B:136:ILE:HG23	2.02	0.41
2:B:209:GLU:HA	2:B:225:ALA:CB	2.51	0.41
2:E:245:PRO:HG2	2:E:248:ASN:HB2	2.02	0.41
2:E:314:GLY:O	2:E:318:TYR:HD1	2.03	0.41
2:K:313:GLU:CD	2:K:313:GLU:H	2.24	0.41
2:B:211:ARG:O	2:B:215:ILE:HG13	2.21	0.41
1:D:34:GLN:OE1	1:D:107:LYS:HB3	2.20	0.41
2:H:88:PRO:HD2	2:H:91:ARG:CD	2.50	0.41
2:H:135:TYR:C	2:H:135:TYR:HD1	2.23	0.41
3:I:31:U:H2'	3:I:32:C:O4'	2.21	0.41
1:J:63:LEU:CD1	1:J:66:ILE:HD11	2.51	0.41
2:K:117:LYS:O	2:K:187:LEU:HD11	2.20	0.41
1:A:54:ILE:HA	1:A:54:ILE:HD13	1.78	0.41
2:B:240:ASN:O	2:B:243:LYS:N	2.54	0.41
1:A:40:ASN:HD22	1:A:40:ASN:H	1.69	0.40
1:A:71:LEU:HD23	1:A:71:LEU:N	2.36	0.40
2:E:234:VAL:HG11	2:E:273:TYR:HE2	1.86	0.40
2:H:211:ARG:HD2	2:H:211:ARG:HA	1.54	0.40
2:H:282:SER:O	2:H:283:LEU:HD12	2.21	0.40
1:J:12:PRO:HG3	1:J:127:LEU:HD21	2.04	0.40
1:A:26:VAL:HG13	1:A:35:LEU:HD11	2.02	0.40
1:A:32:TYR:HD2	1:A:112:LEU:HD11	1.86	0.40
2:E:218:ASN:CA	2:E:221:ILE:HD12	2.33	0.40
1:D:46:LEU:HD13	1:D:72:LEU:HB2	2.02	0.40
1:D:63:LEU:O	1:D:67:LEU:HD13	2.21	0.40
2:H:293:ARG:CD	3:L:41:G:O6	2.56	0.40
2:K:114:ILE:CG2	2:K:187:LEU:HD22	2.52	0.40
2:B:168:SER:HA	2:B:171:ALA:HB3	2.04	0.40
1:G:40:ASN:O	1:G:43:THR:HB	2.22	0.40
2:H:128:LEU:HD22	2:H:129:VAL:HG23	2.04	0.40
1:A:14:ALA:HA	1:A:18:LEU:HD23	2.04	0.40
2:E:301:LEU:O	2:E:305:VAL:HG23	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	126/130 (97%)	110 (87%)	13 (10%)	3 (2%)	6	28
1	D	123/130 (95%)	110 (89%)	11 (9%)	2 (2%)	9	36
1	G	126/130 (97%)	119 (94%)	4 (3%)	3 (2%)	6	28
1	J	124/130 (95%)	113 (91%)	10 (8%)	1 (1%)	19	51
2	B	233/254 (92%)	190 (82%)	36 (16%)	7 (3%)	4	24
2	E	232/254 (91%)	196 (84%)	32 (14%)	4 (2%)	9	35
2	H	231/254 (91%)	189 (82%)	37 (16%)	5 (2%)	6	30
2	K	237/254 (93%)	193 (81%)	34 (14%)	10 (4%)	3	17
All	All	1432/1536 (93%)	1220 (85%)	177 (12%)	35 (2%)	6	28

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	58	ALA
1	D	105	THR
2	K	87	ALA
2	K	128	LEU
2	B	119	SER
2	B	132	ALA
2	B	277	SER
2	H	203	ARG
2	H	277	SER
2	K	132	ALA
2	K	180	SER
1	A	4	ALA
1	A	60	ALA
2	B	210	SER
2	B	311	SER
2	E	160	THR
1	G	66	ILE

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Mol	Chain	Res	Type
2	H	112	LYS
2	K	202	HIS
2	B	142	LEU
2	E	315	LYS
2	H	192	ASP
2	K	151	ASN
2	K	153	GLU
2	K	282	SER
1	A	75	ASP
2	B	122	PHE
2	E	277	SER
1	J	67	LEU
2	K	257	LYS
1	G	65	ILE
2	H	222	ILE
2	E	316	VAL
1	G	49	GLY
2	K	88	PRO

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	111/112 (99%)	92 (83%)	19 (17%)	2 9
1	D	108/112 (96%)	88 (82%)	20 (18%)	1 7
1	G	111/112 (99%)	97 (87%)	14 (13%)	4 19
1	J	109/112 (97%)	88 (81%)	21 (19%)	1 6
2	B	205/219 (94%)	168 (82%)	37 (18%)	1 7
2	E	204/219 (93%)	163 (80%)	41 (20%)	1 5
2	H	203/219 (93%)	178 (88%)	25 (12%)	4 20
2	K	209/219 (95%)	183 (88%)	26 (12%)	4 19
All	All	1260/1324 (95%)	1057 (84%)	203 (16%)	2 10

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	13	LEU
1	A	37	LYS
1	A	41	GLU
1	A	43	THR
1	A	46	LEU
1	A	50	ILE
1	A	64	GLU
1	A	72	LEU
1	A	74	GLU
1	A	76	LYS
1	A	78	VAL
1	A	96	SER
1	A	110	SER
1	A	112	LEU
1	A	121	GLN
1	A	122	SER
1	A	125	ARG
1	A	126	LEU
2	B	90	TYR
2	B	101	VAL
2	B	110	ILE
2	B	120	LYS
2	B	124	GLU
2	B	129	VAL
2	B	133	LEU
2	B	138	THR
2	B	139	VAL
2	B	141	GLU
2	B	142	LEU
2	B	146	LEU
2	B	149	CYS
2	B	154	ASN
2	B	160	THR
2	B	166	VAL
2	B	167	VAL
2	B	169	VAL
2	B	170	THR
2	B	172	SER
2	B	174	THR
2	B	180	SER
2	B	187	LEU
2	B	197	LEU

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Mol	Chain	Res	Type
2	B	203	ARG
2	B	213	SER
2	B	214	PHE
2	B	231	ILE
2	B	234	VAL
2	B	240	ASN
2	B	242	SER
2	B	268	LEU
2	B	282	SER
2	B	286	ASP
2	B	307	SER
2	B	322	ASP
2	B	331	TRP
1	D	9	LYS
1	D	11	TYR
1	D	13	LEU
1	D	15	ASP
1	D	18	LEU
1	D	20	LYS
1	D	24	ASP
1	D	26	VAL
1	D	31	ASN
1	D	41	GLU
1	D	53	PHE
1	D	61	GLU
1	D	63	LEU
1	D	81	VAL
1	D	83	VAL
1	D	85	SER
1	D	96	SER
1	D	112	LEU
1	D	121	GLN
1	D	123	ILE
2	E	94	VAL
2	E	95	ASP
2	E	100	THR
2	E	107	LEU
2	E	110	ILE
2	E	115	ARG
2	E	121	ARG
2	E	139	VAL
2	E	142	LEU

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Mol	Chain	Res	Type
2	E	146	LEU
2	E	149	CYS
2	E	152	ASN
2	E	154	ASN
2	E	160	THR
2	E	164	ILE
2	E	169	VAL
2	E	170	THR
2	E	172	SER
2	E	174	THR
2	E	177	GLN
2	E	181	GLU
2	E	186	ARG
2	E	188	GLU
2	E	193	MET
2	E	198	ASN
2	E	208	VAL
2	E	211	ARG
2	E	214	PHE
2	E	215	ILE
2	E	223	ILE
2	E	227	THR
2	E	231	ILE
2	E	234	VAL
2	E	239	THR
2	E	240	ASN
2	E	283	LEU
2	E	286	ASP
2	E	300	THR
2	E	312	THR
2	E	313	GLU
2	E	322	ASP
1	G	27	GLN
1	G	35	LEU
1	G	40	ASN
1	G	50	ILE
1	G	51	SER
1	G	64	GLU
1	G	68	HIS
1	G	84	ARG
1	G	91	ARG
1	G	112	LEU

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Mol	Chain	Res	Type
1	G	116	ILE
1	G	124	GLU
1	G	127	LEU
1	G	128	VAL
2	H	93	ILE
2	H	99	LEU
2	H	120	LYS
2	H	133	LEU
2	H	135	TYR
2	H	137	ARG
2	H	155	LEU
2	H	158	ILE
2	H	163	THR
2	H	195	LEU
2	H	196	GLU
2	H	197	LEU
2	H	214	PHE
2	H	219	LEU
2	H	226	SER
2	H	227	THR
2	H	231	ILE
2	H	234	VAL
2	H	239	THR
2	H	274	ILE
2	H	281	GLN
2	H	282	SER
2	H	286	ASP
2	H	289	ARG
2	H	312	THR
1	J	5	ASP
1	J	6	VAL
1	J	11	TYR
1	J	18	LEU
1	J	22	LEU
1	J	23	LEU
1	J	29	SER
1	J	37	LYS
1	J	48	ARG
1	J	52	GLU
1	J	64	GLU
1	J	66	ILE
1	J	76	LYS

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Mol	Chain	Res	Type
1	J	81	VAL
1	J	83	VAL
1	J	89	LEU
1	J	105	THR
1	J	107	LYS
1	J	111	GLN
1	J	115	GLN
1	J	126	LEU
2	K	90	TYR
2	K	91	ARG
2	K	108	ASN
2	K	114	ILE
2	K	121	ARG
2	K	122	PHE
2	K	127	SER
2	K	128	LEU
2	K	133	LEU
2	K	135	TYR
2	K	148	LYS
2	K	161	ASN
2	K	173	THR
2	K	174	THR
2	K	180	SER
2	K	182	GLU
2	K	212	MET
2	K	214	PHE
2	K	220	SER
2	K	226	SER
2	K	227	THR
2	K	256	ARG
2	K	257	LYS
2	K	259	LEU
2	K	283	LEU
2	K	312	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	34	GLN
1	A	115	GLN
2	B	97	ASN

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Mol	Chain	Res	Type
2	B	154	ASN
2	B	157	GLN
2	B	161	ASN
2	B	255	GLN
1	D	7	ASN
1	D	31	ASN
1	D	120	GLN
2	E	97	ASN
2	E	152	ASN
2	E	177	GLN
2	E	198	ASN
2	E	240	ASN
2	E	281	GLN
1	G	34	GLN
2	H	97	ASN
2	H	152	ASN
2	H	281	GLN
2	K	98	ASN
2	K	108	ASN
2	K	156	GLN
2	K	178	GLN
2	K	198	ASN
2	K	202	HIS
2	K	281	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	31/32 (96%)	4 (12%)	0
3	F	31/32 (96%)	6 (19%)	0
3	I	31/32 (96%)	3 (9%)	0
3	L	31/32 (96%)	8 (25%)	0
All	All	124/128 (96%)	21 (16%)	0

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	30	G
3	C	36	U
3	C	43	A
3	C	50	G

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Mol	Chain	Res	Type
3	F	32	C
3	F	42	C
3	F	43	A
3	F	44	U
3	F	45	A
3	F	50	G
3	I	33	C
3	I	45	A
3	I	50	G
3	L	32	C
3	L	33	C
3	L	42	C
3	L	43	A
3	L	45	A
3	L	47	U
3	L	48	G
3	L	50	G

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)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	128/130 (98%)	-0.49	0	100	100	81, 109, 179, 224	0
1	D	125/130 (96%)	0.01	5 (4%)	38	36	92, 142, 192, 239	0
1	G	128/130 (98%)	-0.39	1 (0%)	86	86	76, 114, 172, 220	0
1	J	126/130 (96%)	-0.14	2 (1%)	72	70	86, 128, 195, 215	0
2	B	237/254 (93%)	-0.23	3 (1%)	77	77	72, 126, 220, 329	1 (0%)
2	E	236/254 (92%)	-0.34	2 (0%)	86	86	86, 122, 171, 213	0
2	H	235/254 (92%)	0.19	25 (10%)	6	6	80, 135, 271, 314	1 (0%)
2	K	241/254 (94%)	-0.16	8 (3%)	46	44	83, 135, 218, 318	0
3	C	32/32 (100%)	-0.32	0	100	100	106, 121, 163, 183	0
3	F	32/32 (100%)	-0.30	0	100	100	90, 128, 188, 211	0
3	I	32/32 (100%)	-0.32	0	100	100	105, 124, 172, 208	0
3	L	32/32 (100%)	-0.23	0	100	100	91, 128, 181, 247	0
All	All	1584/1664 (95%)	-0.19	46 (2%)	51	50	72, 126, 218, 329	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	151	ASN	6.1
2	H	165	MET	5.7
2	H	130	PRO	5.2
2	H	127	SER	5.0
2	H	162	ALA	4.8
2	H	166	VAL	4.4
1	D	40	ASN	4.3
2	H	128	LEU	4.2
2	K	267	VAL	4.1
2	H	169	VAL	3.9
2	H	175	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	160	THR	3.8
2	H	129	VAL	3.7
2	H	163	THR	3.6
2	K	257	LYS	3.6
2	K	266	SER	3.6
2	H	172	SER	3.5
2	H	147	ASP	3.4
2	H	153	GLU	3.3
1	J	128	VAL	3.3
1	D	4	ALA	3.1
2	K	258	THR	3.0
2	K	256	ARG	3.0
1	D	128	VAL	2.9
1	J	40	ASN	2.8
2	H	146	LEU	2.6
2	E	267	VAL	2.6
2	B	165	MET	2.6
2	H	182	GLU	2.5
2	H	152	ASN	2.5
2	H	124	GLU	2.5
2	E	297	ALA	2.4
1	G	128	VAL	2.3
2	H	120	LYS	2.3
2	H	131	ASN	2.3
2	K	247	CYS	2.2
2	K	151	ASN	2.2
2	H	168	SER	2.1
2	B	267	VAL	2.1
2	H	299	CYS	2.1
1	D	39	ALA	2.1
1	D	108	GLU	2.1
2	H	297	ALA	2.1
2	B	269	PRO	2.0
2	H	150	LYS	2.0
2	K	128	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.