Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:38 am BST

PDB ID	:	5C0X
Title	:	Structure of a 12-subunit nuclear exosome complex bound to structured RNA
Authors	:	Makino, D.L.; Conti, E.
Deposited on	:	2015-06-12
Resolution	:	3.81 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

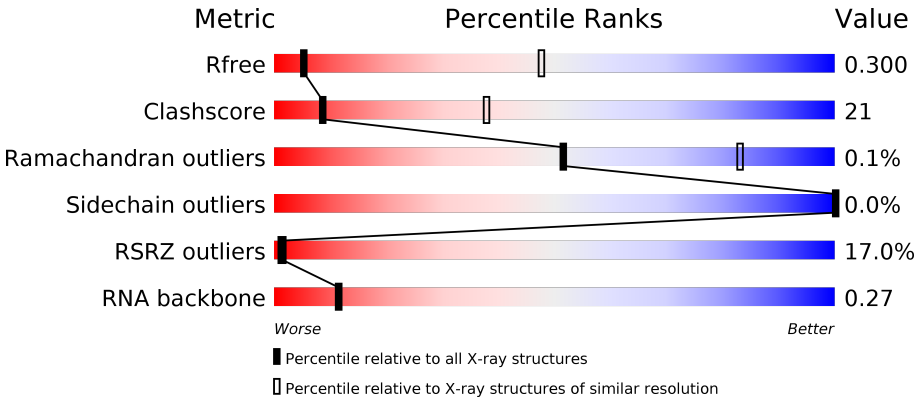
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.81 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	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)
RNA backbone	3102	1037 (4.62-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	305	7% 77% 21% ·
2	B	248	8% 76% 22% ·
3	C	394	7% 61% 25% 14%
4	D	245	5% 74% 17% 9%

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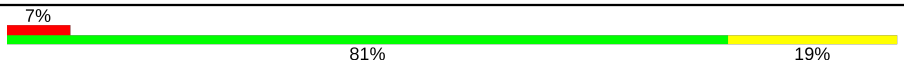
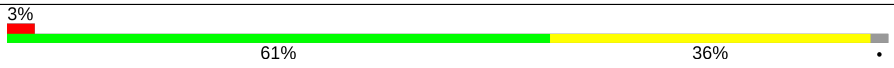
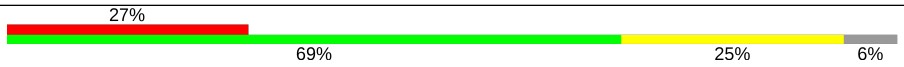
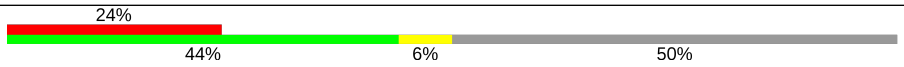
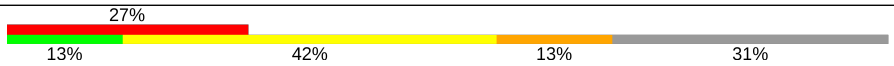
Mol	Chain	Length	Quality of chain
5	E	267	
6	F	250	
7	G	243	
8	H	361	
9	I	295	
10	J	1003	
11	K	695	
12	R	45	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27816 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 Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2304	1444	393	451	16			

- Molecule 2 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1886	1177	335	366	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P46948
B	0	HIS	-	expression tag	UNP P46948

- Molecule 3 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	339	Total	C	N	O	S	0	1	0
			2589	1640	441	497	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	102	SER	ALA	engineered mutation	UNP P25359
C	363	MET	VAL	engineered mutation	UNP P25359

- Molecule 4 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	223	Total	C	N	O	S	0	1	0
			1701	1072	285	334	10			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	GLY	-	expression tag	UNP P53256
D	-20	HIS	-	expression tag	UNP P53256
D	-19	GLY	-	expression tag	UNP P53256
D	-18	ASN	-	expression tag	UNP P53256
D	-17	ASN	-	expression tag	UNP P53256
D	-16	LYS	-	expression tag	UNP P53256
D	-15	GLU	-	expression tag	UNP P53256
D	-14	PRO	-	expression tag	UNP P53256
D	-13	ASN	-	expression tag	UNP P53256
D	-12	THR	-	expression tag	UNP P53256
D	-11	LYS	-	expression tag	UNP P53256
D	-10	ASN	-	expression tag	UNP P53256
D	-9	ARG	-	expression tag	UNP P53256
D	-8	LEU	-	expression tag	UNP P53256
D	-7	ASP	-	expression tag	UNP P53256
D	-6	SER	-	expression tag	UNP P53256
D	-5	ALA	-	expression tag	UNP P53256
D	-4	GLU	-	expression tag	UNP P53256
D	-3	LYS	-	expression tag	UNP P53256
D	-2	LYS	-	expression tag	UNP P53256
D	-1	LYS	-	expression tag	UNP P53256
D	0	LYS	-	expression tag	UNP P53256

- Molecule 5 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	267	Total	C	N	O	S	0	1	0
			2050	1308	338	399	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q12277
E	0	HIS	-	expression tag	UNP Q12277
E	138	ILE	VAL	engineered mutation	UNP Q12277

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	215	Total	C	N	O	S	0	0	0
			1638	1023	273	332	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	75	SER	THR	engineered mutation	UNP P48240
F	161	THR	MET	engineered mutation	UNP P48240

- Molecule 7 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	237	Total	C	N	O	S	0	0	0
			1792	1143	295	344	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP Q08285
G	-1	PRO	-	expression tag	UNP Q08285
G	0	HIS	-	expression tag	UNP Q08285

- Molecule 8 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	293	Total	C	N	O	S	0	0	0
			2236	1393	403	428	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	ARG	-	expression tag	UNP P38792
H	0	SER	-	expression tag	UNP P38792

- Molecule 9 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1653	1034	287	325	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	expression tag	UNP P53859
I	-1	PRO	-	expression tag	UNP P53859
I	0	HIS	-	expression tag	UNP P53859

- Molecule 10 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	944	Total	C	N	O	S	0	1	0
			7427	4693	1304	1395	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	GLY	-	expression tag	UNP Q08162
J	0	ALA	-	expression tag	UNP Q08162
J	171	ASN	ASP	engineered mutation	UNP Q08162
J	551	ASN	ASP	engineered mutation	UNP Q08162

- Molecule 11 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	350	Total	C	N	O	S	0	0	0
			1982	1212	379	389	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	expression tag	UNP Q12149
K	0	ALA	-	expression tag	UNP Q12149
K	2	ALA	THR	engineered mutation	UNP Q12149
K	296	ASN	ASP	engineered mutation	UNP Q12149

- Molecule 12 is a RNA chain called RNA synthetic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	31	Total	C	N	O	P	0	0	0
			557	244	71	211	31			

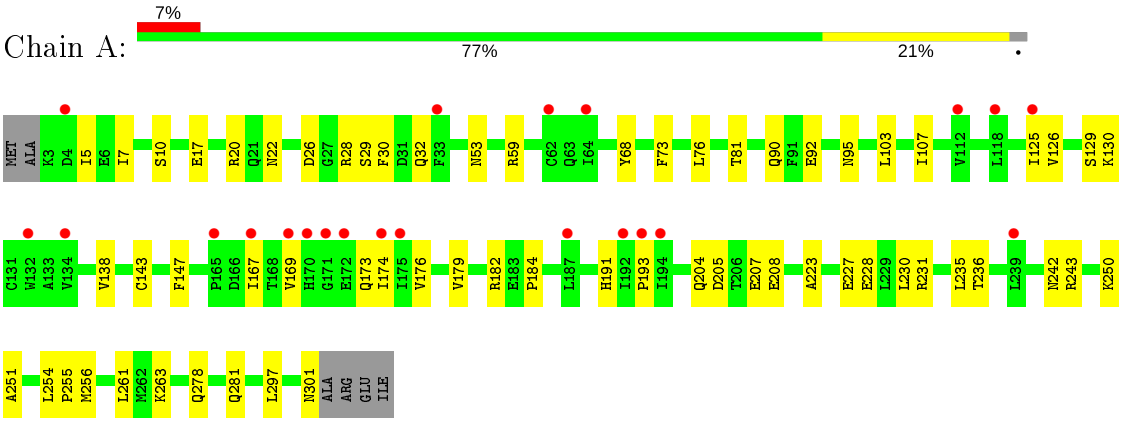
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

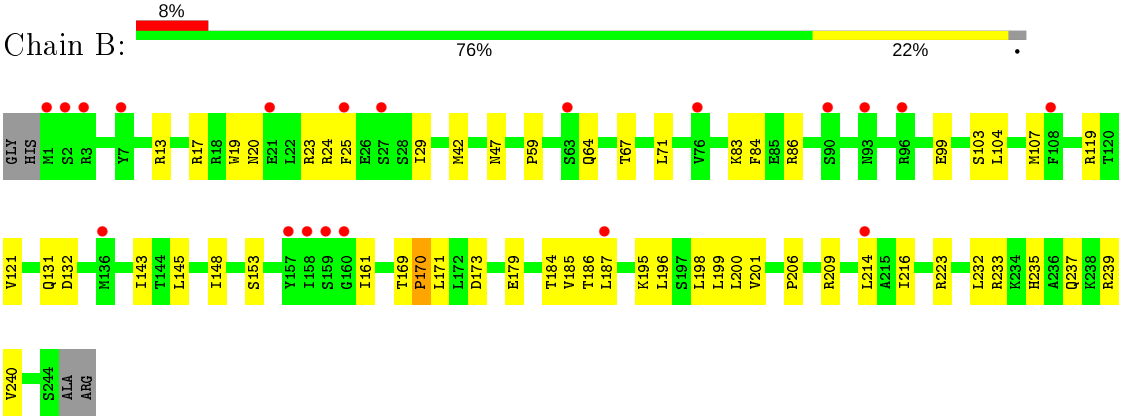
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

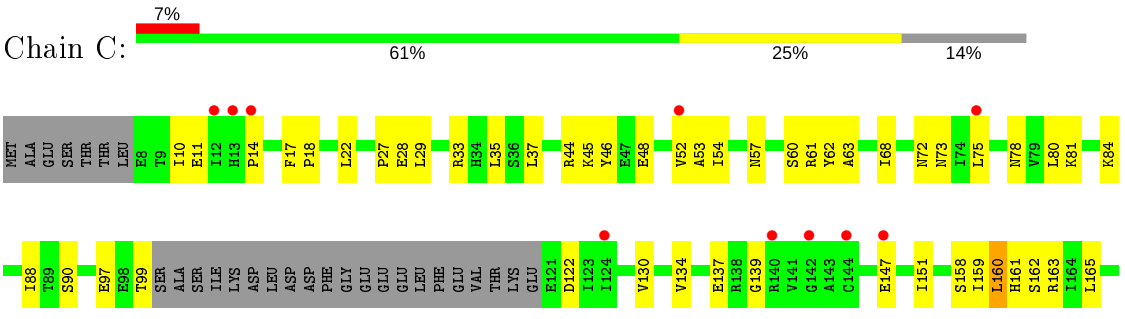
- Molecule 1: Exosome complex component RRP45

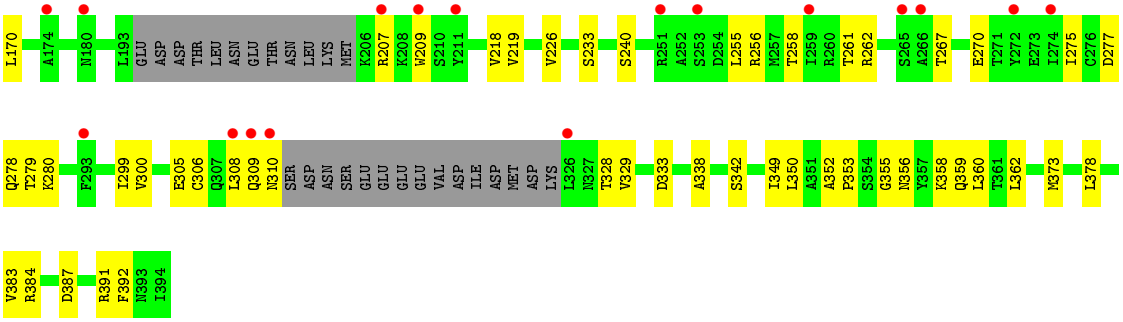


- Molecule 2: Exosome complex component SKI6

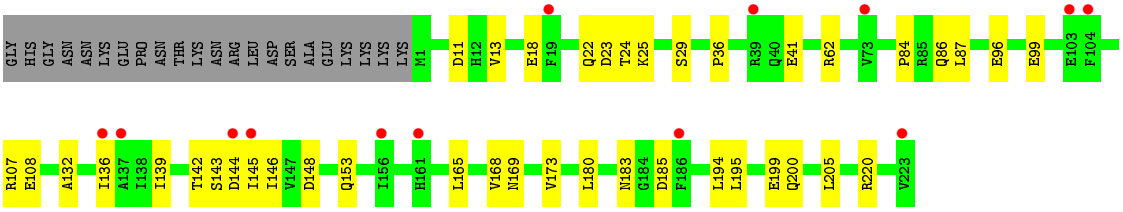


- Molecule 3: Exosome complex component RRP43

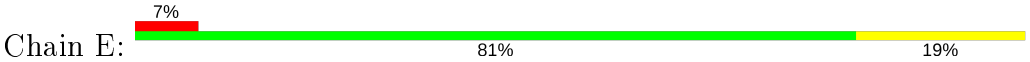


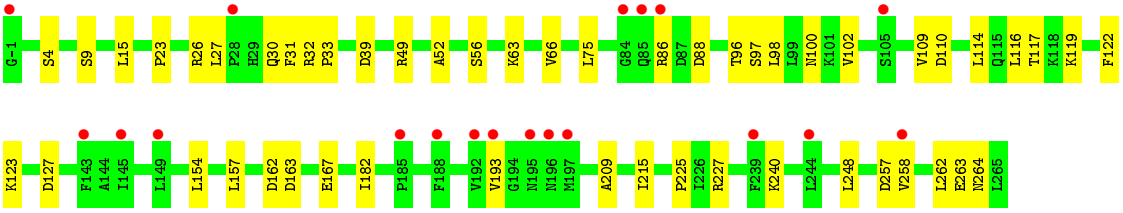


• Molecule 4: Exosome complex component RRP46

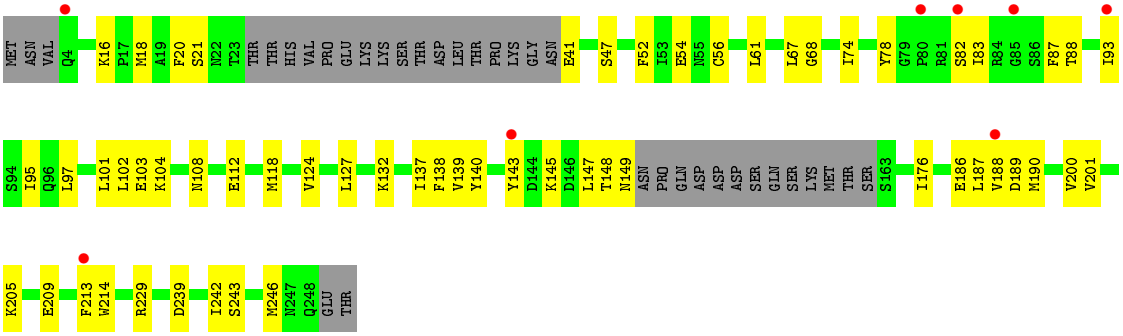


• Molecule 5: Exosome complex component RRP42

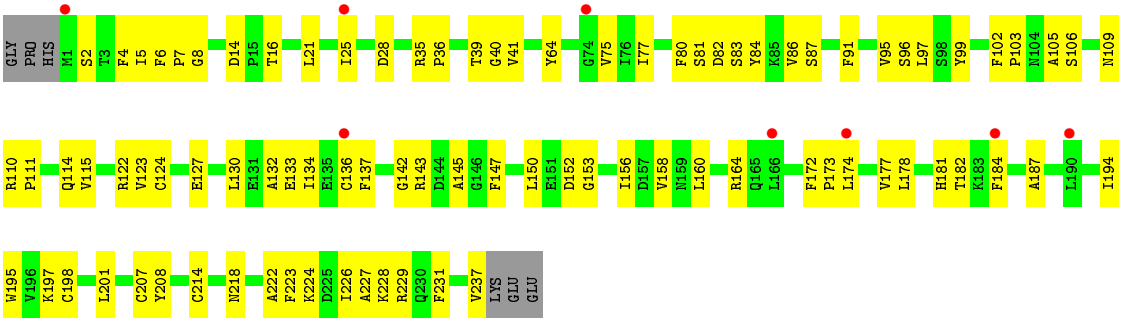




• Molecule 6: Exosome complex component MTR3

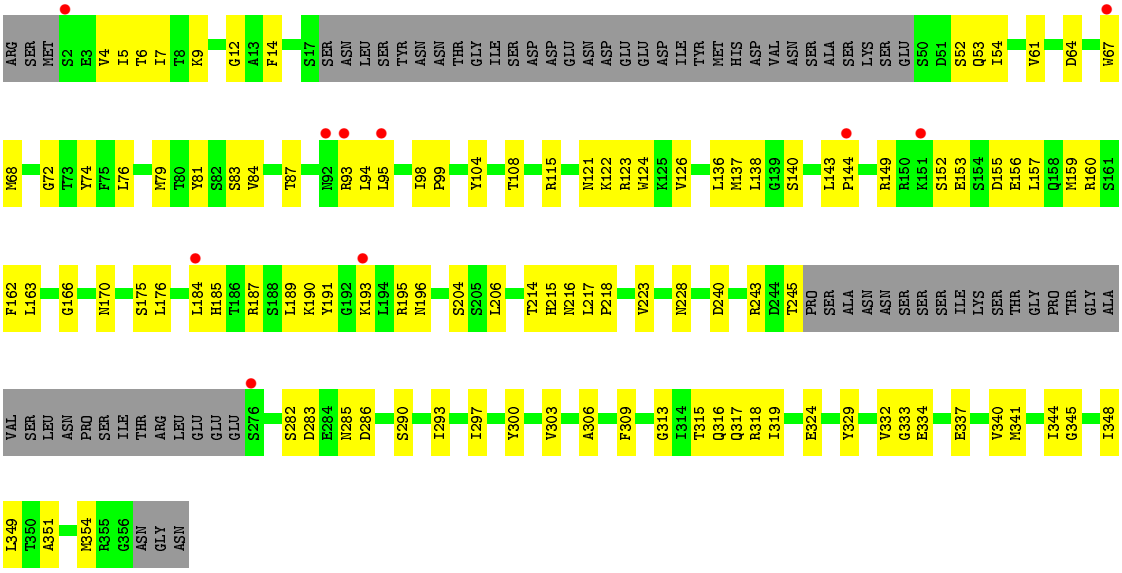


• Molecule 7: Exosome complex component RRP40



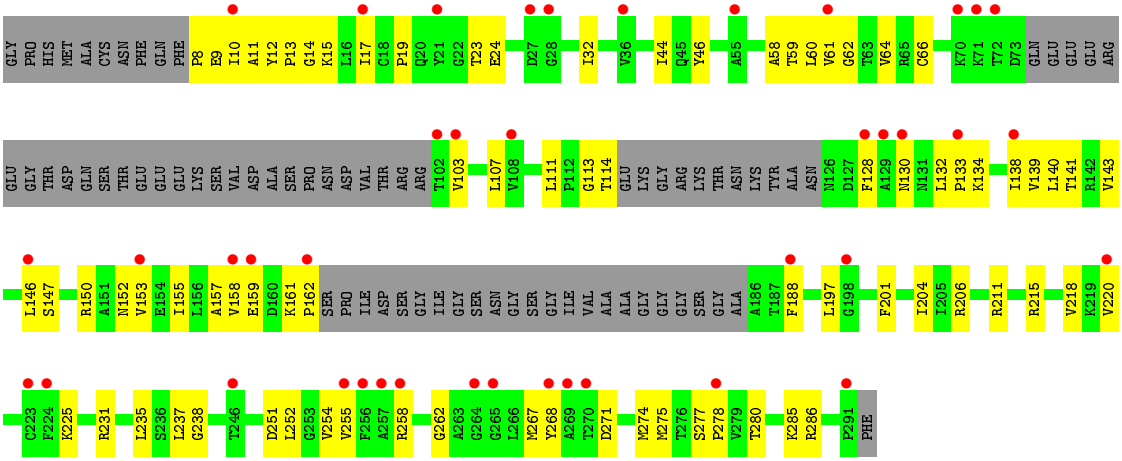
• Molecule 8: Exosome complex component RRP4

Chain H:



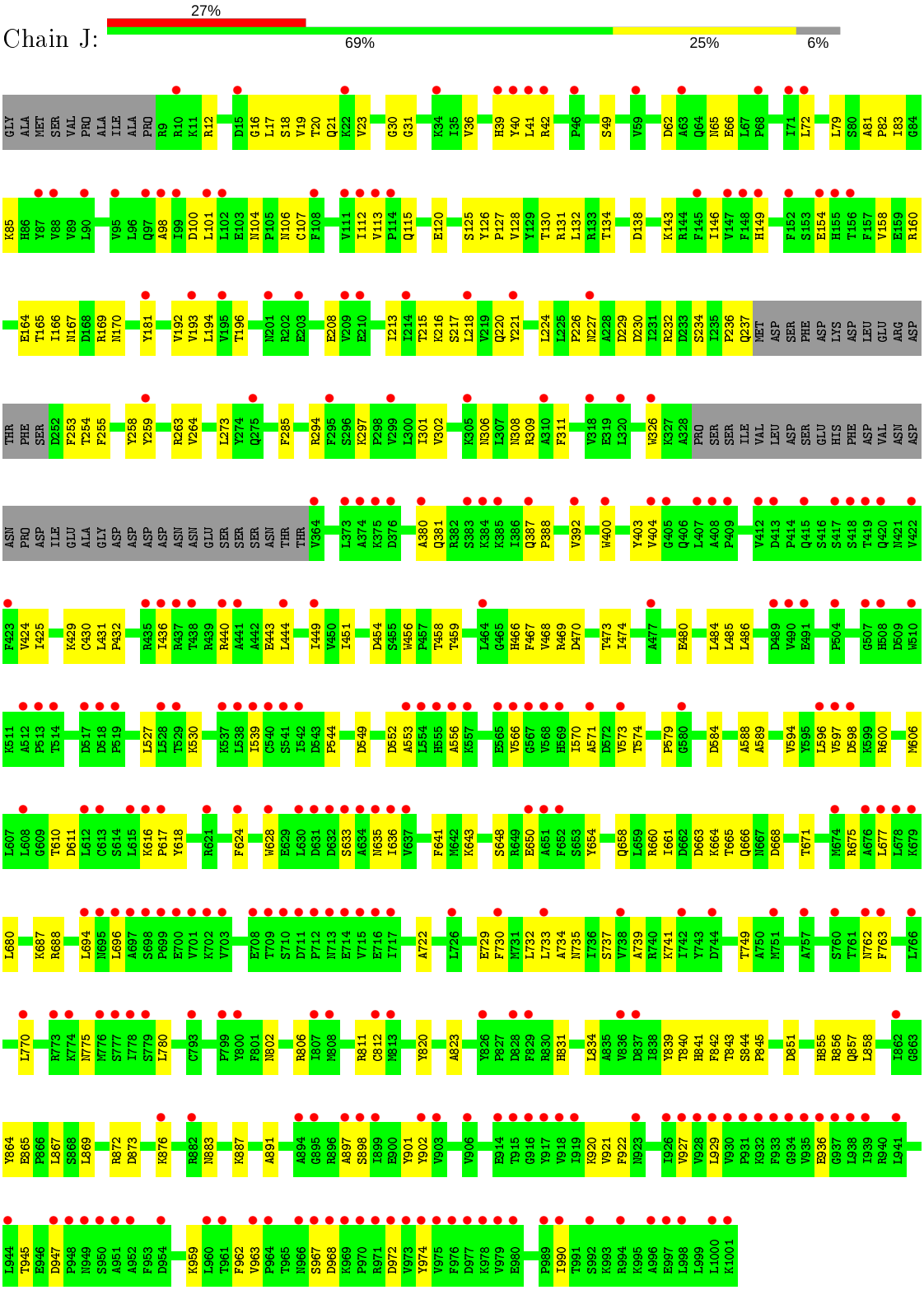
• Molecule 9: Exosome complex component CSL4

Chain I:



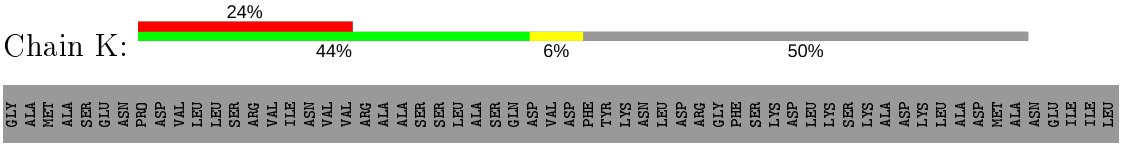
• Molecule 10: Exosome complex exonuclease DIS3

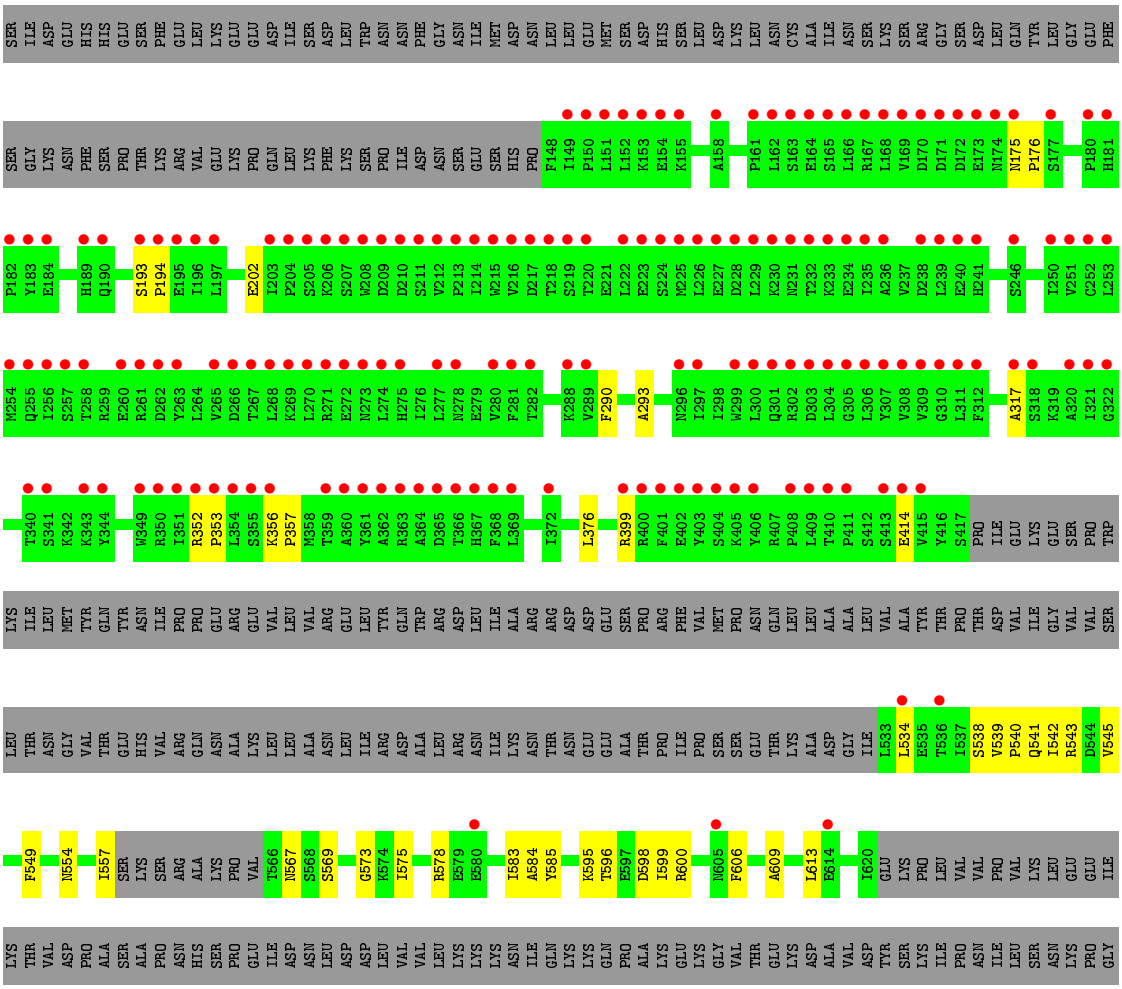
Chain J:



• Molecule 11: Exosome complex exonuclease RRP6

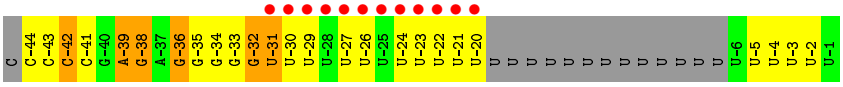
Chain K:





- Molecule 12: RNA synthetic

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.15Å 177.39Å 299.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.89 – 3.81 57.89 – 3.81	Depositor EDS
% Data completeness (in resolution range)	81.5 (57.89-3.81) 81.6 (57.89-3.81)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.295 , 0.300 0.295 , 0.300	Depositor DCC
R_{free} test set	2292 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	159.6	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 181.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	27816	wwPDB-VP
Average B, all atoms (Å^2)	270.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: 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	0.25	0/2340	0.37	0/3161
2	B	0.28	0/1910	0.43	0/2579
3	C	0.25	0/2629	0.41	0/3569
4	D	0.23	0/1722	0.40	0/2339
5	E	0.24	0/2093	0.39	1/2849 (0.0%)
6	F	0.24	0/1660	0.40	0/2241
7	G	0.25	0/1828	0.43	0/2486
8	H	0.26	0/2269	0.40	0/3066
9	I	0.22	0/1676	0.43	0/2277
10	J	0.28	0/7575	0.40	1/10290 (0.0%)
11	K	0.30	0/2001	0.56	0/2778
12	R	0.26	0/615	0.70	0/951
All	All	0.26	0/28318	0.43	2/38586 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	947	ASP	CB-CG-OD2	5.20	122.97	118.30
5	E	110	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2304	0	2265	85	0
2	B	1886	0	1904	59	0
3	C	2589	0	2607	135	0
4	D	1701	0	1755	39	3
5	E	2050	0	2063	74	1
6	F	1638	0	1590	108	0
7	G	1792	0	1747	133	1
8	H	2236	0	2215	159	4
9	I	1653	0	1616	142	0
10	J	7427	0	7352	284	0
11	K	1982	0	1255	45	2
12	R	557	0	281	45	1
13	J	1	0	0	0	0
All	All	27816	0	26650	1120	6

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 21.

All (1120) 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)
5:E:257:ASP:CB	8:H:4:VAL:HG21	1.35	1.57
10:J:467:PHE:CZ	10:J:469:ARG:O	1.63	1.50
5:E:257:ASP:CB	8:H:4:VAL:CG2	2.08	1.30
10:J:467:PHE:CZ	10:J:469:ARG:C	2.04	1.29
1:A:242:ASN:HB3	10:J:872:ARG:NH2	1.45	1.28
9:I:141:THR:HG22	9:I:155:ILE:HA	1.22	1.20
3:C:261:THR:HG22	3:C:262:ARG:H	1.02	1.19
8:H:315:THR:HB	8:H:318:ARG:HG3	1.26	1.18
5:E:257:ASP:HB3	8:H:4:VAL:CG2	1.71	1.15
7:G:86:VAL:HG11	7:G:134:ILE:CD1	1.75	1.14
10:J:467:PHE:CE1	10:J:469:ARG:O	2.00	1.14
10:J:440:ARG:CG	10:J:443:GLU:HB2	1.79	1.12
10:J:467:PHE:HZ	10:J:469:ARG:C	1.42	1.12
5:E:116:LEU:HD11	5:E:157:LEU:HB2	1.17	1.12
10:J:449:ILE:HB	10:J:467:PHE:CE1	1.85	1.11
9:I:23:THR:HG21	11:K:539:VAL:HG13	1.32	1.10
8:H:140:SER:O	8:H:187:ARG:HG2	1.48	1.10
7:G:86:VAL:HG11	7:G:134:ILE:HD13	1.28	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:HG3	1:A:205:ASP:H	1.15	1.10
3:C:72:ASN:HA	6:F:102:LEU:HD21	1.26	1.09
3:C:57:ASN:OD1	3:C:60:SER:HB3	1.52	1.09
5:E:116:LEU:HD11	5:E:157:LEU:CB	1.79	1.09
3:C:360:LEU:HD21	3:C:362:LEU:HD13	1.17	1.09
10:J:18:SER:HB2	10:J:41:LEU:HB2	1.31	1.08
10:J:440:ARG:HG2	10:J:443:GLU:HB2	1.32	1.08
10:J:624:PHE:CE2	10:J:858:LEU:HD23	1.88	1.08
8:H:340:VAL:O	8:H:344:ILE:HG13	1.55	1.07
9:I:11:ALA:HB3	9:I:62:GLY:O	1.55	1.07
7:G:222:ALA:O	7:G:226:ILE:HG12	1.55	1.07
10:J:83:ILE:HG13	10:J:224:LEU:HD21	1.33	1.06
3:C:72:ASN:OD1	6:F:102:LEU:HD22	1.56	1.05
9:I:103:VAL:HG21	11:K:534:LEU:CD1	1.85	1.05
8:H:306:ALA:HA	8:H:341:MET:HE3	1.08	1.04
5:E:116:LEU:HD21	5:E:157:LEU:HD13	1.39	1.02
8:H:306:ALA:HA	8:H:341:MET:CE	1.88	1.02
9:I:132:LEU:HD12	9:I:133:PRO:HD2	1.39	1.02
10:J:945:THR:OG1	10:J:963:VAL:O	1.78	1.01
5:E:116:LEU:CD1	5:E:157:LEU:HD22	1.90	1.01
1:A:143:CYS:HB2	1:A:147:PHE:HZ	1.25	1.00
5:E:75:LEU:HD11	5:E:122:PHE:O	1.61	1.00
10:J:624:PHE:CE2	10:J:858:LEU:CD2	2.44	1.00
7:G:110:ARG:HG3	7:G:111:PRO:HD2	1.39	1.00
9:I:103:VAL:HG21	11:K:534:LEU:HD12	1.43	0.99
4:D:146:ILE:HD13	4:D:153:GLN:NE2	1.77	0.99
1:A:179:VAL:HG13	1:A:184:PRO:HD3	1.44	0.98
7:G:110:ARG:HD3	12:R:-44:C:C5	1.98	0.98
6:F:201:VAL:HG22	6:F:213:PHE:CD1	1.99	0.97
8:H:54:ILE:HD13	8:H:87:THR:HG22	1.46	0.97
5:E:116:LEU:CD1	5:E:157:LEU:HB2	1.95	0.97
6:F:205:LYS:HE3	9:I:46:TYR:CE1	2.00	0.97
6:F:41:GLU:OE2	6:F:229:ARG:NE	1.97	0.97
1:A:90:GLN:NE2	7:G:91:PHE:HZ	1.62	0.97
3:C:261:THR:HG22	3:C:262:ARG:N	1.79	0.96
6:F:87:PHE:CE1	8:H:160:ARG:HD3	2.00	0.95
3:C:360:LEU:CD2	3:C:362:LEU:HD13	1.96	0.95
7:G:4:PHE:CE1	7:G:40:GLY:HA2	2.01	0.95
9:I:12:TYR:CE2	9:I:15:LYS:HD2	2.01	0.95
6:F:188:VAL:HG13	9:I:44:ILE:CD1	1.96	0.94
9:I:113:GLY:O	9:I:114:THR:HG23	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:146:LEU:CD2	9:I:220:VAL:HG12	1.97	0.94
1:A:242:ASN:CB	10:J:872:ARG:NH2	2.31	0.94
10:J:254:THR:HG22	10:J:459:THR:HG22	1.47	0.94
1:A:207:GLU:N	1:A:207:GLU:OE2	2.00	0.94
10:J:258:TYR:CE1	10:J:309:ARG:NH2	2.36	0.93
2:B:17:ARG:NH1	2:B:23:ARG:HG3	1.84	0.93
7:G:106:SER:HB3	7:G:109:ASN:CB	1.97	0.93
1:A:143:CYS:HB2	1:A:147:PHE:CZ	2.02	0.93
6:F:189:ASP:HA	9:I:14:GLY:HA3	1.50	0.92
10:J:17:LEU:HD12	10:J:42:ARG:HA	1.51	0.92
7:G:184:PHE:HB2	7:G:197:LYS:O	1.69	0.91
3:C:158:SER:OG	3:C:359:GLN:OE1	1.87	0.91
8:H:306:ALA:CA	8:H:341:MET:HE3	1.99	0.91
3:C:261:THR:CG2	3:C:262:ARG:H	1.84	0.90
11:K:538:SER:OG	11:K:541:GLN:HG3	1.69	0.90
3:C:360:LEU:HD21	3:C:362:LEU:CD1	2.01	0.90
10:J:610:THR:O	10:J:616:LYS:HE3	1.71	0.90
5:E:257:ASP:HB2	8:H:4:VAL:HG21	0.91	0.90
9:I:139:VAL:HG13	9:I:157:ALA:O	1.71	0.90
10:J:449:ILE:HB	10:J:467:PHE:HE1	1.28	0.90
12:R:-32:G:O2'	12:R:-31:U:C5	2.24	0.90
3:C:88:ILE:HB	3:C:218:VAL:CG2	2.02	0.90
3:C:299:ILE:CG2	3:C:328:THR:HG23	2.02	0.90
10:J:945:THR:HG21	10:J:962:PHE:HB2	1.54	0.89
7:G:110:ARG:HD2	12:R:-44:C:C4	2.07	0.89
5:E:116:LEU:CG	5:E:157:LEU:HD22	2.02	0.89
6:F:201:VAL:CG2	6:F:213:PHE:CD1	2.56	0.89
1:A:22:ASN:HA	1:A:30:PHE:CZ	2.08	0.89
5:E:116:LEU:HG	5:E:157:LEU:HD22	1.55	0.88
6:F:189:ASP:HA	9:I:14:GLY:CA	2.03	0.88
6:F:187:LEU:HB2	9:I:13:PRO:HB3	1.55	0.88
12:R:-33:G:H2'	12:R:-32:G:H5"	1.56	0.88
3:C:61:ARG:CZ	6:F:20:PHE:CE1	2.58	0.87
3:C:17:PHE:HZ	9:I:255:VAL:HG11	1.40	0.87
7:G:95:VAL:HG11	7:G:134:ILE:HG23	1.57	0.87
6:F:188:VAL:HG13	9:I:44:ILE:HD13	1.56	0.87
7:G:102:PHE:HB3	7:G:103:PRO:HD2	1.53	0.86
10:J:694:LEU:HD21	10:J:696:LEU:HG	1.58	0.86
6:F:246:MET:HE1	9:I:10:ILE:HG13	1.56	0.86
8:H:157:LEU:CD1	9:I:235:LEU:HD13	2.05	0.86
12:R:-35:G:O2'	12:R:-34:G:H5'	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:214:CYS:SG	7:G:223:PHE:CD1	2.68	0.85
8:H:83:SER:O	8:H:84:VAL:HG13	1.74	0.85
9:I:146:LEU:HD22	9:I:220:VAL:HG12	1.59	0.85
10:J:12:ARG:NH1	10:J:154:GLU:OE2	2.10	0.85
12:R:-33:G:C2'	12:R:-32:G:H5"	2.08	0.84
5:E:66:VAL:HG21	10:J:30:GLY:O	1.77	0.84
10:J:425:ILE:HG21	10:J:990:ILE:O	1.76	0.84
8:H:140:SER:O	8:H:187:ARG:CG	2.24	0.84
9:I:274:MET:SD	9:I:285:LYS:HG2	2.17	0.84
1:A:73:PHE:CZ	3:C:261:THR:OG1	2.29	0.84
9:I:146:LEU:CD2	9:I:220:VAL:CG1	2.55	0.84
5:E:257:ASP:HB3	8:H:4:VAL:HG23	1.58	0.84
3:C:299:ILE:HG23	3:C:328:THR:HG23	1.60	0.84
10:J:101:LEU:HD13	10:J:234:SER:HB2	1.60	0.83
1:A:143:CYS:CB	1:A:147:PHE:CZ	2.60	0.83
8:H:157:LEU:HD11	9:I:235:LEU:HD13	1.60	0.83
12:R:-42:C:H6	12:R:-42:C:O5'	1.61	0.83
7:G:106:SER:HB3	7:G:109:ASN:HB2	1.59	0.83
4:D:144:ASP:OD1	4:D:145:ILE:N	2.12	0.83
9:I:225:LYS:HG3	9:I:286:ARG:CZ	2.08	0.83
1:A:204:GLN:HG3	1:A:205:ASP:N	1.94	0.83
9:I:12:TYR:CZ	9:I:15:LYS:HB2	2.14	0.82
7:G:110:ARG:CG	7:G:111:PRO:HD2	2.09	0.82
8:H:124:TRP:CZ2	8:H:159:MET:HB3	2.13	0.82
7:G:110:ARG:CD	12:R:-44:C:C4	2.62	0.82
10:J:236:PRO:HA	10:J:466:HIS:ND1	1.94	0.82
3:C:350:LEU:HD12	3:C:359:GLN:HG2	1.60	0.82
8:H:67:TRP:CE3	8:H:93:ARG:O	2.32	0.82
7:G:184:PHE:HB3	7:G:198:CYS:SG	2.19	0.82
10:J:694:LEU:CD2	10:J:696:LEU:HG	2.10	0.82
5:E:116:LEU:HD11	5:E:157:LEU:HD22	1.60	0.81
8:H:193:LYS:NZ	8:H:283:ASP:OD1	2.12	0.81
1:A:173:GLN:HA	3:C:99:THR:HG23	1.63	0.81
7:G:86:VAL:HG11	7:G:134:ILE:HD11	1.60	0.81
7:G:156:ILE:HG12	7:G:208:TYR:CD2	2.15	0.81
7:G:156:ILE:HD11	7:G:208:TYR:HA	1.62	0.81
1:A:22:ASN:HD22	1:A:30:PHE:HE2	1.26	0.80
2:B:19:TRP:CE2	2:B:20:ASN:HB3	2.17	0.80
5:E:227:ARG:NH1	6:F:112:GLU:OE2	2.15	0.80
10:J:694:LEU:HD21	10:J:696:LEU:CG	2.11	0.80
9:I:23:THR:HG21	11:K:539:VAL:CG1	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:257:ASP:HB2	8:H:4:VAL:CG2	1.88	0.80
9:I:113:GLY:O	9:I:114:THR:CG2	2.30	0.80
1:A:5:ILE:HD11	1:A:90:GLN:HG2	1.63	0.80
12:R:-31:U:OP1	12:R:-31:U:C4'	2.30	0.80
10:J:624:PHE:CZ	10:J:858:LEU:HD23	2.15	0.80
7:G:136:CYS:O	7:G:147:PHE:CB	2.30	0.79
7:G:99:TYR:HA	7:G:102:PHE:HE2	1.46	0.79
9:I:128:PHE:HE2	9:I:158:VAL:HG23	1.46	0.79
5:E:97:SER:HB2	6:F:108:ASN:HB3	1.62	0.79
5:E:116:LEU:HD11	5:E:157:LEU:CD2	2.12	0.79
8:H:315:THR:CB	8:H:318:ARG:HG3	2.09	0.79
8:H:54:ILE:CD1	8:H:87:THR:HG22	2.12	0.79
1:A:242:ASN:HB3	10:J:872:ARG:CZ	2.12	0.78
12:R:-36:G:H2'	12:R:-35:G:H8	1.48	0.78
9:I:139:VAL:HG11	9:I:155:ILE:HG23	1.65	0.78
2:B:20:ASN:O	2:B:223:ARG:NH1	2.17	0.78
6:F:87:PHE:CE2	9:I:238:GLY:O	2.37	0.78
10:J:311:PHE:CE2	10:J:431:LEU:HG	2.18	0.78
5:E:116:LEU:HD11	5:E:157:LEU:CG	2.12	0.78
3:C:72:ASN:CA	6:F:102:LEU:HD21	2.12	0.78
12:R:-41:C:O5'	12:R:-41:C:H6	1.66	0.78
2:B:19:TRP:HZ3	2:B:216:ILE:HD12	1.48	0.78
10:J:112[A]:ILE:HD13	10:J:181:TYR:CE1	2.18	0.77
10:J:112[B]:ILE:HD13	10:J:181:TYR:CE1	2.18	0.77
9:I:139:VAL:HG22	9:I:158:VAL:HG22	1.66	0.77
2:B:233:ARG:O	2:B:237:GLN:HG2	1.84	0.77
8:H:72:GLY:O	8:H:83:SER:N	2.13	0.77
9:I:143:VAL:HA	9:I:153:VAL:HG12	1.66	0.77
7:G:227:ALA:O	7:G:231:PHE:CD2	2.37	0.77
9:I:132:LEU:HD12	9:I:133:PRO:CD	2.15	0.77
10:J:404:VAL:HG21	10:J:486:LEU:HD11	1.67	0.77
1:A:90:GLN:NE2	7:G:91:PHE:CZ	2.50	0.77
9:I:13:PRO:HD3	9:I:61:VAL:CG2	2.14	0.77
7:G:214:CYS:SG	7:G:223:PHE:CG	2.78	0.76
9:I:13:PRO:HD3	9:I:61:VAL:HG22	1.66	0.76
5:E:257:ASP:CB	8:H:4:VAL:HG23	2.14	0.76
10:J:844:SER:N	10:J:851:ASP:OD2	2.18	0.76
10:J:624:PHE:CZ	10:J:858:LEU:HG	2.19	0.76
9:I:277:SER:HB3	9:I:280:THR:OG1	1.83	0.76
12:R:-31:U:OP1	12:R:-31:U:H4'	1.86	0.76
1:A:22:ASN:HA	1:A:30:PHE:HZ	1.47	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:271:ASP:HB2	9:I:274:MET:HB2	1.67	0.76
10:J:126:TYR:N	10:J:127:PRO:HD2	2.01	0.76
10:J:945:THR:OG1	10:J:963:VAL:C	2.24	0.76
11:K:554:ASN:O	11:K:557:ILE:HG22	1.85	0.76
1:A:130:LYS:HD2	1:A:174:ILE:HD11	1.67	0.76
3:C:328:THR:HG21	3:C:373:MET:HG3	1.68	0.76
6:F:87:PHE:CD1	8:H:160:ARG:NH1	2.54	0.76
1:A:73:PHE:CE1	3:C:261:THR:OG1	2.39	0.76
5:E:119:LYS:HB3	5:E:163:ASP:OD2	1.86	0.76
10:J:194:LEU:HB3	10:J:215:THR:HG22	1.66	0.76
10:J:253:PHE:O	10:J:254:THR:HG23	1.84	0.76
1:A:278:GLN:O	1:A:281:GLN:HG2	1.85	0.75
6:F:201:VAL:CG2	6:F:213:PHE:HD1	1.99	0.75
6:F:88:THR:OG1	6:F:132:LYS:HA	1.84	0.75
8:H:309:PHE:HB3	8:H:341:MET:HE2	1.67	0.75
6:F:246:MET:CE	9:I:10:ILE:HG13	2.16	0.75
8:H:351:ALA:HA	8:H:354:MET:CE	2.16	0.75
10:J:17:LEU:HD11	10:J:42:ARG:HG2	1.68	0.75
3:C:57:ASN:OD1	3:C:60:SER:CB	2.33	0.75
4:D:136:ILE:HG21	4:D:194:LEU:CD1	2.16	0.75
7:G:95:VAL:HG22	7:G:132:ALA:HB3	1.67	0.75
6:F:87:PHE:CE1	8:H:160:ARG:CD	2.69	0.74
9:I:12:TYR:CE1	9:I:15:LYS:HB2	2.21	0.74
11:K:569:SER:HB3	11:K:573:GLY:HA3	1.70	0.74
7:G:110:ARG:HD3	12:R:-44:C:C6	2.22	0.74
6:F:188:VAL:HG13	9:I:44:ILE:HD11	1.69	0.74
9:I:267:MET:HG2	9:I:277:SER:HB2	1.70	0.74
7:G:110:ARG:CD	12:R:-44:C:C5	2.71	0.74
6:F:201:VAL:HG22	6:F:213:PHE:HD1	1.45	0.74
3:C:72:ASN:OD1	6:F:102:LEU:CD2	2.34	0.73
8:H:351:ALA:HA	8:H:354:MET:HE3	1.70	0.73
10:J:610:THR:O	10:J:616:LYS:CE	2.36	0.73
3:C:72:ASN:CG	6:F:102:LEU:HD22	2.09	0.73
8:H:83:SER:O	8:H:84:VAL:CG1	2.37	0.73
6:F:205:LYS:HE3	9:I:46:TYR:CD1	2.22	0.73
6:F:67:LEU:HG	6:F:68:GLY:N	2.04	0.73
8:H:152:SER:HB3	8:H:155:ASP:OD2	1.88	0.73
10:J:530:LYS:HD3	10:J:864:TYR:HA	1.70	0.73
12:R:-39:A:HO2'	12:R:-38:G:C4'	2.01	0.73
7:G:95:VAL:HG13	7:G:132:ALA:CB	2.19	0.73
10:J:258:TYR:CZ	10:J:309:ARG:NH2	2.56	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:538:SER:OG	11:K:541:GLN:CG	2.35	0.73
10:J:467:PHE:HZ	10:J:469:ARG:O	1.26	0.73
10:J:579:PRO:HG3	10:J:856:ARG:NH1	2.04	0.73
10:J:635:ASN:OD1	10:J:687:LYS:NZ	2.20	0.73
12:R:-32:G:O2'	12:R:-31:U:H5	1.68	0.73
10:J:811:ARG:NH2	10:J:936:GLU:OE2	2.22	0.72
10:J:589:ALA:O	10:J:887:LYS:HD2	1.90	0.72
12:R:-36:G:H2'	12:R:-35:G:C8	2.23	0.72
1:A:143:CYS:SG	1:A:147:PHE:CZ	2.82	0.72
4:D:22:GLN:HG2	4:D:23:ASP:H	1.53	0.72
10:J:234:SER:O	10:J:466:HIS:CD2	2.42	0.72
12:R:-33:G:C3'	12:R:-32:G:H5"	2.19	0.72
2:B:83:LYS:HE3	2:B:131:GLN:OE1	1.90	0.72
7:G:95:VAL:CG1	7:G:134:ILE:HG23	2.20	0.72
7:G:106:SER:HB3	7:G:109:ASN:HB3	1.70	0.72
9:I:128:PHE:CZ	9:I:133:PRO:HD3	2.25	0.72
7:G:95:VAL:HG13	7:G:132:ALA:C	2.10	0.72
8:H:153:GLU:O	8:H:156:GLU:HG2	1.90	0.72
10:J:573:VAL:CG2	10:J:845:PRO:HB2	2.20	0.72
8:H:67:TRP:HE3	8:H:93:ARG:O	1.70	0.72
8:H:216:ASN:HD21	8:H:240:ASP:HB3	1.54	0.71
12:R:-43:C:H2'	12:R:-42:C:C6	2.24	0.71
8:H:160:ARG:HA	8:H:163:LEU:O	1.90	0.71
10:J:624:PHE:HZ	10:J:858:LEU:HG	1.54	0.71
11:K:538:SER:HG	11:K:541:GLN:HG3	1.53	0.71
10:J:404:VAL:CG2	10:J:486:LEU:HD11	2.20	0.71
4:D:136:ILE:HG21	4:D:194:LEU:HD11	1.73	0.71
10:J:945:THR:HB	10:J:962:PHE:CD1	2.25	0.71
8:H:196:ASN:OD1	8:H:286:ASP:N	2.21	0.71
7:G:227:ALA:HB1	7:G:231:PHE:HE2	1.56	0.70
1:A:167:ILE:CD1	1:A:176:VAL:HA	2.20	0.70
5:E:240:LYS:HD3	6:F:209:GLU:HG2	1.73	0.70
5:E:240:LYS:NZ	6:F:209:GLU:OE2	2.23	0.70
10:J:62:ASP:OD1	10:J:66:GLU:N	2.22	0.70
8:H:215:HIS:HB3	8:H:316:GLN:NE2	2.06	0.70
10:J:594:VAL:HG12	10:J:891:ALA:HA	1.73	0.70
10:J:449:ILE:CB	10:J:467:PHE:HE1	2.04	0.70
3:C:328:THR:HG22	3:C:373:MET:SD	2.32	0.70
10:J:72:LEU:HD11	10:J:146:ILE:CG2	2.22	0.70
9:I:159:GLU:OE2	9:I:231:ARG:NE	2.24	0.70
10:J:130:THR:O	10:J:134:THR:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:TYR:CA	7:G:102:PHE:HE2	2.05	0.70
10:J:663:ASP:OD1	10:J:664:LYS:N	2.25	0.70
8:H:309:PHE:HB2	8:H:341:MET:HE1	1.73	0.69
4:D:195:LEU:O	4:D:199:GLU:HG3	1.92	0.69
7:G:184:PHE:CE2	7:G:207:CYS:SG	2.85	0.69
8:H:149:ARG:HH12	8:H:152:SER:CB	2.05	0.69
6:F:93:ILE:CD1	6:F:127:LEU:HD21	2.23	0.69
6:F:189:ASP:OD1	9:I:14:GLY:HA3	1.92	0.69
10:J:126:TYR:N	10:J:127:PRO:CD	2.55	0.69
2:B:23:ARG:O	2:B:24:ARG:C	2.26	0.69
5:E:9:SER:HB3	8:H:285:ASN:ND2	2.08	0.69
10:J:253:PHE:O	10:J:254:THR:CG2	2.40	0.69
7:G:224:LYS:O	7:G:228:LYS:HG3	1.93	0.69
10:J:72:LEU:CD1	10:J:146:ILE:HG21	2.23	0.69
11:K:569:SER:CB	11:K:573:GLY:HA3	2.22	0.69
2:B:148:ILE:HG21	2:B:232:LEU:HD21	1.73	0.69
3:C:61:ARG:HG3	3:C:62:TYR:CD2	2.28	0.69
3:C:72:ASN:CG	6:F:102:LEU:CD2	2.61	0.69
8:H:315:THR:HB	8:H:318:ARG:CG	2.15	0.69
9:I:132:LEU:CD1	9:I:133:PRO:HD2	2.21	0.69
3:C:299:ILE:HG23	3:C:328:THR:CG2	2.23	0.68
10:J:449:ILE:HB	10:J:467:PHE:CD1	2.26	0.68
5:E:75:LEU:HD12	5:E:123:LYS:HA	1.75	0.68
7:G:102:PHE:HB3	7:G:103:PRO:CD	2.23	0.68
2:B:240:VAL:HG21	8:H:54:ILE:HD11	1.75	0.68
9:I:139:VAL:CG1	9:I:155:ILE:HG23	2.24	0.68
10:J:624:PHE:CZ	10:J:858:LEU:CD2	2.74	0.68
10:J:624:PHE:CZ	10:J:858:LEU:CG	2.76	0.68
11:K:317:ALA:HB1	11:K:376:LEU:CB	2.24	0.68
1:A:176:VAL:HG13	1:A:176:VAL:O	1.94	0.68
2:B:42:MET:SD	2:B:145:LEU:HD12	2.34	0.68
8:H:149:ARG:HH12	8:H:152:SER:HB3	1.58	0.68
6:F:246:MET:HE1	9:I:10:ILE:CG1	2.24	0.68
9:I:60:LEU:HD11	9:I:130:ASN:OD1	1.93	0.68
3:C:61:ARG:CZ	6:F:20:PHE:CZ	2.76	0.68
8:H:143:LEU:HB3	8:H:144:PRO:HD2	1.76	0.68
9:I:11:ALA:CB	9:I:62:GLY:O	2.37	0.68
2:B:19:TRP:CZ3	2:B:216:ILE:HD12	2.28	0.68
6:F:187:LEU:HB2	9:I:13:PRO:CB	2.23	0.68
5:E:75:LEU:HD11	5:E:122:PHE:C	2.14	0.68
8:H:315:THR:HG22	8:H:317:GLN:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:571:ALA:O	10:J:845:PRO:HG3	1.93	0.68
11:K:539:VAL:HB	11:K:540:PRO:HD3	1.76	0.68
7:G:97:LEU:HB2	7:G:134:ILE:HG13	1.77	0.67
10:J:72:LEU:CD1	10:J:146:ILE:CG2	2.71	0.67
10:J:259:TYR:CD2	10:J:263:ARG:HD3	2.28	0.67
10:J:633:SER:HB3	10:J:635:ASN:HD21	1.59	0.67
3:C:278:GLN:HB2	6:F:21:SER:O	1.93	0.67
10:J:596:LEU:HD22	10:J:898:SER:HB2	1.76	0.67
7:G:158:VAL:HG11	7:G:194:ILE:HD12	1.76	0.67
4:D:142:THR:HG22	4:D:144:ASP:HB2	1.76	0.67
7:G:97:LEU:HB2	7:G:134:ILE:CG1	2.25	0.67
7:G:99:TYR:HA	7:G:102:PHE:CE2	2.29	0.67
3:C:88:ILE:HB	3:C:218:VAL:HG22	1.74	0.67
7:G:214:CYS:HB3	7:G:223:PHE:CZ	2.31	0.66
10:J:72:LEU:HD11	10:J:146:ILE:HG23	1.77	0.66
7:G:222:ALA:C	7:G:226:ILE:HG12	2.15	0.66
8:H:332:VAL:C	8:H:334:GLU:H	1.99	0.66
10:J:574:THR:CG2	10:J:856:ARG:HG2	2.26	0.66
2:B:17:ARG:NH1	2:B:23:ARG:CG	2.58	0.66
3:C:17:PHE:CZ	9:I:255:VAL:HG11	2.27	0.66
1:A:90:GLN:CD	7:G:91:PHE:HZ	1.98	0.66
10:J:12:ARG:HH12	10:J:154:GLU:CD	1.99	0.66
6:F:188:VAL:O	9:I:14:GLY:HA2	1.95	0.66
5:E:257:ASP:CG	8:H:4:VAL:CG2	2.63	0.66
10:J:255:PHE:HB2	10:J:458:THR:HA	1.78	0.66
11:K:596:THR:O	11:K:599:ILE:HG12	1.96	0.66
10:J:234:SER:HA	10:J:467:PHE:O	1.96	0.66
7:G:156:ILE:HG12	7:G:208:TYR:CE2	2.30	0.66
1:A:143:CYS:CB	1:A:147:PHE:HZ	2.00	0.66
7:G:81:SER:O	7:G:82:ASP:HB2	1.96	0.66
8:H:214:THR:O	8:H:243:ARG:NH2	2.29	0.66
10:J:549:ASP:OD1	10:J:600:ARG:NH1	2.29	0.66
5:E:26:ARG:NH1	5:E:32:ARG:HG3	2.11	0.65
7:G:97:LEU:CD1	7:G:134:ILE:O	2.43	0.65
10:J:259:TYR:CE2	10:J:263:ARG:NE	2.63	0.65
1:A:167:ILE:HD11	1:A:176:VAL:HG23	1.79	0.65
2:B:17:ARG:HH12	2:B:173:ASP:HB3	1.61	0.65
8:H:126:VAL:HG11	8:H:184:LEU:HD12	1.77	0.65
8:H:309:PHE:CB	8:H:341:MET:CE	2.73	0.65
9:I:128:PHE:CE2	9:I:158:VAL:HG23	2.30	0.65
3:C:61:ARG:HD2	3:C:62:TYR:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:141:THR:HG22	9:I:155:ILE:CA	2.14	0.65
10:J:115:GLN:HB2	10:J:149:HIS:HA	1.78	0.65
6:F:67:LEU:HG	6:F:68:GLY:H	1.60	0.65
7:G:7:PRO:HD3	7:G:39:THR:HG22	1.77	0.65
9:I:231:ARG:NH1	9:I:252:LEU:HD23	2.11	0.65
3:C:328:THR:CG2	3:C:373:MET:SD	2.85	0.65
7:G:214:CYS:HA	7:G:223:PHE:CE1	2.32	0.65
11:K:609:ALA:O	11:K:613:LEU:CB	2.44	0.65
1:A:68:TYR:CE2	1:A:76:LEU:HD22	2.32	0.65
3:C:391:ARG:HD2	3:C:392:PHE:CZ	2.32	0.65
7:G:227:ALA:O	7:G:231:PHE:HD2	1.77	0.65
3:C:299:ILE:HA	3:C:329:VAL:O	1.97	0.64
10:J:556:ALA:HB2	10:J:677:LEU:HD21	1.78	0.64
3:C:255:LEU:HD12	3:C:256:ARG:N	2.12	0.64
10:J:440:ARG:HG3	10:J:443:GLU:HB2	1.77	0.64
5:E:264:ASN:HB3	8:H:9:LYS:HE3	1.80	0.64
6:F:188:VAL:CG1	9:I:44:ILE:HD13	2.26	0.64
8:H:140:SER:O	8:H:187:ARG:CD	2.45	0.64
1:A:26:ASP:OD2	1:A:28:ARG:NE	2.29	0.64
5:E:109:VAL:HG13	5:E:182:ILE:HD11	1.80	0.64
6:F:93:ILE:HD11	6:F:127:LEU:HD21	1.79	0.64
1:A:22:ASN:ND2	1:A:30:PHE:HE2	1.95	0.64
3:C:352:ALA:O	3:C:355:GLY:N	2.29	0.64
11:K:538:SER:HB2	11:K:540:PRO:HD2	1.79	0.64
1:A:5:ILE:CD1	1:A:90:GLN:HG2	2.28	0.64
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.79	0.64
8:H:153:GLU:OE2	9:I:215:ARG:NH2	2.30	0.64
8:H:290:SER:OG	8:H:293:ILE:HG13	1.98	0.64
9:I:141:THR:OG1	9:I:153:VAL:HG21	1.98	0.64
2:B:13:ARG:HD3	2:B:171:LEU:HD22	1.78	0.63
3:C:61:ARG:HD2	3:C:62:TYR:CE2	2.34	0.63
8:H:332:VAL:O	8:H:334:GLU:N	2.31	0.63
10:J:285:PHE:CZ	10:J:430:CYS:HA	2.33	0.63
8:H:149:ARG:NH1	8:H:155:ASP:OD1	2.31	0.63
12:R:-43:C:O5'	12:R:-43:C:H6	1.80	0.63
2:B:64:GLN:O	2:B:64:GLN:HG3	1.99	0.63
5:E:116:LEU:CD1	5:E:157:LEU:CD2	2.69	0.63
7:G:123:VAL:HG22	7:G:134:ILE:HG22	1.81	0.63
10:J:467:PHE:HZ	10:J:470:ASP:N	1.94	0.63
10:J:83:ILE:HG13	10:J:224:LEU:CD2	2.22	0.63
6:F:87:PHE:CZ	8:H:160:ARG:CD	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:225:LYS:HG3	9:I:286:ARG:NH2	2.13	0.63
5:E:258:VAL:HG23	8:H:4:VAL:HG11	1.81	0.63
10:J:921:VAL:O	10:J:922:PHE:HD1	1.81	0.63
10:J:556:ALA:HB2	10:J:677:LEU:CD2	2.30	0.62
5:E:75:LEU:CD1	5:E:122:PHE:O	2.45	0.62
3:C:61:ARG:NH2	6:F:20:PHE:CE1	2.67	0.62
7:G:95:VAL:HG13	7:G:132:ALA:HB3	1.79	0.62
8:H:108:THR:HB	8:H:176:LEU:HD13	1.81	0.62
5:E:257:ASP:OD2	8:H:4:VAL:CG2	2.47	0.62
1:A:29:SER:HB3	1:A:32:GLN:HB2	1.80	0.62
3:C:305:GLU:O	3:C:305:GLU:HG2	1.98	0.62
10:J:762:ASN:HB3	10:J:812:CYS:HB2	1.81	0.62
6:F:87:PHE:CZ	8:H:160:ARG:NE	2.67	0.62
10:J:945:THR:HG1	10:J:963:VAL:C	2.01	0.62
5:E:257:ASP:CG	8:H:4:VAL:HG21	2.15	0.62
10:J:484:LEU:HD11	10:J:897:ALA:C	2.20	0.62
10:J:921:VAL:O	10:J:922:PHE:CD1	2.53	0.62
12:R:-39:A:O2'	12:R:-38:G:O5'	2.18	0.62
4:D:13:VAL:HG11	4:D:29:SER:HB2	1.80	0.62
10:J:259:TYR:CD2	10:J:263:ARG:NE	2.67	0.62
5:E:263:GLU:O	5:E:263:GLU:HG3	1.99	0.62
6:F:205:LYS:HG2	9:I:46:TYR:HE1	1.64	0.62
9:I:231:ARG:NH1	9:I:251:ASP:O	2.32	0.62
10:J:107:CYS:O	10:J:143:LYS:NZ	2.33	0.62
5:E:33:PRO:HG3	8:H:337:GLU:OE2	1.98	0.62
8:H:115:ARG:C	8:H:126:VAL:HG23	2.20	0.62
8:H:215:HIS:HB3	8:H:316:GLN:CD	2.20	0.62
3:C:134:VAL:HG11	3:C:151:ILE:HB	1.81	0.62
10:J:449:ILE:CB	10:J:467:PHE:CE1	2.75	0.62
4:D:146:ILE:HD13	4:D:153:GLN:HE22	1.64	0.61
8:H:309:PHE:CB	8:H:341:MET:HE2	2.30	0.61
10:J:552:ASP:OD2	12:R:-2:U:H5"	2.00	0.61
7:G:97:LEU:HD12	7:G:134:ILE:O	2.00	0.61
9:I:225:LYS:CG	9:I:286:ARG:CZ	2.78	0.61
10:J:400:TRP:HA	10:J:403:TYR:OH	2.00	0.61
3:C:52:VAL:HG23	3:C:384:ARG:HH22	1.65	0.61
2:B:153:SER:HB3	8:H:83:SER:OG	1.99	0.61
1:A:167:ILE:HD13	1:A:176:VAL:HA	1.82	0.61
10:J:633:SER:HB3	10:J:635:ASN:ND2	2.15	0.61
11:K:539:VAL:N	11:K:540:PRO:CD	2.64	0.61
4:D:136:ILE:CG2	4:D:194:LEU:HD11	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HD21	2:B:199:LEU:HD13	1.81	0.61
3:C:90:SER:HB3	6:F:101:LEU:HD13	1.83	0.61
4:D:142:THR:O	4:D:143:SER:HB3	2.00	0.61
10:J:125:SER:OG	10:J:128:VAL:HB	2.01	0.61
3:C:328:THR:HG21	3:C:373:MET:CG	2.30	0.61
3:C:75:LEU:HD11	6:F:18:MET:HE1	1.81	0.61
10:J:208:GLU:O	10:J:208:GLU:HG2	2.00	0.61
10:J:236:PRO:HB3	10:J:466:HIS:CE1	2.36	0.60
8:H:61:VAL:HG11	8:H:95:LEU:HD21	1.83	0.60
9:I:150:ARG:HD2	9:I:204:ILE:CG2	2.31	0.60
4:D:142:THR:CG2	4:D:144:ASP:HB2	2.31	0.60
10:J:285:PHE:HE1	10:J:430:CYS:O	1.83	0.60
10:J:424:VAL:HG11	10:J:436:ILE:HD11	1.82	0.60
3:C:61:ARG:NH1	6:F:20:PHE:CZ	2.69	0.60
8:H:157:LEU:HD13	9:I:235:LEU:HB3	1.83	0.60
5:E:75:LEU:HD21	5:E:114:LEU:CB	2.31	0.60
9:I:113:GLY:C	9:I:114:THR:HG23	2.22	0.60
3:C:48:GLU:HG2	11:K:584:ALA:HB2	1.82	0.60
2:B:86:ARG:HB2	5:E:63:LYS:HD3	1.84	0.60
2:B:179:GLU:HG2	2:B:184:THR:HG21	1.82	0.60
6:F:201:VAL:HG21	6:F:213:PHE:CD1	2.37	0.60
10:J:216:LYS:HB2	10:J:221:TYR:HB2	1.84	0.60
3:C:258:THR:HG22	3:C:267:THR:HG22	1.82	0.60
9:I:128:PHE:CE1	9:I:133:PRO:HD3	2.36	0.60
10:J:101:LEU:HD13	10:J:234:SER:CB	2.30	0.60
10:J:259:TYR:CD2	10:J:263:ARG:CD	2.85	0.60
4:D:22:GLN:HG2	4:D:23:ASP:N	2.16	0.59
7:G:184:PHE:CB	7:G:198:CYS:SG	2.88	0.59
10:J:440:ARG:CG	10:J:443:GLU:CB	2.69	0.59
3:C:61:ARG:NH1	6:F:20:PHE:CE1	2.70	0.59
7:G:152:ASP:CG	7:G:153:GLY:H	2.05	0.59
3:C:17:PHE:HZ	9:I:255:VAL:CG1	2.13	0.59
1:A:130:LYS:HD3	1:A:174:ILE:HG13	1.84	0.59
1:A:243:ARG:HG2	1:A:243:ARG:O	2.01	0.59
1:A:68:TYR:HE2	1:A:76:LEU:HD22	1.68	0.59
7:G:222:ALA:HB1	7:G:226:ILE:CG1	2.33	0.59
6:F:190:MET:HG2	9:I:13:PRO:O	2.02	0.59
10:J:255:PHE:O	10:J:458:THR:CG2	2.51	0.59
10:J:624:PHE:CE2	10:J:858:LEU:HD21	2.34	0.59
10:J:617:PRO:HA	10:J:648:SER:HB3	1.85	0.59
1:A:173:GLN:HA	3:C:99:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:GLU:OE2	6:F:229:ARG:CZ	2.50	0.59
8:H:193:LYS:CE	8:H:283:ASP:OD1	2.51	0.59
3:C:122:ASP:O	3:C:163:ARG:NH2	2.36	0.59
6:F:97:LEU:HD22	6:F:139:VAL:HB	1.85	0.59
8:H:67:TRP:CZ3	8:H:93:ARG:C	2.76	0.59
1:A:204:GLN:CG	1:A:205:ASP:H	1.98	0.59
4:D:136:ILE:HG21	4:D:194:LEU:HD12	1.84	0.59
5:E:262:LEU:HD13	8:H:7:ILE:HD13	1.85	0.58
9:I:146:LEU:CD2	9:I:220:VAL:HG11	2.33	0.58
6:F:186:GLU:HA	9:I:59:THR:O	2.02	0.58
10:J:106:ASN:O	10:J:227:ASN:ND2	2.36	0.58
10:J:100:ASP:HB3	10:J:468:VAL:HG13	1.84	0.58
10:J:81:ALA:HB1	10:J:82:PRO:HA	1.84	0.58
8:H:121:ASN:OD1	8:H:122:LYS:N	2.37	0.58
1:A:59:ARG:NH2	4:D:96:GLU:OE1	2.34	0.58
3:C:84:LYS:HE3	6:F:54:GLU:HG3	1.85	0.58
2:B:86:ARG:NH1	5:E:127:ASP:OD2	2.36	0.58
10:J:694:LEU:HD21	10:J:696:LEU:CD1	2.33	0.58
10:J:217:SER:O	10:J:220:GLN:N	2.37	0.58
7:G:4:PHE:CZ	7:G:40:GLY:HA2	2.38	0.58
9:I:128:PHE:O	9:I:128:PHE:CD1	2.57	0.58
10:J:259:TYR:CG	10:J:263:ARG:HD3	2.38	0.58
9:I:141:THR:CG2	9:I:155:ILE:HG13	2.33	0.58
10:J:79:LEU:CD2	10:J:226:PRO:HD3	2.34	0.58
1:A:7:ILE:HG21	1:A:230:LEU:HD21	1.86	0.57
3:C:45:LYS:HG2	3:C:46:TYR:H	1.69	0.57
2:B:23:ARG:NE	2:B:173:ASP:OD1	2.37	0.57
7:G:110:ARG:CG	7:G:111:PRO:CD	2.82	0.57
8:H:149:ARG:NH1	8:H:152:SER:CB	2.67	0.57
10:J:440:ARG:O	10:J:440:ARG:HG2	2.03	0.57
6:F:187:LEU:O	9:I:59:THR:HA	2.04	0.57
7:G:99:TYR:C	7:G:102:PHE:HE2	2.08	0.57
10:J:573:VAL:HB	10:J:845:PRO:HB2	1.86	0.57
1:A:242:ASN:CB	10:J:872:ARG:HH21	2.14	0.57
3:C:362:LEU:HB2	4:D:180:LEU:HB3	1.86	0.57
6:F:200:VAL:HB	6:F:214:TRP:HB3	1.86	0.57
9:I:8:PRO:HB2	9:I:64:VAL:HB	1.87	0.57
10:J:120:GLU:OE2	10:J:170:ASN:ND2	2.31	0.57
8:H:340:VAL:HG12	8:H:344:ILE:HD11	1.85	0.57
9:I:146:LEU:HD23	9:I:220:VAL:HG11	1.86	0.57
10:J:696:LEU:HD12	12:R:-5:U:H1'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:611:ASP:HA	10:J:616:LYS:HE3	1.87	0.57
5:E:75:LEU:HD21	5:E:114:LEU:HB2	1.87	0.57
2:B:23:ARG:NH2	2:B:173:ASP:OD1	2.37	0.57
6:F:87:PHE:HE1	8:H:160:ARG:HD3	1.64	0.57
12:R:-43:C:H2'	12:R:-42:C:C5	2.39	0.57
6:F:246:MET:SD	9:I:10:ILE:HG13	2.45	0.56
3:C:299:ILE:HG21	3:C:328:THR:HG23	1.83	0.56
9:I:150:ARG:HD2	9:I:204:ILE:HG21	1.86	0.56
10:J:237:GLN:O	10:J:454:ASP:HB3	2.04	0.56
10:J:574:THR:HG23	10:J:856:ARG:HG2	1.87	0.56
1:A:125:ILE:CG2	1:A:169:VAL:HG21	2.35	0.56
3:C:255:LEU:HD12	3:C:256:ARG:O	2.05	0.56
10:J:574:THR:HG21	10:J:856:ARG:HG2	1.88	0.56
6:F:41:GLU:OE2	6:F:229:ARG:NH2	2.37	0.56
8:H:309:PHE:CB	8:H:341:MET:HE1	2.35	0.56
10:J:196:THR:O	10:J:217:SER:HA	2.05	0.56
10:J:309:ARG:HD2	10:J:456:TRP:O	2.05	0.56
8:H:140:SER:HB2	8:H:185:HIS:HB2	1.87	0.56
10:J:104:ASN:O	10:J:143:LYS:NZ	2.25	0.56
10:J:309:ARG:CD	10:J:456:TRP:O	2.53	0.56
5:E:9:SER:HB3	8:H:285:ASN:HD22	1.70	0.56
12:R:-36:G:O2'	12:R:-35:G:H5'	2.06	0.56
2:B:13:ARG:NH1	2:B:171:LEU:HB3	2.21	0.56
7:G:156:ILE:CD1	7:G:208:TYR:HA	2.33	0.56
3:C:207:ARG:NH1	3:C:270:GLU:O	2.39	0.56
7:G:82:ASP:O	7:G:83:SER:HB3	2.06	0.56
3:C:61:ARG:CD	3:C:62:TYR:CZ	2.89	0.56
7:G:130:LEU:HD12	9:I:147:SER:HA	1.87	0.56
9:I:13:PRO:HD3	9:I:61:VAL:HG23	1.88	0.56
9:I:23:THR:HG22	9:I:24:GLU:N	2.21	0.56
10:J:308:ASN:HB3	10:J:392:VAL:HG22	1.87	0.55
3:C:45:LYS:HG2	3:C:46:TYR:N	2.20	0.55
9:I:159:GLU:HG2	9:I:188:PHE:CE2	2.41	0.55
2:B:29:ILE:HD11	2:B:145:LEU:HD22	1.87	0.55
8:H:300:TYR:O	8:H:303:VAL:HG22	2.06	0.55
9:I:13:PRO:CD	9:I:61:VAL:HG22	2.36	0.55
10:J:539:ILE:HG23	10:J:553:ALA:HB1	1.89	0.55
9:I:231:ARG:HH11	9:I:252:LEU:HD23	1.71	0.55
3:C:299:ILE:CG2	3:C:328:THR:CG2	2.79	0.55
7:G:222:ALA:O	7:G:226:ILE:CG1	2.44	0.55
10:J:253:PHE:C	10:J:254:THR:HG23	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:HB3	10:J:872:ARG:HH21	1.58	0.55
2:B:23:ARG:HE	2:B:173:ASP:CG	2.10	0.55
3:C:134:VAL:HG11	3:C:151:ILE:CG2	2.37	0.55
7:G:110:ARG:HD3	12:R:-44:C:C4	2.33	0.55
4:D:142:THR:HG22	4:D:144:ASP:CB	2.36	0.55
5:E:227:ARG:HD2	6:F:214:TRP:CE3	2.42	0.55
7:G:222:ALA:HB1	7:G:226:ILE:HG13	1.88	0.55
8:H:104:TYR:CD1	8:H:228:ASN:HA	2.42	0.55
10:J:467:PHE:CZ	10:J:469:ARG:CA	2.89	0.55
10:J:539:ILE:HG22	10:J:648:SER:HA	1.89	0.55
3:C:165[B]:LEU:HD21	3:C:170:LEU:HD11	1.89	0.55
7:G:6:PHE:HB3	7:G:7:PRO:HD2	1.88	0.55
8:H:83:SER:C	8:H:84:VAL:HG13	2.25	0.55
10:J:72:LEU:CD1	10:J:146:ILE:HG23	2.36	0.55
5:E:257:ASP:HB3	8:H:4:VAL:CB	2.34	0.54
9:I:9:GLU:O	9:I:10:ILE:HD13	2.06	0.54
10:J:309:ARG:HB3	10:J:456:TRP:CD2	2.42	0.54
4:D:84:PRO:O	4:D:86:GLN:HG2	2.06	0.54
7:G:127:GLU:HB2	7:G:130:LEU:HB3	1.88	0.54
8:H:315:THR:O	8:H:319:ILE:HG13	2.07	0.54
3:C:147:GLU:O	3:C:151:ILE:HG13	2.06	0.54
3:C:160:LEU:HD12	3:C:160:LEU:O	2.06	0.54
7:G:102:PHE:O	7:G:105:ALA:HB2	2.08	0.54
7:G:97:LEU:HD13	7:G:134:ILE:O	2.07	0.54
8:H:156:GLU:O	8:H:159:MET:HG3	2.07	0.54
9:I:138:ILE:HG21	9:I:159:GLU:OE1	2.08	0.54
10:J:309:ARG:NE	10:J:456:TRP:O	2.40	0.54
5:E:15:LEU:HD11	5:E:23:PRO:HD3	1.90	0.54
5:E:96:THR:O	5:E:100:ASN:ND2	2.36	0.54
7:G:142:GLY:O	7:G:143:ARG:CB	2.56	0.54
8:H:340:VAL:O	8:H:344:ILE:CG1	2.44	0.54
8:H:351:ALA:HA	8:H:354:MET:HE2	1.88	0.54
11:K:569:SER:HB3	11:K:573:GLY:CA	2.38	0.54
6:F:103:GLU:O	6:F:104:LYS:HD2	2.07	0.54
6:F:147:LEU:C	6:F:149:ASN:H	2.12	0.54
7:G:5:ILE:HD11	7:G:36:PRO:HG3	1.88	0.54
9:I:139:VAL:HG12	9:I:140:LEU:N	2.23	0.54
9:I:12:TYR:CE2	9:I:15:LYS:HB2	2.43	0.54
4:D:107:ARG:NH2	4:D:148:ASP:OD1	2.41	0.54
7:G:4:PHE:CE1	7:G:40:GLY:CA	2.84	0.54
9:I:12:TYR:CD2	9:I:15:LYS:HD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:230:ASP:OD1	10:J:230:ASP:O	2.25	0.54
2:B:19:TRP:CD2	2:B:20:ASN:HB3	2.43	0.53
3:C:139:GLY:HA2	6:F:138:PHE:CE1	2.43	0.53
9:I:285:LYS:O	9:I:286:ARG:HD3	2.08	0.53
10:J:160:ARG:NH1	10:J:164:GLU:O	2.41	0.53
10:J:193:VAL:HG11	10:J:221:TYR:CD1	2.42	0.53
10:J:641:PHE:CG	10:J:858:LEU:HD11	2.43	0.53
11:K:569:SER:OG	11:K:573:GLY:HA3	2.08	0.53
3:C:61:ARG:CD	3:C:62:TYR:CE2	2.91	0.53
7:G:137:PHE:HD1	7:G:145:ALA:HB2	1.72	0.53
9:I:103:VAL:HG21	11:K:534:LEU:HD13	1.83	0.53
7:G:7:PRO:HD3	7:G:39:THR:CG2	2.39	0.53
8:H:124:TRP:O	8:H:136:LEU:N	2.39	0.53
3:C:350:LEU:HD12	3:C:359:GLN:CG	2.37	0.53
3:C:349:ILE:HD13	3:C:378:LEU:HD23	1.90	0.53
10:J:641:PHE:CE1	10:J:741:LYS:HB2	2.42	0.53
11:K:599:ILE:HG13	11:K:600:ARG:N	2.24	0.53
3:C:28:GLU:HG2	3:C:342:SER:HB3	1.89	0.53
8:H:193:LYS:HE2	8:H:283:ASP:OD1	2.09	0.53
8:H:332:VAL:C	8:H:334:GLU:N	2.62	0.53
10:J:98:ALA:HB2	10:J:236:PRO:HG3	1.90	0.53
8:H:53:GLN:O	8:H:54:ILE:HD13	2.09	0.53
9:I:146:LEU:HD21	9:I:220:VAL:HG12	1.87	0.53
8:H:195:ARG:HH11	8:H:282:SER:N	2.07	0.53
12:R:-39:A:HO2'	12:R:-38:G:C5'	2.22	0.53
6:F:61:LEU:HD23	6:F:74:ILE:HG12	1.89	0.52
10:J:165:THR:HG22	10:J:167:ASN:H	1.75	0.52
9:I:225:LYS:HB2	9:I:286:ARG:NH1	2.24	0.52
10:J:297:LYS:O	10:J:381:GLN:NE2	2.43	0.52
10:J:485:LEU:HD21	10:J:596:LEU:HD11	1.92	0.52
7:G:182:THR:HG23	7:G:184:PHE:HD2	1.74	0.52
6:F:88:THR:OG1	6:F:132:LYS:CA	2.57	0.52
7:G:214:CYS:HB3	7:G:223:PHE:CE2	2.44	0.52
9:I:103:VAL:HG11	11:K:534:LEU:HD13	1.92	0.52
10:J:661:ILE:HG23	10:J:675:ARG:HG2	1.92	0.52
2:B:187:LEU:HD22	2:B:196:LEU:HD13	1.91	0.52
3:C:391:ARG:HD2	3:C:392:PHE:CE2	2.44	0.52
3:C:88:ILE:HB	3:C:218:VAL:HG23	1.87	0.52
8:H:337:GLU:O	8:H:341:MET:HG3	2.10	0.52
10:J:309:ARG:HD2	10:J:456:TRP:CD1	2.45	0.52
10:J:668:ASP:OD1	10:J:671:THR:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD23	2:B:99:GLU:HG3	1.91	0.52
5:E:116:LEU:CD1	5:E:157:LEU:CB	2.68	0.52
7:G:237:VAL:HG22	7:G:237:VAL:O	2.10	0.52
7:G:28:ASP:OD2	7:G:35:ARG:NH1	2.43	0.52
8:H:345:GLY:O	8:H:349:LEU:HG	2.10	0.52
7:G:99:TYR:O	7:G:102:PHE:CE2	2.63	0.52
3:C:68:ILE:HD12	3:C:279:THR:HG23	1.92	0.51
8:H:121:ASN:CG	8:H:122:LYS:H	2.13	0.51
8:H:124:TRP:HZ2	8:H:159:MET:HB3	1.72	0.51
10:J:100:ASP:HB3	10:J:468:VAL:CG1	2.39	0.51
1:A:17:GLU:HG3	7:G:201:LEU:HD13	1.92	0.51
1:A:22:ASN:ND2	1:A:30:PHE:CE2	2.68	0.51
3:C:22:LEU:HD11	3:C:29:LEU:HD23	1.93	0.51
3:C:75:LEU:HD21	6:F:18:MET:HE1	1.93	0.51
10:J:530:LYS:HB2	10:J:864:TYR:CE1	2.45	0.51
10:J:480:GLU:HG3	10:J:901:TYR:CE1	2.45	0.51
7:G:156:ILE:CG1	7:G:208:TYR:CD2	2.91	0.51
1:A:125:ILE:HG22	1:A:169:VAL:HG21	1.92	0.51
1:A:5:ILE:HD11	1:A:90:GLN:CG	2.37	0.51
8:H:309:PHE:HB3	8:H:341:MET:CE	2.33	0.51
7:G:99:TYR:O	7:G:102:PHE:CD2	2.63	0.51
10:J:18:SER:O	10:J:41:LEU:N	2.40	0.51
10:J:660:ARG:NH2	10:J:668:ASP:OD2	2.42	0.51
7:G:110:ARG:HB3	12:R:-44:C:C5	2.46	0.51
10:J:125:SER:C	10:J:127:PRO:HD2	2.31	0.51
10:J:12:ARG:NH1	10:J:154:GLU:CD	2.61	0.51
10:J:527:LEU:HD11	10:J:865:GLU:CD	2.31	0.51
7:G:187:ALA:HB3	7:G:195:TRP:HB3	1.93	0.51
4:D:22:GLN:CG	4:D:23:ASP:H	2.17	0.51
6:F:47:SER:HA	11:K:567:ASN:OD1	2.11	0.51
7:G:214:CYS:CA	7:G:223:PHE:CE1	2.94	0.51
9:I:13:PRO:CD	9:I:61:VAL:CG2	2.87	0.51
10:J:839:TYR:OH	12:R:-3:U:OP1	2.24	0.51
2:B:153:SER:HB3	8:H:83:SER:HG	1.75	0.51
2:B:67:THR:HB	2:B:119:ARG:CZ	2.41	0.51
10:J:573:VAL:CB	10:J:845:PRO:HB2	2.40	0.51
11:K:290:PHE:CB	11:K:293:ALA:HB2	2.41	0.51
3:C:309:GLN:O	3:C:310:ASN:CB	2.59	0.50
7:G:227:ALA:HB1	7:G:231:PHE:CE2	2.40	0.50
8:H:124:TRP:HB2	8:H:136:LEU:HB3	1.94	0.50
10:J:628:TRP:CH2	10:J:734:ALA:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:573:VAL:HG21	10:J:845:PRO:HB2	1.92	0.50
9:I:103:VAL:CG2	11:K:534:LEU:HD12	2.29	0.50
2:B:59:PRO:HG3	2:B:121:VAL:HG23	1.93	0.50
10:J:618:TYR:OH	10:J:650:GLU:OE1	2.22	0.50
10:J:749:THR:O	10:J:857:GLN:NE2	2.43	0.50
10:J:963:VAL:HG23	10:J:963:VAL:O	2.10	0.50
3:C:219:VAL:HG11	3:C:226:VAL:HG21	1.93	0.50
6:F:148:THR:O	6:F:149:ASN:C	2.48	0.50
6:F:242:ILE:HG13	6:F:243:SER:N	2.25	0.50
7:G:214:CYS:CB	7:G:223:PHE:CE1	2.95	0.50
10:J:264:VAL:HA	10:J:273:LEU:HD12	1.92	0.50
10:J:285:PHE:CE1	10:J:430:CYS:O	2.64	0.50
10:J:440:ARG:CD	10:J:443:GLU:HB2	2.41	0.50
3:C:387:ASP:OD2	3:C:391:ARG:NH2	2.39	0.50
4:D:142:THR:CG2	4:D:144:ASP:CB	2.90	0.50
6:F:137:ILE:HG21	6:F:176:ILE:HG23	1.92	0.50
8:H:126:VAL:CG1	8:H:184:LEU:HD12	2.39	0.50
9:I:197:LEU:O	9:I:197:LEU:HG	2.10	0.50
10:J:62:ASP:O	10:J:65:ASN:N	2.39	0.50
10:J:636:ILE:HD11	10:J:733:LEU:HD11	1.93	0.50
10:J:694:LEU:HD21	10:J:696:LEU:HD11	1.93	0.50
7:G:77:ILE:HD13	7:G:87:SER:HB2	1.93	0.50
1:A:90:GLN:CD	7:G:91:PHE:CZ	2.83	0.50
10:J:326:TRP:CZ3	10:J:380:ALA:HB2	2.47	0.50
7:G:95:VAL:HG13	7:G:132:ALA:O	2.12	0.50
10:J:527:LEU:CD1	10:J:865:GLU:CD	2.80	0.50
6:F:148:THR:O	6:F:149:ASN:O	2.30	0.50
12:R:-31:U:O4'	12:R:-31:U:P	2.70	0.50
1:A:10:SER:HB3	7:G:152:ASP:O	2.12	0.50
1:A:179:VAL:O	1:A:182:ARG:O	2.30	0.50
2:B:67:THR:HB	2:B:119:ARG:NH2	2.27	0.50
9:I:12:TYR:CE2	9:I:15:LYS:CD	2.87	0.50
8:H:160:ARG:O	8:H:163:LEU:O	2.30	0.49
10:J:309:ARG:HD2	10:J:456:TRP:CG	2.46	0.49
10:J:668:ASP:O	10:J:668:ASP:OD1	2.30	0.49
9:I:19:PRO:HB3	11:K:545:VAL:CG1	2.42	0.49
10:J:570:ILE:HG23	10:J:843:THR:O	2.12	0.49
10:J:663:ASP:HB2	10:J:665:THR:OG1	2.11	0.49
10:J:628:TRP:CZ2	10:J:734:ALA:HA	2.47	0.49
10:J:217:SER:O	10:J:218:LEU:C	2.49	0.49
8:H:152:SER:HB3	8:H:155:ASP:CG	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:VAL:CG2	10:J:31:GLY:HA2	2.43	0.49
6:F:201:VAL:CG2	6:F:213:PHE:CE1	2.96	0.49
8:H:318:ARG:HD3	8:H:348:ILE:HG21	1.95	0.49
10:J:285:PHE:HZ	10:J:429:LYS:O	1.95	0.49
1:A:103:LEU:O	1:A:107:ILE:HG12	2.12	0.49
3:C:350:LEU:CD1	3:C:359:GLN:HG2	2.38	0.49
7:G:152:ASP:CG	7:G:153:GLY:N	2.65	0.49
9:I:146:LEU:HD22	9:I:220:VAL:CG1	2.29	0.49
3:C:255:LEU:HD11	10:J:294:ARG:NE	2.28	0.49
3:C:57:ASN:HB2	3:C:240:SER:OG	2.13	0.49
10:J:49:SER:HA	10:J:72:LEU:HB2	1.94	0.49
4:D:132:ALA:HB1	4:D:205:LEU:HD23	1.94	0.49
8:H:140:SER:HA	8:H:187:ARG:HD2	1.94	0.49
6:F:87:PHE:CE1	8:H:160:ARG:NH1	2.81	0.49
8:H:206:LEU:HB3	8:H:313:GLY:HA2	1.94	0.49
10:J:134:THR:O	10:J:138:ASP:HB2	2.12	0.49
10:J:285:PHE:HZ	10:J:430:CYS:HA	1.75	0.49
10:J:311:PHE:HE2	10:J:431:LEU:CD2	2.26	0.49
10:J:544:PRO:HD3	10:J:654:TYR:HE2	1.78	0.49
11:K:538:SER:OG	11:K:541:GLN:CB	2.61	0.48
1:A:204:GLN:CG	1:A:205:ASP:N	2.66	0.48
2:B:187:LEU:HD11	2:B:214:LEU:HA	1.94	0.48
5:E:39:ASP:O	8:H:12:GLY:HA2	2.12	0.48
7:G:181:HIS:ND1	7:G:231:PHE:CZ	2.81	0.48
8:H:157:LEU:HD13	9:I:235:LEU:HD13	1.92	0.48
6:F:56:CYS:HB3	6:F:78:TYR:CZ	2.48	0.48
7:G:21:LEU:HD22	7:G:25:ILE:HG21	1.94	0.48
1:A:92:GLU:HB2	1:A:95:ASN:HB2	1.95	0.48
3:C:81:LYS:HD3	11:K:578:ARG:HB3	1.96	0.48
8:H:126:VAL:HG11	8:H:184:LEU:CD1	2.42	0.48
10:J:311:PHE:CE2	10:J:431:LEU:CG	2.93	0.48
10:J:842:PHE:HE1	10:J:855:HIS:HA	1.78	0.48
2:B:83:LYS:HE3	2:B:131:GLN:CD	2.33	0.48
3:C:275:ILE:HG21	6:F:21:SER:HB3	1.95	0.48
10:J:920:LYS:HB2	10:J:927:VAL:HB	1.96	0.48
10:J:98:ALA:HB2	10:J:236:PRO:CD	2.43	0.48
11:K:352:ARG:HA	11:K:353:PRO:C	2.34	0.48
3:C:88:ILE:HG22	6:F:101:LEU:HD11	1.95	0.48
7:G:14:ASP:OD2	7:G:16:THR:OG1	2.31	0.48
7:G:96:SER:OG	7:G:133:GLU:HG2	2.14	0.48
5:E:116:LEU:HG	5:E:117:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TYR:CE2	1:A:76:LEU:CD2	2.97	0.48
5:E:49:ARG:HD2	8:H:14:PHE:CE1	2.49	0.48
7:G:177:VAL:O	7:G:181:HIS:ND1	2.47	0.48
7:G:181:HIS:ND1	7:G:231:PHE:CE2	2.82	0.48
3:C:161:HIS:ND1	4:D:183:ASN:HB3	2.29	0.48
5:E:31:PHE:CB	8:H:5:ILE:HD12	2.44	0.48
7:G:97:LEU:HB2	7:G:134:ILE:CD1	2.44	0.48
8:H:155:ASP:O	8:H:159:MET:HG3	2.14	0.48
10:J:802:ASN:OD1	10:J:806:ARG:NH2	2.47	0.48
12:R:-43:C:O5'	12:R:-43:C:C6	2.65	0.48
3:C:278:GLN:NE2	6:F:20:PHE:HB3	2.29	0.48
9:I:139:VAL:HG11	9:I:155:ILE:CG2	2.39	0.48
10:J:158:VAL:O	10:J:169:ARG:NH1	2.47	0.48
4:D:36:PRO:HG2	4:D:41:GLU:HG2	1.96	0.47
6:F:83:ILE:O	6:F:83:ILE:HG22	2.13	0.47
7:G:97:LEU:HB2	7:G:134:ILE:HD11	1.95	0.47
9:I:285:LYS:O	9:I:286:ARG:CD	2.61	0.47
3:C:384:ARG:NH1	11:K:583:ILE:HD11	2.29	0.47
9:I:128:PHE:HZ	9:I:133:PRO:CG	2.28	0.47
10:J:311:PHE:CD2	10:J:431:LEU:HG	2.49	0.47
10:J:570:ILE:CG2	10:J:845:PRO:HD3	2.43	0.47
3:C:37:LEU:HD12	11:K:606:PHE:HD1	1.79	0.47
1:A:143:CYS:SG	1:A:147:PHE:CE2	3.05	0.47
8:H:162:PHE:CD2	8:H:163:LEU:HG	2.50	0.47
8:H:175:SER:C	8:H:176:LEU:HD12	2.34	0.47
11:K:539:VAL:N	11:K:540:PRO:HD2	2.29	0.47
12:R:-39:A:O2'	12:R:-38:G:C4'	2.63	0.47
1:A:126:VAL:HG23	1:A:130:LYS:H	1.80	0.47
2:B:235:HIS:O	2:B:239:ARG:HG2	2.14	0.47
6:F:16:LYS:NZ	6:F:16:LYS:HB3	2.29	0.47
9:I:161:LYS:O	9:I:162:PRO:C	2.52	0.47
10:J:12:ARG:NH2	10:J:16:GLY:O	2.48	0.47
10:J:668:ASP:OD1	10:J:671:THR:OG1	2.31	0.47
1:A:208:GLU:HA	8:H:76:LEU:HD22	1.96	0.47
4:D:139:ILE:CD1	4:D:146:ILE:HD12	2.44	0.47
1:A:126:VAL:HG23	1:A:129:SER:HB2	1.97	0.47
1:A:191:HIS:CE1	1:A:193:PRO:HG3	2.50	0.47
11:K:542:ILE:O	11:K:545:VAL:HB	2.15	0.47
3:C:10:ILE:HG22	3:C:11:GLU:N	2.29	0.47
5:E:27:LEU:HB2	5:E:30:GLN:HG2	1.96	0.47
8:H:340:VAL:HG12	8:H:344:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:134:LYS:HD2	9:I:237:LEU:HD21	1.97	0.47
10:J:79:LEU:HD22	10:J:226:PRO:HD3	1.97	0.47
7:G:80:PHE:CD2	7:G:81:SER:O	2.68	0.47
8:H:157:LEU:HD21	9:I:206:ARG:CZ	2.45	0.47
9:I:139:VAL:CG1	9:I:140:LEU:N	2.78	0.47
6:F:87:PHE:HE2	9:I:238:GLY:O	1.93	0.47
8:H:217:LEU:HD11	8:H:223:VAL:HG12	1.96	0.47
8:H:195:ARG:NE	8:H:282:SER:O	2.39	0.47
10:J:694:LEU:CG	10:J:696:LEU:HG	2.44	0.47
12:R:-31:U:OP1	12:R:-31:U:O4'	2.32	0.47
3:C:139:GLY:HA3	6:F:78:TYR:CD2	2.50	0.46
9:I:128:PHE:CZ	9:I:133:PRO:CD	2.97	0.46
8:H:293:ILE:O	8:H:297:ILE:HG12	2.15	0.46
10:J:867:LEU:O	10:J:872:ARG:NH1	2.44	0.46
10:J:869:LEU:HD23	10:J:872:ARG:NH1	2.30	0.46
2:B:23:ARG:O	2:B:25:PHE:N	2.49	0.46
3:C:387:ASP:OD2	11:K:585:TYR:OH	2.22	0.46
7:G:99:TYR:C	7:G:102:PHE:CE2	2.87	0.46
5:E:33:PRO:CG	8:H:337:GLU:OE2	2.63	0.46
9:I:150:ARG:NE	9:I:204:ILE:HD13	2.30	0.46
10:J:72:LEU:HD13	10:J:146:ILE:HG21	1.95	0.46
10:J:841:HIS:HB3	10:J:851:ASP:OD1	2.16	0.46
8:H:140:SER:O	8:H:187:ARG:NE	2.48	0.46
8:H:218:PRO:HG2	8:H:300:TYR:OH	2.16	0.46
8:H:64:ASP:OD2	8:H:93:ARG:NH1	2.47	0.46
10:J:473:THR:HG22	10:J:474:ILE:N	2.30	0.46
10:J:845:PRO:HA	10:J:851:ASP:HB2	1.98	0.46
1:A:261:LEU:HD12	2:B:196:LEU:HD12	1.97	0.46
2:B:71:LEU:HB2	2:B:121:VAL:HG22	1.97	0.46
3:C:10:ILE:CG2	3:C:11:GLU:N	2.78	0.46
3:C:280:LYS:NZ	3:C:280:LYS:HB3	2.30	0.46
3:C:28:GLU:HG2	3:C:342:SER:CB	2.45	0.46
6:F:239:ASP:O	6:F:242:ILE:HG12	2.15	0.46
9:I:150:ARG:HD2	9:I:204:ILE:HD13	1.98	0.46
10:J:770:LEU:O	10:J:775:ASN:N	2.49	0.46
2:B:153:SER:HA	8:H:83:SER:O	2.16	0.46
7:G:4:PHE:HD2	7:G:6:PHE:CE1	2.33	0.46
10:J:12:ARG:NH2	10:J:154:GLU:OE1	2.48	0.46
2:B:17:ARG:NH1	2:B:173:ASP:HB3	2.30	0.46
2:B:19:TRP:CZ2	2:B:20:ASN:HB3	2.51	0.46
3:C:57:ASN:O	3:C:63:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:205:LYS:HG2	9:I:46:TYR:CE1	2.48	0.46
10:J:641:PHE:CD1	10:J:741:LYS:HG2	2.49	0.46
5:E:163:ASP:HA	5:E:167:GLU:HA	1.98	0.46
5:E:75:LEU:O	5:E:75:LEU:HG	2.16	0.46
7:G:86:VAL:CG1	7:G:134:ILE:HD11	2.38	0.46
10:J:820:TYR:CZ	10:J:823:ALA:HB2	2.50	0.46
10:J:831:HIS:CE1	10:J:834:LEU:HG	2.51	0.46
11:K:317:ALA:CB	11:K:376:LEU:CB	2.92	0.46
3:C:255:LEU:CD1	3:C:256:ARG:N	2.77	0.46
3:C:308:LEU:HD22	11:K:613:LEU:CB	2.46	0.46
3:C:54:ILE:HB	3:C:78:ASN:HD21	1.81	0.46
5:E:75:LEU:HD23	5:E:114:LEU:HD12	1.98	0.46
7:G:75:VAL:O	7:G:75:VAL:HG13	2.15	0.46
7:G:84:TYR:HB2	7:G:97:LEU:HB3	1.98	0.46
9:I:211:ARG:CZ	9:I:218:VAL:HG22	2.46	0.46
10:J:18:SER:N	10:J:41:LEU:O	2.38	0.46
10:J:424:VAL:CG1	10:J:436:ILE:HD11	2.46	0.46
10:J:436:ILE:HD11	10:J:451:ILE:HG21	1.98	0.46
10:J:467:PHE:CE2	10:J:469:ARG:C	2.80	0.46
10:J:663:ASP:O	10:J:664:LYS:CB	2.64	0.46
5:E:86:ARG:HG2	5:E:88:ASP:H	1.81	0.45
3:C:73:ASN:H	6:F:102:LEU:HD11	1.81	0.45
9:I:285:LYS:C	9:I:286:ARG:HG2	2.37	0.45
10:J:566:VAL:HG21	10:J:680:LEU:HD13	1.97	0.45
12:R:-32:G:O2'	12:R:-31:U:C6	2.59	0.45
2:B:206:PRO:HB2	2:B:209:ARG:HD3	1.99	0.45
4:D:165:LEU:HD11	4:D:199:GLU:HG2	1.99	0.45
6:F:246:MET:CE	9:I:10:ILE:CG1	2.89	0.45
9:I:23:THR:CG2	9:I:24:GLU:N	2.79	0.45
3:C:261:THR:CG2	3:C:262:ARG:N	2.52	0.45
5:E:98:LEU:O	5:E:102:VAL:HG23	2.16	0.45
6:F:82:SER:HA	9:I:201:PHE:CE1	2.51	0.45
7:G:130:LEU:CD1	9:I:147:SER:HA	2.45	0.45
10:J:688:ARG:NH1	10:J:732:LEU:HD12	2.31	0.45
1:A:207:GLU:HG3	8:H:74:TYR:HD2	1.82	0.45
3:C:45:LYS:CG	3:C:46:TYR:H	2.29	0.45
4:D:168:VAL:HB	7:G:8:GLY:O	2.16	0.45
5:E:215:ILE:HD13	5:E:248:LEU:HD23	1.99	0.45
12:R:-39:A:C2'	12:R:-38:G:O5'	2.64	0.45
6:F:67:LEU:CG	6:F:68:GLY:H	2.25	0.45
7:G:160:LEU:O	7:G:164:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:138:LEU:HD22	8:H:159:MET:SD	2.57	0.45
12:R:-42:C:H2'	12:R:-41:C:C6	2.51	0.45
12:R:-42:C:C6	12:R:-42:C:O5'	2.54	0.45
9:I:12:TYR:CZ	9:I:15:LYS:CB	2.93	0.45
10:J:229:ASP:HA	10:J:232:ARG:HE	1.80	0.45
10:J:98:ALA:HB2	10:J:236:PRO:HD3	1.99	0.45
10:J:302:VAL:O	10:J:306:ASN:ND2	2.43	0.45
10:J:660:ARG:NE	10:J:666:GLN:OE1	2.49	0.45
5:E:193:VAL:HG22	5:E:209:ALA:HA	1.99	0.45
6:F:201:VAL:HG21	6:F:213:PHE:CE1	2.51	0.45
6:F:52:PHE:CE2	6:F:61:LEU:HB2	2.52	0.45
10:J:224:LEU:HG	10:J:224:LEU:O	2.16	0.45
10:J:285:PHE:CE1	10:J:430:CYS:C	2.90	0.45
10:J:440:ARG:HG3	10:J:443:GLU:CG	2.47	0.45
3:C:14:PRO:HG3	9:I:268:TYR:CE2	2.52	0.45
6:F:143:TYR:HE2	6:F:145:LYS:HE2	1.82	0.45
10:J:739:ALA:HB2	10:J:840:THR:HG22	1.99	0.45
2:B:187:LEU:CD2	2:B:199:LEU:HD13	2.47	0.45
7:G:134:ILE:O	7:G:134:ILE:HG13	2.17	0.45
5:E:257:ASP:CG	8:H:4:VAL:HG23	2.36	0.45
10:J:387:GLN:HA	10:J:388:PRO:HD3	1.80	0.45
10:J:311:PHE:CE2	10:J:431:LEU:CD2	2.99	0.45
11:K:538:SER:HG	11:K:541:GLN:H	1.63	0.45
5:E:75:LEU:CD2	5:E:114:LEU:HD12	2.46	0.45
1:A:208:GLU:HA	8:H:76:LEU:CD2	2.46	0.45
8:H:79:MET:HB3	8:H:81:TYR:CE1	2.51	0.45
6:F:124:VAL:HG12	6:F:187:LEU:HD22	1.99	0.44
7:G:4:PHE:HD2	7:G:6:PHE:CZ	2.36	0.44
10:J:326:TRP:HZ3	10:J:380:ALA:HB2	1.82	0.44
3:C:218:VAL:HG23	3:C:218:VAL:O	2.16	0.44
3:C:387:ASP:CG	3:C:391:ARG:HH21	2.20	0.44
6:F:95:ILE:H	6:F:118:MET:HE3	1.82	0.44
10:J:79:LEU:HD13	10:J:224:LEU:HG	1.98	0.44
7:G:81:SER:OG	12:R:-31:U:OP2	2.23	0.44
9:I:62:GLY:HA3	9:I:111:LEU:O	2.17	0.44
10:J:929:LEU:HD13	10:J:936:GLU:HG2	1.99	0.44
4:D:99:GLU:OE2	4:D:108:GLU:HG3	2.17	0.44
8:H:124:TRP:CZ2	8:H:159:MET:HE3	2.52	0.44
9:I:159:GLU:CD	9:I:231:ARG:HE	2.17	0.44
10:J:440:ARG:HG3	10:J:443:GLU:CB	2.45	0.44
10:J:680:LEU:HB2	10:J:730:PHE:HZ	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:300:VAL:HG23	3:C:329:VAL:HB	1.99	0.44
7:G:152:ASP:OD1	7:G:153:GLY:N	2.50	0.44
10:J:236:PRO:HA	10:J:466:HIS:CE1	2.51	0.44
2:B:169:THR:HA	2:B:170:PRO:HD3	1.67	0.44
8:H:216:ASN:OD1	8:H:243:ARG:NH1	2.50	0.44
8:H:195:ARG:NH1	8:H:282:SER:N	2.65	0.44
8:H:67:TRP:CE3	8:H:93:ARG:C	2.91	0.44
8:H:68:MET:O	8:H:94:LEU:HD12	2.18	0.44
9:I:150:ARG:HD2	9:I:204:ILE:HG23	1.99	0.44
3:C:134:VAL:HG11	3:C:151:ILE:CB	2.45	0.44
3:C:97:GLU:HG2	3:C:209:TRP:CD1	2.52	0.44
10:J:326:TRP:CZ3	10:J:380:ALA:CB	3.00	0.44
3:C:162:SER:HB3	3:C:358:LYS:CB	2.48	0.44
5:E:15:LEU:HD23	5:E:193:VAL:HG21	2.00	0.44
7:G:95:VAL:HG11	7:G:134:ILE:CG2	2.38	0.44
6:F:87:PHE:CZ	8:H:160:ARG:CZ	3.00	0.44
8:H:170:ASN:HB2	8:H:191:TYR:HA	2.00	0.44
10:J:236:PRO:HA	10:J:466:HIS:CG	2.53	0.44
1:A:297:LEU:O	1:A:301:ASN:HB2	2.17	0.44
1:A:5:ILE:CG1	1:A:90:GLN:HG2	2.47	0.44
3:C:139:GLY:HA3	6:F:78:TYR:CG	2.53	0.44
6:F:186:GLU:HG2	9:I:60:LEU:HD21	2.00	0.44
7:G:106:SER:CB	7:G:109:ASN:HB3	2.44	0.44
10:J:688:ARG:NH1	10:J:729:GLU:OE2	2.51	0.44
5:E:33:PRO:HG3	8:H:337:GLU:CD	2.38	0.43
6:F:186:GLU:HB3	9:I:59:THR:HB	2.00	0.43
9:I:66:CYS:HA	9:I:107:LEU:O	2.18	0.43
10:J:131:ARG:O	10:J:134:THR:OG1	2.34	0.43
7:G:181:HIS:CE1	7:G:231:PHE:CE2	3.06	0.43
10:J:81:ALA:CB	10:J:82:PRO:HA	2.45	0.43
12:R:-35:G:C2'	12:R:-34:G:H5'	2.47	0.43
3:C:73:ASN:H	6:F:102:LEU:CD1	2.31	0.43
10:J:181:TYR:HB3	10:J:192:VAL:HG11	1.99	0.43
10:J:597:VAL:HB	10:J:902:TYR:HD2	1.84	0.43
10:J:643:LYS:HD2	10:J:864:TYR:CE2	2.53	0.43
10:J:873:ASP:HB3	10:J:876:LYS:HB2	2.00	0.43
12:R:-39:A:O2'	12:R:-38:G:C5'	2.66	0.43
3:C:27:PRO:HB3	3:C:338:ALA:HA	2.00	0.43
6:F:186:GLU:HG2	9:I:60:LEU:CD2	2.48	0.43
10:J:735:ASN:HB3	10:J:840:THR:O	2.18	0.43
1:A:176:VAL:CG1	1:A:176:VAL:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:258:ARG:HB2	9:I:262:GLY:HA2	2.00	0.43
10:J:112[A]:ILE:HD13	10:J:181:TYR:CZ	2.53	0.43
10:J:112[B]:ILE:HD13	10:J:181:TYR:CZ	2.53	0.43
5:E:66:VAL:HG21	10:J:31:GLY:HA2	2.00	0.43
10:J:431:LEU:HA	10:J:432:PRO:HD3	1.88	0.43
10:J:959:LYS:HD3	10:J:972:ASP:OD2	2.19	0.43
1:A:254:LEU:HD12	1:A:255:PRO:HD2	2.01	0.43
3:C:277:ASP:OD1	3:C:280:LYS:N	2.45	0.43
1:A:169:VAL:HG22	1:A:174:ILE:CD1	2.49	0.43
1:A:204:GLN:HG3	1:A:205:ASP:OD1	2.18	0.43
1:A:228:GLU:HG3	1:A:231:ARG:CZ	2.49	0.43
2:B:17:ARG:HH11	2:B:23:ARG:HG3	1.78	0.43
7:G:214:CYS:HB3	7:G:223:PHE:CE1	2.53	0.43
10:J:255:PHE:N	10:J:458:THR:HB	2.34	0.43
10:J:579:PRO:HA	10:J:584:ASP:OD2	2.19	0.43
10:J:606:MET:O	10:J:610:THR:OG1	2.24	0.43
12:R:-3:U:H2'	12:R:-2:U:C6	2.54	0.43
1:A:167:ILE:HD12	1:A:176:VAL:HA	1.99	0.43
10:J:213:ILE:HG12	10:J:215:THR:HG23	2.00	0.43
3:C:33:ARG:NH1	3:C:306:CYS:HA	2.34	0.43
4:D:62:ARG:NH2	4:D:108:GLU:OE2	2.50	0.43
5:E:52:ALA:HB3	5:E:56:SER:HB2	2.00	0.43
6:F:87:PHE:CE1	8:H:160:ARG:CZ	3.02	0.43
9:I:138:ILE:CG2	9:I:159:GLU:OE1	2.66	0.43
10:J:112[A]:ILE:HD13	10:J:181:TYR:CD1	2.54	0.43
10:J:112[B]:ILE:HD13	10:J:181:TYR:CD1	2.54	0.43
8:H:190:LYS:HE3	8:H:191:TYR:CZ	2.53	0.43
9:I:141:THR:HG21	9:I:155:ILE:HG13	2.00	0.43
9:I:150:ARG:CD	9:I:204:ILE:HD13	2.49	0.43
10:J:12:ARG:NH1	10:J:154:GLU:OE1	2.52	0.43
10:J:17:LEU:CD1	10:J:42:ARG:HA	2.37	0.43
8:H:121:ASN:CG	8:H:122:LYS:N	2.71	0.42
9:I:32:ILE:HB	9:I:103:VAL:HG12	2.01	0.42
6:F:246:MET:CE	9:I:10:ILE:CD1	2.97	0.42
10:J:216:LYS:HD2	10:J:220:GLN:HG2	2.00	0.42
9:I:19:PRO:HG3	11:K:549:PHE:HB2	2.01	0.42
7:G:172:PHE:HA	7:G:173:PRO:HD3	1.78	0.42
8:H:215:HIS:CD2	8:H:316:GLN:OE1	2.72	0.42
10:J:113:VAL:HG11	10:J:132:LEU:HD21	2.02	0.42
10:J:959:LYS:HE2	10:J:974:TYR:HE1	1.84	0.42
2:B:23:ARG:CZ	2:B:173:ASP:OD1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LYS:O	2:B:198:LEU:HA	2.18	0.42
2:B:84:PHE:O	5:E:63:LYS:NZ	2.38	0.42
4:D:18:GLU:OE2	4:D:25:LYS:HD2	2.19	0.42
5:E:4:SER:HB3	8:H:166:GLY:O	2.19	0.42
7:G:106:SER:HB3	7:G:109:ASN:H	1.83	0.42
7:G:114:GLN:O	7:G:115:VAL:C	2.58	0.42
8:H:84:VAL:HG21	8:H:99:PRO:HG3	2.01	0.42
2:B:186:THR:HB	2:B:200:LEU:HB3	2.01	0.42
5:E:122:PHE:HD2	5:E:154:LEU:HD13	1.85	0.42
7:G:4:PHE:CD2	7:G:6:PHE:CZ	3.07	0.42
8:H:138:LEU:HD22	8:H:156:GLU:HA	2.01	0.42
9:I:254:VAL:HG12	9:I:275:MET:HE3	2.01	0.42
3:C:353:PRO:C	3:C:355:GLY:N	2.70	0.42
3:C:52:VAL:CG2	3:C:384:ARG:HH22	2.31	0.42
10:J:440:ARG:NH2	10:J:444:LEU:HD21	2.34	0.42
10:J:945:THR:HB	10:J:962:PHE:HD1	1.79	0.42
3:C:309:GLN:HG3	3:C:310:ASN:N	2.34	0.42
8:H:155:ASP:O	8:H:159:MET:CG	2.68	0.42
10:J:17:LEU:HD11	10:J:42:ARG:NH1	2.35	0.42
10:J:112[B]:ILE:CD1	10:J:181:TYR:CE1	2.97	0.42
1:A:107:ILE:HG21	1:A:236:THR:HG21	2.02	0.42
3:C:352:ALA:O	3:C:355:GLY:CA	2.67	0.42
7:G:64:TYR:HA	7:G:160:LEU:HD11	2.01	0.42
1:A:278:GLN:O	1:A:281:GLN:CG	2.62	0.42
3:C:362:LEU:HD22	4:D:180:LEU:HD23	2.01	0.42
6:F:67:LEU:CG	6:F:68:GLY:N	2.73	0.42
6:F:88:THR:OG1	6:F:132:LYS:N	2.52	0.42
8:H:124:TRP:CH2	8:H:159:MET:HE3	2.54	0.42
3:C:130:VAL:HG22	3:C:159:ILE:HD12	2.01	0.42
3:C:305:GLU:O	3:C:305:GLU:CG	2.67	0.42
3:C:383:VAL:HG12	11:K:585:TYR:CD2	2.54	0.42
10:J:570:ILE:HG22	10:J:845:PRO:HD3	2.02	0.42
3:C:353:PRO:C	3:C:355:GLY:H	2.23	0.42
3:C:44:ARG:NH2	3:C:333:ASP:HB3	2.34	0.42
7:G:122:ARG:NH2	7:G:124:CYS:HB3	2.34	0.42
12:R:-33:G:C3'	12:R:-32:G:C5'	2.94	0.42
8:H:5:ILE:HG12	8:H:6:THR:N	2.35	0.41
10:J:641:PHE:HZ	10:J:737:SER:O	2.03	0.41
10:J:763:PHE:CG	10:J:780:LEU:HD21	2.56	0.41
11:K:175:ASN:HA	11:K:176:PRO:HD3	1.74	0.41
1:A:223:ALA:HB1	1:A:227:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:HB3	10:J:872:ARG:HH22	1.66	0.41
3:C:134:VAL:O	3:C:134:VAL:HG13	2.21	0.41
3:C:356:ASN:HB3	4:D:185:ASP:OD1	2.20	0.41
5:E:102:VAL:HG22	5:E:225:PRO:HD2	2.01	0.41
10:J:23:VAL:HB	10:J:36:VAL:HG22	2.01	0.41
10:J:588:ALA:O	10:J:883:ASN:OD1	2.38	0.41
10:J:596:LEU:HB3	10:J:898:SER:OG	2.20	0.41
10:J:98:ALA:HB2	10:J:236:PRO:CG	2.50	0.41
1:A:81:THR:HG22	1:A:138:VAL:HB	2.02	0.41
1:A:169:VAL:HG22	1:A:174:ILE:HD12	2.02	0.41
1:A:235:LEU:HD22	1:A:261:LEU:HD22	2.01	0.41
2:B:47:ASN:OD1	2:B:132:ASP:N	2.52	0.41
2:B:240:VAL:HG21	8:H:54:ILE:CD1	2.47	0.41
3:C:137:GLU:CD	6:F:140:TYR:CE1	2.93	0.41
7:G:95:VAL:CG1	7:G:132:ALA:O	2.68	0.41
7:G:2:SER:OG	7:G:41:VAL:HG22	2.20	0.41
11:K:356:LYS:N	11:K:357:PRO:CD	2.83	0.41
3:C:61:ARG:NH1	6:F:20:PHE:CE2	2.89	0.41
1:A:207:GLU:HG3	8:H:74:TYR:CD2	2.56	0.41
3:C:29:LEU:HB2	9:I:258:ARG:HH22	1.85	0.41
10:J:285:PHE:HE1	10:J:430:CYS:C	2.24	0.41
10:J:85:LYS:HE2	10:J:85:LYS:HB2	1.92	0.41
8:H:189:LEU:HD12	8:H:190:LYS:N	2.35	0.41
10:J:834:LEU:HD21	12:R:-4:U:H4'	2.03	0.41
11:K:595:LYS:HB2	11:K:598:ASP:HB2	2.01	0.41
2:B:206:PRO:HG3	10:J:869:LEU:HD11	2.02	0.41
4:D:220:ARG:HA	7:G:218:ASN:HD22	1.85	0.41
8:H:123:ARG:HG2	8:H:137:MET:HA	2.03	0.41
8:H:67:TRP:HZ3	8:H:93:ARG:C	2.21	0.41
10:J:301:ILE:HD13	10:J:392:VAL:HG12	2.03	0.41
10:J:658:GLN:OE1	10:J:722:ALA:HB3	2.20	0.41
1:A:251:ALA:HA	2:B:198:LEU:HD12	2.03	0.41
2:B:185:VAL:HG22	2:B:201:VAL:HG22	2.03	0.41
7:G:102:PHE:CB	7:G:103:PRO:HD2	2.38	0.41
7:G:178:LEU:HD13	7:G:184:PHE:HZ	1.85	0.41
9:I:143:VAL:HG22	9:I:153:VAL:HG12	2.03	0.41
9:I:277:SER:HA	9:I:278:PRO:HD3	1.84	0.41
7:G:174:LEU:O	7:G:177:VAL:HG22	2.20	0.41
10:J:19:VAL:HB	10:J:40:TYR:CD2	2.56	0.41
3:C:33:ARG:HH12	3:C:306:CYS:HA	1.85	0.41
4:D:220:ARG:HA	7:G:218:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:110:ARG:HD2	12:R:-44:C:N3	2.34	0.41
3:C:17:PHE:CZ	9:I:255:VAL:CG1	2.98	0.41
10:J:694:LEU:CD2	10:J:696:LEU:CD1	2.99	0.41
10:J:967:SER:OG	10:J:968:ASP:N	2.53	0.41
4:D:168:VAL:HG23	4:D:173:VAL:HB	2.02	0.40
8:H:98:ILE:HA	8:H:99:PRO:HD3	1.94	0.40
9:I:152:ASN:OD1	9:I:204:ILE:HG12	2.22	0.40
9:I:17:ILE:HD11	9:I:58:ALA:HB2	2.03	0.40
10:J:165:THR:HG22	10:J:166:ILE:N	2.36	0.40
10:J:20:THR:OG1	10:J:21:GLN:N	2.54	0.40
1:A:263:LYS:HB3	1:A:263:LYS:HE2	1.97	0.40
2:B:103:SER:O	2:B:107:MET:HG3	2.21	0.40
2:B:104:LEU:HD13	2:B:143:ILE:HD11	2.03	0.40
2:B:161:ILE:HD12	2:B:161:ILE:HA	1.95	0.40
3:C:80:LEU:HD23	3:C:233:SER:HB2	2.04	0.40
4:D:136:ILE:CG2	4:D:194:LEU:CD1	2.92	0.40
8:H:104:TYR:HB2	8:H:204:SER:CB	2.52	0.40
8:H:309:PHE:HB2	8:H:341:MET:CE	2.39	0.40
3:C:53:ALA:CB	11:K:575:ILE:HD11	2.51	0.40
7:G:110:ARG:HB2	12:R:-44:C:N4	2.36	0.40
1:A:53:ASN:HB3	4:D:11:ASP:OD2	2.22	0.40
2:B:240:VAL:HG11	8:H:52:SER:HB2	2.02	0.40
6:F:93:ILE:HD12	6:F:127:LEU:HD21	2.02	0.40
10:J:902:TYR:HA	10:J:902:TYR:HD1	1.81	0.40
11:K:399:ARG:CB	11:K:414:GLU:O	2.70	0.40
1:A:17:GLU:OE2	1:A:20:ARG:NE	2.52	0.40
1:A:256:MET:O	2:B:195:LYS:HA	2.22	0.40
3:C:275:ILE:CG2	6:F:21:SER:HB3	2.51	0.40
4:D:24:THR:OG1	4:D:107:ARG:NH1	2.54	0.40
5:E:75:LEU:HD21	5:E:114:LEU:HB3	2.01	0.40
10:J:255:PHE:O	10:J:458:THR:HG21	2.20	0.40
3:C:35:LEU:O	3:C:46:TYR:OH	2.39	0.40
7:G:150:LEU:HD13	7:G:195:TRP:CG	2.56	0.40
8:H:67:TRP:CE3	8:H:95:LEU:HB2	2.56	0.40
10:J:20:THR:HG23	10:J:39:HIS:HB3	2.03	0.40
11:K:193:SER:HA	11:K:194:PRO:HD3	1.89	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:GLN:NE2	8:H:329:TYR:CE1[1_655]	1.52	0.68
7:G:229:ARG:NH1	12:R:-39:A:N6[4_545]	1.88	0.32
8:H:245:THR:C	11:K:202:GLU:O[1_455]	1.88	0.32
5:E:162:ASP:OD1	11:K:543:ARG:NH2[3_554]	1.97	0.23
4:D:200:GLN:NE2	8:H:329:TYR:CD1[1_655]	1.98	0.22
4:D:169:ASN:ND2	8:H:324:GLU:OE1[1_655]	2.13	0.07

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	297/305 (97%)	290 (98%)	7 (2%)	0	100	100
2	B	242/248 (98%)	237 (98%)	4 (2%)	1 (0%)	34	70
3	C	332/394 (84%)	312 (94%)	19 (6%)	1 (0%)	41	74
4	D	222/245 (91%)	218 (98%)	4 (2%)	0	100	100
5	E	266/267 (100%)	250 (94%)	16 (6%)	0	100	100
6	F	209/250 (84%)	197 (94%)	12 (6%)	0	100	100
7	G	235/243 (97%)	226 (96%)	9 (4%)	0	100	100
8	H	287/361 (80%)	278 (97%)	8 (3%)	1 (0%)	41	74
9	I	214/295 (72%)	208 (97%)	6 (3%)	0	100	100
10	J	939/1003 (94%)	899 (96%)	39 (4%)	1 (0%)	51	83
11	K	344/695 (50%)	330 (96%)	14 (4%)	0	100	100
All	All	3587/4306 (83%)	3445 (96%)	138 (4%)	4 (0%)	51	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	333	GLY
2	B	170	PRO
10	J	598	ASP

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Mol	Chain	Res	Type
3	C	18	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	255/266 (96%)	255 (100%)	0	100 100
2	B	210/219 (96%)	210 (100%)	0	100 100
3	C	282/350 (81%)	281 (100%)	1 (0%)	91 95
4	D	196/216 (91%)	196 (100%)	0	100 100
5	E	238/241 (99%)	238 (100%)	0	100 100
6	F	181/219 (83%)	181 (100%)	0	100 100
7	G	194/211 (92%)	194 (100%)	0	100 100
8	H	243/313 (78%)	243 (100%)	0	100 100
9	I	174/242 (72%)	174 (100%)	0	100 100
10	J	816/901 (91%)	816 (100%)	0	100 100
11	K	81/636 (13%)	81 (100%)	0	100 100
All	All	2870/3814 (75%)	2869 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	HIS
1	A	191	HIS
2	B	237	GLN
3	C	73	ASN

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Mol	Chain	Res	Type
6	F	49	HIS
6	F	206	ASN
7	G	218	ASN
10	J	855	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	29/45 (64%)	15 (51%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	-42	C
12	R	-39	A
12	R	-38	G
12	R	-36	G
12	R	-32	G
12	R	-31	U
12	R	-30	U
12	R	-29	U
12	R	-27	U
12	R	-26	U
12	R	-24	U
12	R	-23	U
12	R	-22	U
12	R	-21	U
12	R	-20	U

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	299/305 (98%)	0.35	22 (7%) 14 11	168, 206, 270, 304	0
2	B	244/248 (98%)	0.58	20 (8%) 11 9	162, 209, 280, 314	0
3	C	339/394 (86%)	0.51	27 (7%) 12 10	205, 234, 301, 333	0
4	D	223/245 (91%)	0.44	13 (5%) 23 18	170, 206, 259, 300	0
5	E	267/267 (100%)	0.47	19 (7%) 16 12	179, 216, 267, 309	0
6	F	215/250 (86%)	0.34	8 (3%) 41 33	189, 221, 266, 308	0
7	G	237/243 (97%)	0.19	8 (3%) 45 37	167, 203, 253, 283	0
8	H	293/361 (81%)	0.21	10 (3%) 45 37	175, 209, 263, 286	0
9	I	222/295 (75%)	0.94	41 (18%) 1 1	205, 244, 291, 345	0
10	J	944/1003 (94%)	1.46	274 (29%) 0 0	238, 377, 429, 458	0
11	K	350/695 (50%)	2.51	170 (48%) 0 0	227, 378, 404, 428	0
12	R	31/45 (68%)	3.37	12 (38%) 0 0	265, 295, 398, 401	0
All	All	3664/4351 (84%)	0.93	624 (17%) 1 1	162, 242, 405, 458	0

All (624) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	270	LEU	16.1
10	J	553	ALA	15.2
12	R	-27	U	14.3
12	R	-26	U	13.5
12	R	-28	U	13.2
10	J	698	SER	13.2
10	J	554	LEU	13.1
10	J	699	PRO	13.0
10	J	701	VAL	12.7
11	K	269	LYS	12.5
11	K	170	ASP	12.5

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Mol	Chain	Res	Type	RSRZ
11	K	307	TYR	11.2
11	K	216	VAL	10.6
10	J	697	ALA	10.6
11	K	217	ASP	10.4
12	R	-20	U	10.2
11	K	207	SER	10.1
11	K	210	ASP	10.1
10	J	937	GLY	10.1
11	K	267	THR	10.0
12	R	-25	U	9.7
10	J	703	VAL	9.6
11	K	151	LEU	9.6
11	K	171	ASP	9.4
11	K	308	VAL	9.3
11	K	209	ASP	9.2
11	K	271	ARG	9.1
12	R	-29	U	9.1
10	J	973	VAL	9.1
10	J	407	LEU	9.0
10	J	926	ILE	9.0
11	K	208	TRP	8.8
11	K	273	ASN	8.8
10	J	615	LEU	8.8
11	K	218	THR	8.5
10	J	968	ASP	8.5
10	J	556	ALA	8.4
10	J	976	PHE	8.3
10	J	933	PHE	8.3
11	K	205	SER	8.3
11	K	365	ASP	8.2
3	C	265	SER	8.2
11	K	252	CYS	8.2
10	J	700	GLU	8.1
11	K	274	LEU	8.1
11	K	206	LYS	8.0
3	C	309	GLN	7.9
12	R	-24	U	7.8
11	K	195	GLU	7.7
11	K	350	ARG	7.7
10	J	1001	LYS	7.7
11	K	165	SER	7.7
10	J	902	TYR	7.6

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Mol	Chain	Res	Type	RSRZ
10	J	566	VAL	7.6
11	K	364	ALA	7.5
10	J	972	ASP	7.5
11	K	305	GLY	7.4
11	K	306	LEU	7.4
10	J	935	VAL	7.3
11	K	353	PRO	7.2
9	I	269	ALA	7.2
10	J	1000	LEU	7.2
11	K	196	ILE	7.2
11	K	219	SER	7.0
11	K	341	SER	6.8
10	J	932	LYS	6.8
10	J	903	VAL	6.8
11	K	253	LEU	6.8
10	J	934	GLY	6.8
11	K	266	ASP	6.8
10	J	507	GLY	6.7
10	J	998	LEU	6.7
10	J	730	PHE	6.6
11	K	213	PRO	6.6
10	J	971	ARG	6.6
10	J	990	ILE	6.6
11	K	238	ASP	6.5
10	J	320	LEU	6.5
11	K	163	SER	6.5
10	J	569	HIS	6.5
11	K	254	MET	6.4
11	K	260	GLU	6.4
10	J	970	PRO	6.4
12	R	-30	U	6.4
10	J	980	GLU	6.4
10	J	837	ASP	6.3
12	R	-23	U	6.3
11	K	173	GLU	6.2
10	J	540	CYS	6.1
11	K	150	PRO	6.1
11	K	230	LYS	6.1
10	J	634	ALA	6.1
10	J	979	VAL	6.1
11	K	368	PHE	6.1
10	J	996	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
11	K	304	LEU	6.0
10	J	632	ASP	6.0
11	K	152	LEU	6.0
3	C	142	GLY	6.0
11	K	309	VAL	6.0
10	J	950	SER	6.0
11	K	153	LYS	5.9
11	K	227	GLU	5.9
10	J	969	LYS	5.9
11	K	268	LEU	5.9
9	I	291	PRO	5.9
10	J	696	LEU	5.8
10	J	710	SER	5.8
10	J	529	THR	5.8
10	J	931	PRO	5.8
11	K	231	ASN	5.8
10	J	422	VAL	5.8
11	K	272	GLU	5.8
12	R	-21	U	5.7
11	K	303	ASP	5.7
11	K	300	LEU	5.7
11	K	369	LEU	5.6
10	J	489	ASP	5.6
10	J	733	LEU	5.6
10	J	715	VAL	5.6
10	J	555	HIS	5.5
10	J	677	LEU	5.5
10	J	147	VAL	5.5
10	J	928	VAL	5.5
10	J	776	MET	5.5
10	J	148	PHE	5.4
10	J	633	SER	5.4
11	K	194	PRO	5.4
11	K	211	SER	5.4
10	J	408	ALA	5.4
11	K	166	LEU	5.4
12	R	-22	U	5.3
11	K	312	PHE	5.3
10	J	504	PRO	5.3
11	K	310	GLY	5.3
11	K	362	ALA	5.3
10	J	90	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
11	K	226	LEU	5.2
10	J	567	GLY	5.2
10	J	438	THR	5.2
10	J	763	PHE	5.2
10	J	829	PHE	5.2
10	J	149	HIS	5.2
11	K	182	PRO	5.1
8	H	2	SER	5.1
9	I	28	GLY	5.1
11	K	349	TRP	5.1
10	J	936	GLU	5.1
11	K	212	VAL	5.1
10	J	826	TYR	5.0
10	J	714	GLU	4.9
10	J	947	ASP	4.9
11	K	228	ASP	4.9
10	J	964	PRO	4.9
10	J	597	VAL	4.9
11	K	234	GLU	4.9
11	K	183	TYR	4.9
10	J	385	LYS	4.9
10	J	565	GLU	4.9
10	J	949	ASN	4.8
11	K	359	THR	4.8
11	K	281	PHE	4.8
10	J	364	VAL	4.8
10	J	997	GLU	4.8
11	K	265	VAL	4.8
10	J	944	LEU	4.8
10	J	409	PRO	4.8
10	J	97	GLN	4.8
10	J	919	ILE	4.8
9	I	268	TYR	4.8
11	K	400	ARG	4.7
9	I	102	THR	4.7
11	K	172	ASP	4.7
11	K	261	ARG	4.7
10	J	899	ILE	4.7
10	J	98	ALA	4.7
10	J	318	VAL	4.7
11	K	257	SER	4.7
11	K	256	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
11	K	229	LEU	4.6
10	J	405	GLY	4.6
10	J	807	ILE	4.6
1	A	165	PRO	4.6
7	G	74	GLY	4.6
10	J	777	SER	4.6
1	A	172	GLU	4.6
10	J	713	ASN	4.6
2	B	2	SER	4.5
10	J	437	ARG	4.5
11	K	174	ASN	4.5
3	C	266	ALA	4.5
5	E	86	ARG	4.5
10	J	636	ILE	4.5
5	E	84	GLY	4.5
9	I	103	VAL	4.5
9	I	162	PRO	4.4
10	J	449	ILE	4.4
11	K	402	GLU	4.4
10	J	513	PRO	4.4
10	J	101	LEU	4.4
10	J	918	VAL	4.4
10	J	966	ASN	4.4
11	K	301	GLN	4.4
2	B	63	SER	4.4
3	C	308	LEU	4.4
10	J	517	ASP	4.3
10	J	927	VAL	4.3
3	C	251	ARG	4.3
10	J	992	SER	4.3
11	K	204	PRO	4.3
10	J	938	LEU	4.3
10	J	376	ASP	4.3
10	J	628	TRP	4.3
11	K	414	GLU	4.3
10	J	808	MET	4.2
10	J	952	ALA	4.2
11	K	161	PRO	4.2
1	A	62	CYS	4.2
11	K	189	HIS	4.2
10	J	712	PRO	4.2
4	D	145	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
10	J	778	ILE	4.1
10	J	836	VAL	4.1
10	J	678	LEU	4.1
10	J	975	VAL	4.1
11	K	363	ARG	4.1
10	J	989	PRO	4.1
10	J	895	GLY	4.0
9	I	188	PHE	4.0
10	J	916	GLY	4.0
8	H	95	LEU	4.0
10	J	112[A]	ILE	4.0
2	B	157	TYR	4.0
10	J	404	VAL	4.0
11	K	413	SER	4.0
11	K	225	MET	4.0
9	I	138	ILE	4.0
10	J	510	TRP	4.0
5	E	105	SER	3.9
3	C	293	PHE	3.9
10	J	951	ALA	3.9
3	C	140	ARG	3.9
10	J	275	GLN	3.9
10	J	557	LYS	3.9
5	E	197	MET	3.9
10	J	906	VAL	3.9
10	J	10	ARG	3.8
10	J	596	LEU	3.8
11	K	214	ILE	3.8
10	J	528	LEU	3.8
9	I	270	THR	3.8
10	J	930	VAL	3.8
10	J	616	LYS	3.8
11	K	164	GLU	3.7
11	K	181	HIS	3.7
9	I	21	TYR	3.7
11	K	361	TYR	3.7
10	J	441	ALA	3.7
2	B	158	ILE	3.7
10	J	978	LYS	3.7
11	K	239	LEU	3.7
3	C	310	ASN	3.6
10	J	310	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
10	J	508	HIS	3.6
3	C	180	ASN	3.6
10	J	571	ALA	3.6
10	J	967	SER	3.6
4	D	19	PHE	3.6
11	K	408	PRO	3.6
11	K	352	ARG	3.6
10	J	542	ILE	3.6
10	J	929	LEU	3.6
11	K	311	LEU	3.6
11	K	223	GLU	3.6
10	J	608	LEU	3.6
5	E	193	VAL	3.6
10	J	210	GLU	3.6
10	J	766	LEU	3.6
4	D	223	VAL	3.5
4	D	136	ILE	3.5
10	J	813	MET	3.5
11	K	241	HIS	3.5
4	D	137	ALA	3.5
10	J	380	ALA	3.5
10	J	695	ASN	3.5
10	J	915	THR	3.5
10	J	423	PHE	3.5
10	J	709	THR	3.5
10	J	894	ALA	3.5
10	J	898	SER	3.5
10	J	418	SER	3.5
2	B	7	TYR	3.5
10	J	774	LYS	3.5
11	K	410	THR	3.5
10	J	650	GLU	3.5
1	A	194	ILE	3.4
9	I	27	ASP	3.4
10	J	113	VAL	3.4
10	J	87	TYR	3.4
10	J	412	VAL	3.4
11	K	162	LEU	3.3
11	K	372	ILE	3.3
9	I	264	GLY	3.3
10	J	88	VAL	3.3
10	J	862	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
10	J	974	TYR	3.3
11	K	251	VAL	3.3
11	K	415	VAL	3.3
10	J	387	GLN	3.3
5	E	145	ILE	3.3
11	K	149	ILE	3.3
10	J	420	GLN	3.3
11	K	175	ASN	3.3
11	K	222	LEU	3.3
10	J	326	TRP	3.3
11	K	169	VAL	3.3
3	C	272	TYR	3.3
10	J	702	LYS	3.3
11	K	167	ARG	3.2
10	J	708	GLU	3.2
11	K	258	THR	3.2
2	B	159	SER	3.2
2	B	93	ASN	3.2
11	K	278	ASN	3.2
10	J	417	SER	3.2
6	F	85	GLY	3.2
2	B	160	GLY	3.2
9	I	128	PHE	3.2
1	A	239	LEU	3.2
11	K	180	PRO	3.2
11	K	158	ALA	3.2
11	K	220	THR	3.2
1	A	125	ILE	3.2
2	B	3	ARG	3.2
10	J	726	LEU	3.2
11	K	255	GLN	3.1
11	K	168	LEU	3.1
1	A	169	VAL	3.1
9	I	130	ASN	3.1
10	J	154	GLU	3.1
11	K	262	ASP	3.1
10	J	155	HIS	3.1
10	J	295	PHE	3.1
11	K	240	GLU	3.1
1	A	64	ILE	3.1
10	J	917	TYR	3.1
9	I	159	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
11	K	299	TRP	3.1
3	C	274	ILE	3.1
11	K	366	THR	3.1
10	J	519	PRO	3.1
10	J	613	CYS	3.1
11	K	235	ILE	3.1
10	J	580	GLY	3.1
10	J	108	PHE	3.1
10	J	259	TYR	3.1
10	J	413	ASP	3.0
10	J	635	ASN	3.0
10	J	114	PRO	3.0
3	C	207	ARG	3.0
10	J	961	THR	3.0
10	J	41	LEU	3.0
10	J	514	THR	3.0
10	J	651	ALA	3.0
10	J	15	ASP	3.0
10	J	762	ASN	3.0
9	I	258	ARG	3.0
6	F	82	SER	3.0
11	K	250	ILE	3.0
9	I	133	PRO	3.0
11	K	215	TRP	3.0
5	E	185	PRO	3.0
5	E	188	PHE	3.0
11	K	233	LYS	3.0
10	J	652	PHE	3.0
11	K	317	ALA	2.9
10	J	674	MET	2.9
10	J	46	PRO	2.9
10	J	977	ASP	2.9
6	F	213	PHE	2.9
8	H	67	TRP	2.9
3	C	52	VAL	2.9
4	D	161	HIS	2.9
10	J	541	SER	2.9
11	K	340	THR	2.9
10	J	598	ASP	2.9
10	J	227	ASN	2.9
10	J	218	LEU	2.9
10	J	156	THR	2.8

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Mol	Chain	Res	Type	RSRZ
11	K	280	VAL	2.8
10	J	102	LEU	2.8
9	I	198	GLY	2.8
11	K	405	LYS	2.8
11	K	320	ALA	2.8
10	J	779	SER	2.8
11	K	318	SER	2.8
10	J	963	VAL	2.8
6	F	143	TYR	2.8
10	J	415	GLN	2.8
9	I	158	VAL	2.8
10	J	111	VAL	2.8
10	J	624	PHE	2.8
11	K	401	PHE	2.8
10	J	221	TYR	2.8
6	F	80	PRO	2.8
11	K	288	LYS	2.8
10	J	419	THR	2.8
8	H	93	ARG	2.8
11	K	177	SER	2.8
11	K	344	TYR	2.8
10	J	72	LEU	2.8
10	J	383	SER	2.8
1	A	33	PHE	2.8
10	J	770	LEU	2.8
10	J	573	VAL	2.8
10	J	537	LYS	2.7
11	K	154	GLU	2.7
10	J	436	ILE	2.7
11	K	224	SER	2.7
10	J	400	TRP	2.7
10	J	717	ILE	2.7
10	J	630	LEU	2.7
10	J	812	CYS	2.7
10	J	631	ASP	2.7
11	K	275	HIS	2.7
2	B	25	PHE	2.7
9	I	70	LYS	2.7
11	K	302	ARG	2.7
7	G	190	LEU	2.7
11	K	282	THR	2.7
10	J	384	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
10	J	491	GLU	2.7
9	I	36	VAL	2.7
11	K	184	GLU	2.7
3	C	124	ILE	2.7
4	D	156	ILE	2.7
10	J	617	PRO	2.6
9	I	256	PHE	2.6
10	J	444	LEU	2.6
11	K	354	LEU	2.6
10	J	876	LYS	2.6
10	J	751	MET	2.6
10	J	374	ALA	2.6
9	I	17	ILE	2.6
5	E	28	PRO	2.6
5	E	244	LEU	2.6
10	J	68	PRO	2.6
2	B	1	MET	2.6
2	B	187	LEU	2.6
3	C	211	TYR	2.6
10	J	742	ILE	2.6
10	J	477	ALA	2.6
10	J	923	ASN	2.6
11	K	155	LYS	2.6
9	I	278	PRO	2.6
10	J	299	VAL	2.6
9	I	71	LYS	2.6
11	K	355	SER	2.6
9	I	72	THR	2.6
10	J	145	PHE	2.6
3	C	144	CYS	2.5
9	I	61	VAL	2.5
10	J	181	TYR	2.5
10	J	621	ARG	2.5
10	J	994	ARG	2.5
10	J	694	LEU	2.5
11	K	614	GLU	2.5
11	K	232	THR	2.5
1	A	192	ILE	2.5
11	K	356	LYS	2.5
11	K	409	LEU	2.5
10	J	95	VAL	2.5
1	A	132	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	14	PRO	2.5
8	H	276	SER	2.5
11	K	399	ARG	2.5
10	J	464	LEU	2.5
10	J	568	VAL	2.5
11	K	406	TYR	2.5
2	B	90	SER	2.5
10	J	209	VAL	2.5
10	J	954	ASP	2.5
10	J	760	SER	2.5
10	J	711	ASP	2.5
10	J	373	LEU	2.5
11	K	411	PRO	2.5
7	G	166	LEU	2.5
10	J	214	ILE	2.5
11	K	351	ILE	2.5
4	D	144	ASP	2.4
8	H	184	LEU	2.4
11	K	343	LYS	2.4
10	J	799	PRO	2.4
9	I	10	ILE	2.4
11	K	193	SER	2.4
11	K	404	SER	2.4
10	J	152	PHE	2.4
11	K	197	LEU	2.4
1	A	171	GLY	2.4
10	J	793	CYS	2.4
10	J	679	LYS	2.4
10	J	744	ASP	2.4
10	J	195	VAL	2.4
1	A	174	ILE	2.4
9	I	265	GLY	2.4
5	E	192	VAL	2.4
1	A	167	ILE	2.4
5	E	143	PHE	2.4
5	E	239	PHE	2.4
10	J	193	VAL	2.4
3	C	174	ALA	2.4
6	F	4	GLN	2.4
11	K	203	ILE	2.4
9	I	255	VAL	2.4
3	C	12	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
11	K	367	HIS	2.4
10	J	897	ALA	2.4
1	A	170	HIS	2.3
9	I	129	ALA	2.3
10	J	512	ALA	2.3
10	J	40	TYR	2.3
1	A	193	PRO	2.3
11	K	605	ASN	2.3
7	G	174	LEU	2.3
11	K	534	LEU	2.3
3	C	326	LEU	2.3
5	E	196	ASN	2.3
9	I	220	VAL	2.3
10	J	42	ARG	2.3
10	J	39	HIS	2.3
9	I	146	LEU	2.3
3	C	259	ILE	2.3
10	J	375	LYS	2.3
10	J	948	PRO	2.3
12	R	-31	U	2.3
10	J	637	VAL	2.3
10	J	71	ILE	2.3
10	J	305	LYS	2.3
10	J	518	ASP	2.3
10	J	22	LYS	2.3
3	C	253	SER	2.2
9	I	224	PHE	2.2
7	G	184	PHE	2.2
9	I	246	THR	2.2
7	G	136	CYS	2.2
10	J	203	GLU	2.2
2	B	108	PHE	2.2
11	K	190	GLN	2.2
11	K	297	ILE	2.2
9	I	223	CYS	2.2
10	J	716	GLU	2.2
10	J	539	ILE	2.2
5	E	85	GLN	2.2
4	D	39	ARG	2.2
11	K	360	ALA	2.2
11	K	296	ASN	2.2
6	F	93	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
8	H	151	LYS	2.2
3	C	209	TRP	2.2
10	J	490	VAL	2.2
10	J	612	LEU	2.2
11	K	246	SER	2.2
5	E	258	VAL	2.2
8	H	144	PRO	2.2
8	H	92	ASN	2.2
10	J	773	ARG	2.2
11	K	536	THR	2.2
6	F	188	VAL	2.2
3	C	13	HIS	2.2
3	C	147	GLU	2.1
4	D	186	PHE	2.1
2	B	21	GLU	2.1
1	A	112	VAL	2.1
9	I	153	VAL	2.1
1	A	118	LEU	2.1
2	B	214	LEU	2.1
10	J	59	VAL	2.1
4	D	103	GLU	2.1
8	H	193	LYS	2.1
2	B	96	ARG	2.1
3	C	75	LEU	2.1
11	K	321	ILE	2.1
2	B	136	MET	2.1
5	E	149	LEU	2.1
10	J	63	ALA	2.1
1	A	187	LEU	2.1
10	J	99	ILE	2.1
1	A	134	VAL	2.1
10	J	440	ARG	2.1
4	D	104	PHE	2.1
9	I	257	ALA	2.1
1	A	175	ILE	2.1
10	J	800	TYR	2.1
10	J	435	ARG	2.1
10	J	941	LEU	2.1
9	I	55	ALA	2.1
11	K	263	TYR	2.1
10	J	201	ASN	2.1
10	J	392	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	25	ILE	2.1
10	J	882	ARG	2.1
2	B	76	VAL	2.1
11	K	277	LEU	2.1
10	J	939	ILE	2.0
5	E	195	ASN	2.0
10	J	914	GLU	2.0
11	K	580	GLU	2.0
10	J	757	ALA	2.0
4	D	73	VAL	2.0
10	J	828	ASP	2.0
11	K	289	VAL	2.0
10	J	34	LYS	2.0
2	B	27	SER	2.0
10	J	676	ALA	2.0
11	K	403	TYR	2.0
1	A	4	ASP	2.0
5	E	-1	GLY	2.0
11	K	322	GLY	2.0
10	J	538	LEU	2.0
10	J	738	VAL	2.0
7	G	1	MET	2.0
11	K	236	ALA	2.0
9	I	108	VAL	2.0
10	J	960	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 carbohydrates 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
13	ZN	J	1101	1/1	0.73	0.04	298,298,298,298	0

6.5 Other polymers (i)

There are no such residues in this entry.