



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:08 AM UTC

PDB ID : 5C0X / pdb_00005c0x
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 types of validation reports are described at

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

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

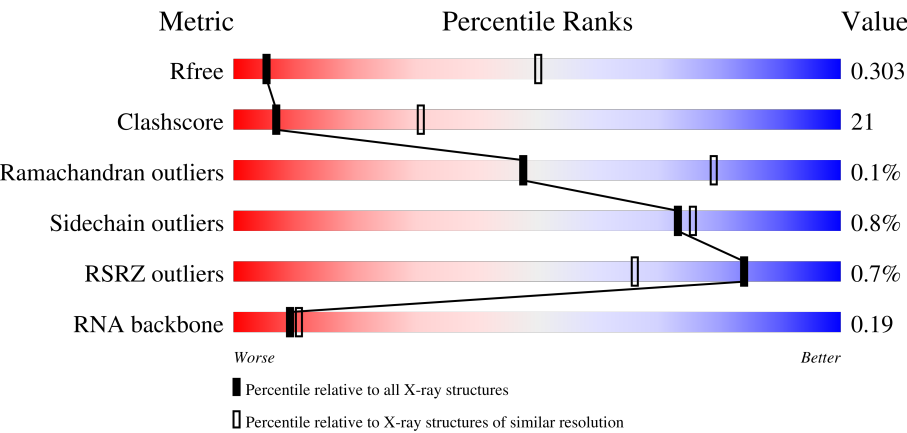
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance 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}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)
RNA backbone	3983	1009 (4.52-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	2% 76% 22%
2	B	248	2% 75% 23%
3	C	394	% 60% 25% 14%
4	D	245	73% 17% 9%

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Mol	Chain	Length	Quality of chain
5	E	267	2%79%21%
6	F	250	%63%22%•14%
7	G	243	60%36%••
8	H	361	51%30%•19%
9	I	295	%48%26%•25%
10	J	1003	68%26%•6%
11	K	695	43%7%50%
12	R	45	13%42%13%31%

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			

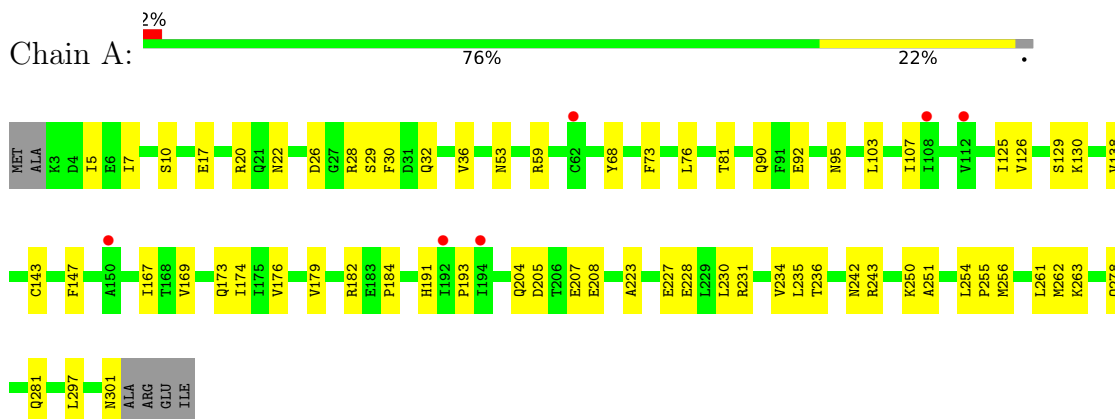
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

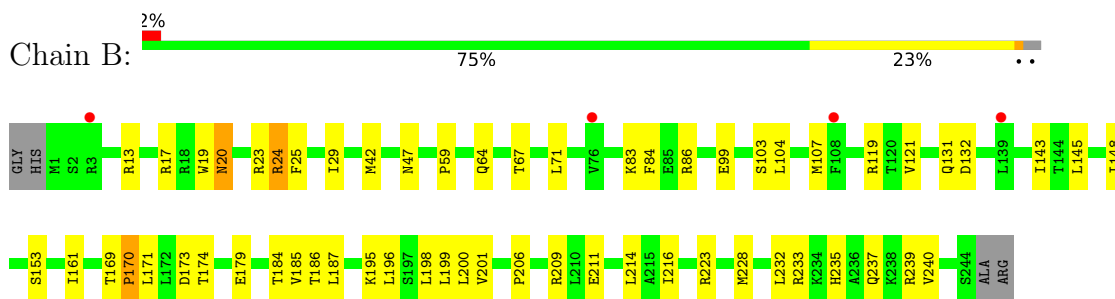
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

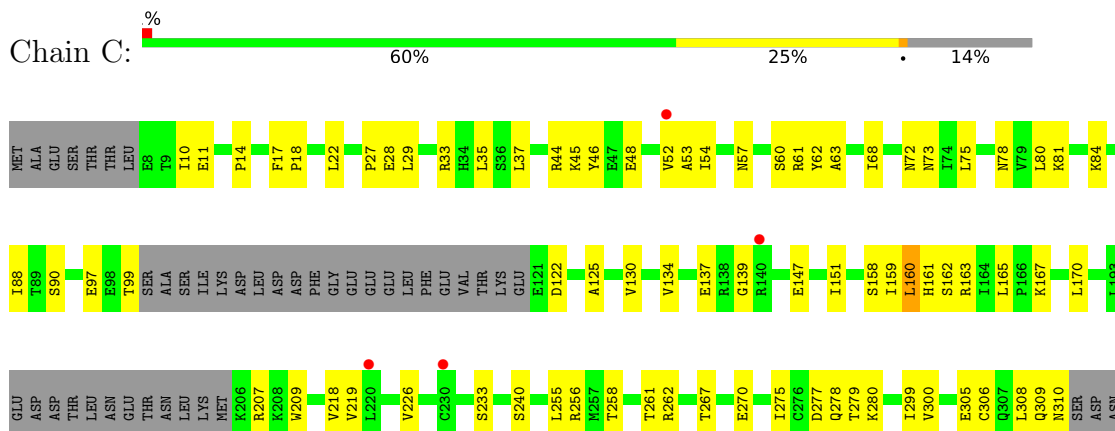
- Molecule 1: Exosome complex component RRP45



- Molecule 2: Exosome complex component SKI6



- Molecule 3: Exosome complex component RRP43





• Molecule 4: Exosome complex component RRP46

Chain D: 73% 17% 9%



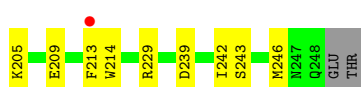
• Molecule 5: Exosome complex component RRP42

Chain E: 2% 79% 21%



• Molecule 6: Exosome complex component MTR3

Chain F: 63% 22% 14%



• Molecule 7: Exosome complex component RRP40

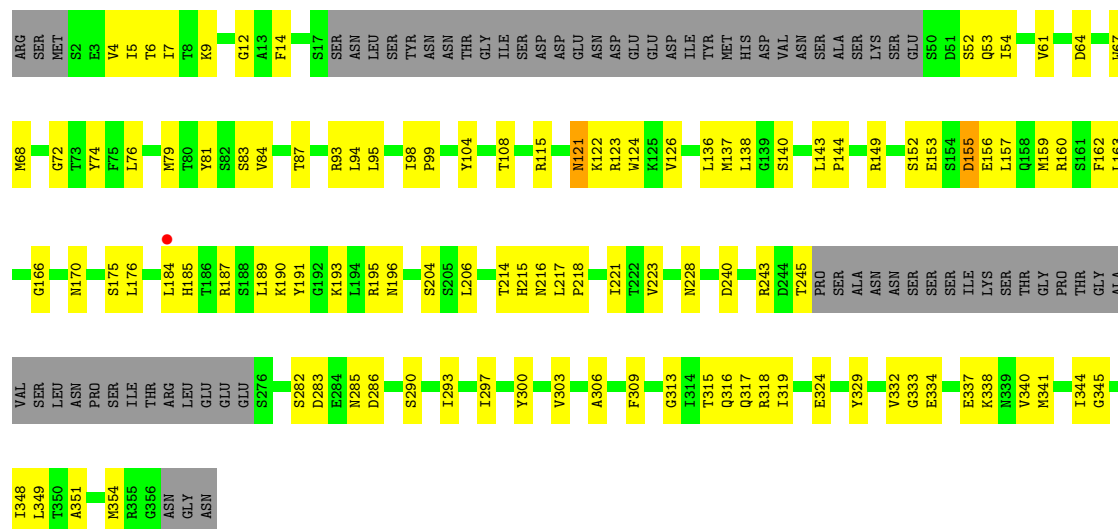
Chain G: 60% 36% 4%





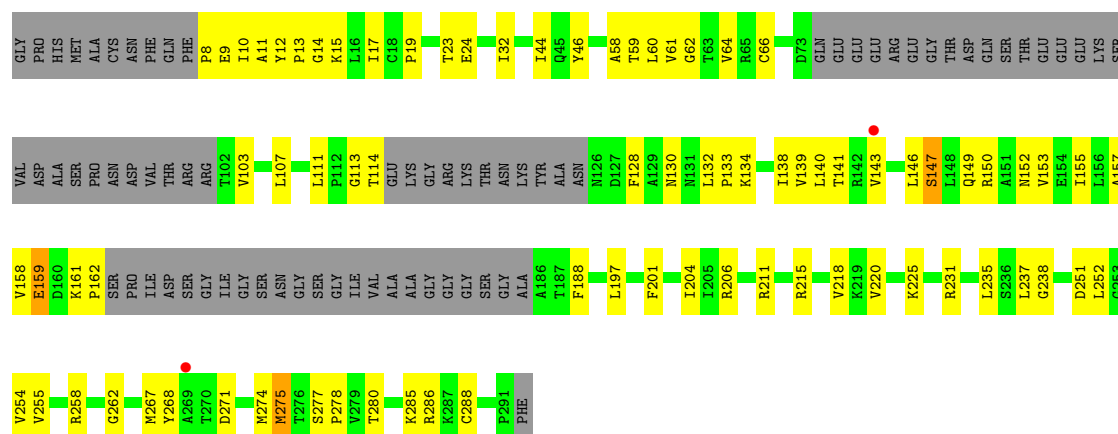
• Molecule 8: Exosome complex component RRP4

Chain H: 51% 30% 19%



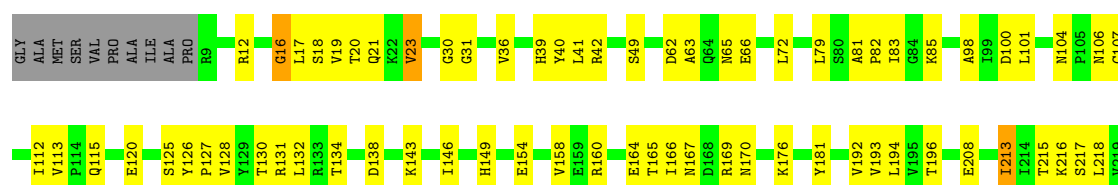
• Molecule 9: Exosome complex component CSL4

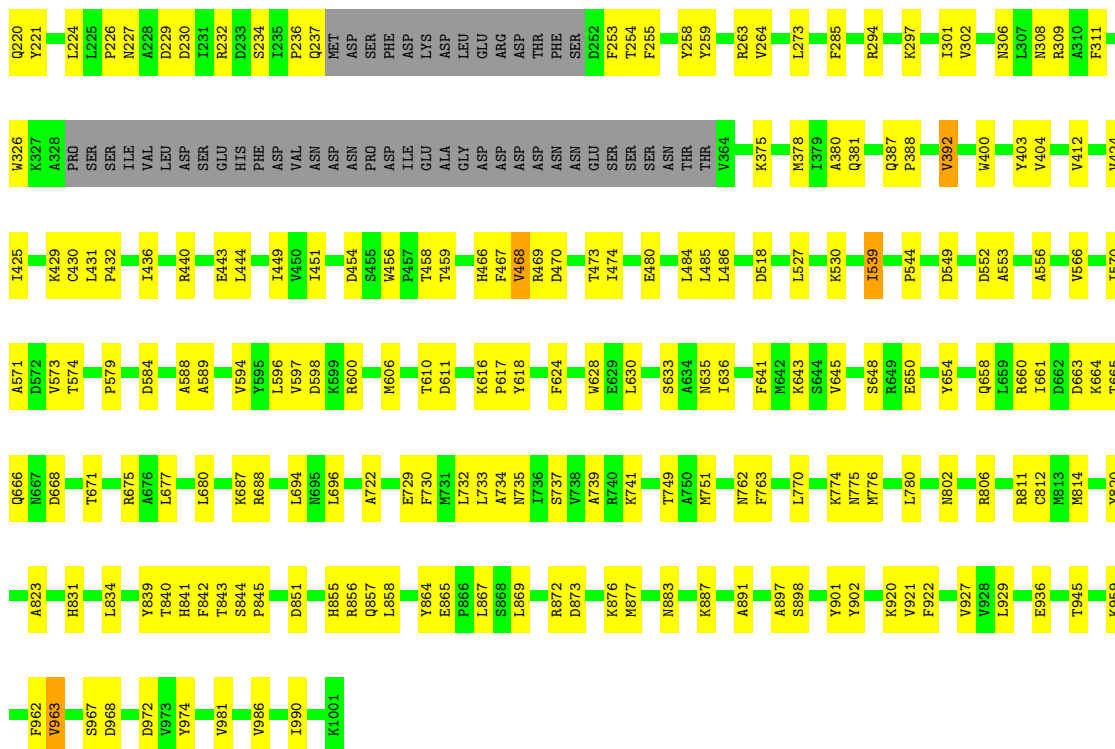
Chain I: 48% 26% 25%



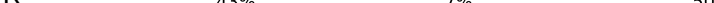
• Molecule 10: Exosome complex exonuclease DIS3

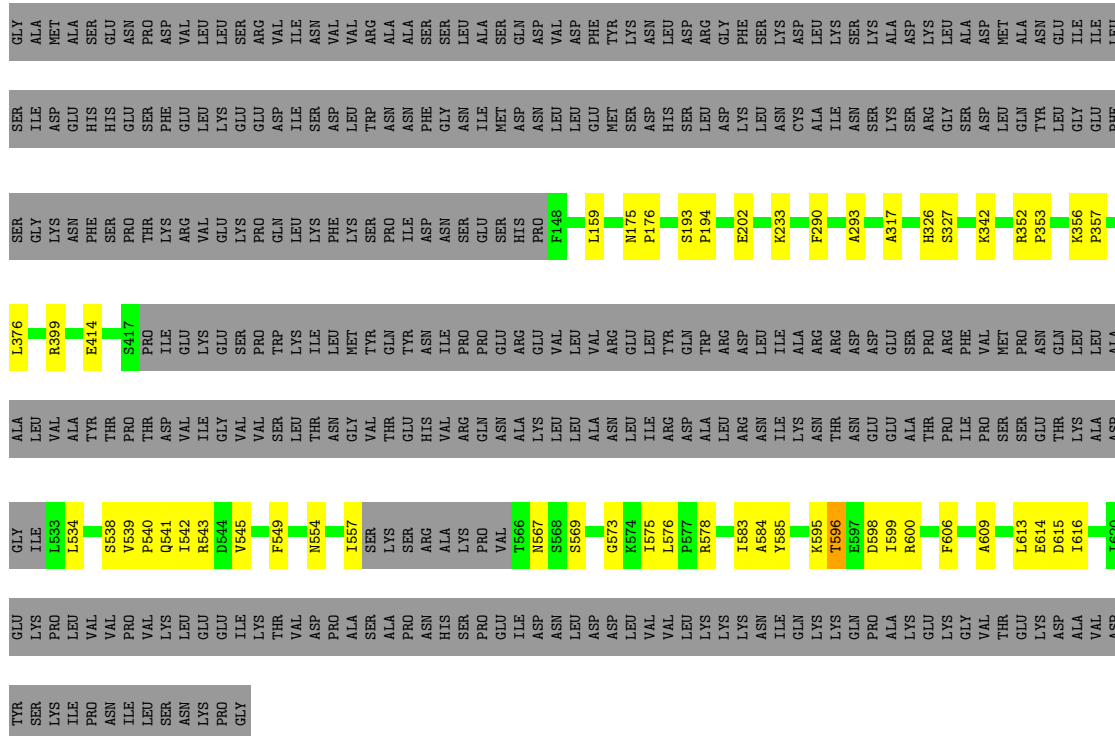
Chain J: 68% 26% 6%





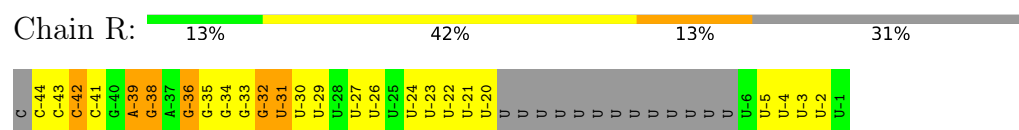
- Molecule 11: Exosome complex exonuclease RRP6

Chain K:  43% 7% 50%



- Molecule 12: RNA synthetic

Chain R:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.295 , 0.300 0.296 , 0.303	Depositor DCC
R_{free} test set	2292 reflections (4.08%)	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)	0.31 , 213.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.33	0/2340	0.70	0/3161
2	B	0.35	0/1910	0.75	3/2579 (0.1%)
3	C	0.34	0/2629	0.72	1/3569 (0.0%)
4	D	0.33	0/1722	0.75	2/2339 (0.1%)
5	E	0.33	0/2093	0.70	0/2849
6	F	0.32	0/1660	0.75	2/2241 (0.1%)
7	G	0.31	0/1828	0.84	7/2486 (0.3%)
8	H	0.31	0/2269	0.73	2/3066 (0.1%)
9	I	0.30	0/1676	0.77	3/2277 (0.1%)
10	J	0.35	0/7575	0.74	6/10290 (0.1%)
11	K	0.49	0/2001	1.05	9/2778 (0.3%)
12	R	0.38	0/615	0.68	0/951
All	All	0.35	0/28318	0.77	35/38586 (0.1%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	342	LYS	N-CA-C	9.23	121.42	111.36
11	K	615	ASP	N-CA-C	8.49	120.54	111.28
11	K	159	LEU	N-CA-C	-7.87	104.20	113.88
2	B	20	ASN	N-CA-C	6.81	121.30	112.92
2	B	24	ARG	N-CA-C	-6.71	100.24	110.30
10	J	468	VAL	N-CA-C	6.61	117.24	111.56
3	C	354	SER	N-CA-C	-6.46	105.12	112.87
6	F	85	GLY	N-CA-C	6.16	120.12	112.73
6	F	101	LEU	N-CA-C	6.14	118.06	111.36
11	K	616	ILE	N-CA-C	6.09	117.07	108.36
11	K	614	GLU	N-CA-C	5.82	117.62	111.28
11	K	596	THR	N-CA-C	-5.79	104.97	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	338	LYS	N-CA-C	5.70	117.49	111.28
7	G	152	ASP	CB-CA-C	-5.63	110.10	116.63
7	G	156	ILE	N-CA-C	5.57	116.13	108.12
2	B	174	THR	N-CA-C	5.55	117.90	110.35
11	K	576	LEU	CA-C-N	-5.52	116.08	121.65
11	K	576	LEU	C-N-CA	-5.52	116.08	121.65
7	G	11	PHE	CA-C-N	5.44	124.90	119.24
7	G	11	PHE	C-N-CA	5.44	124.90	119.24
8	H	121	ASN	CB-CA-C	-5.43	110.33	116.63
4	D	22	GLN	CB-CA-C	-5.40	110.37	116.63
9	I	147	SER	N-CA-C	-5.39	101.10	109.24
7	G	102	PHE	CA-C-N	5.33	124.97	119.05
7	G	102	PHE	C-N-CA	5.33	124.97	119.05
10	J	963	VAL	CA-C-N	5.21	125.21	119.89
10	J	963	VAL	C-N-CA	5.21	125.21	119.89
10	J	518	ASP	CA-C-N	5.14	124.58	119.24
10	J	518	ASP	C-N-CA	5.14	124.58	119.24
9	I	159	GLU	N-CA-C	5.13	117.48	110.55
7	G	222	ALA	N-CA-C	5.10	116.84	111.28
10	J	16	GLY	N-CA-C	-5.09	108.22	115.30
9	I	149	GLN	N-CA-C	5.07	116.81	111.28
11	K	233	LYS	N-CA-C	-5.04	107.17	113.72
4	D	140	LYS	N-CA-C	5.00	116.42	111.07

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	87	0
2	B	1886	0	1904	63	0
3	C	2589	0	2607	136	0
4	D	1701	0	1755	39	3
5	E	2050	0	2063	78	1
6	F	1638	0	1590	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1792	0	1747	136	1
8	H	2236	0	2215	160	4
9	I	1653	0	1616	146	0
10	J	7427	0	7352	291	0
11	K	1982	0	1255	46	2
12	R	557	0	281	43	1
13	J	1	0	0	0	0
All	All	27816	0	26650	1144	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 (1144) 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
10:J:467:PHE:CZ	10:J:469:ARG:C	2.04	1.33
5:E:257:ASP:CB	8:H:4:VAL:CG2	2.08	1.30
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
10:J:467:PHE:HZ	10:J:469:ARG:C	1.42	1.17
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
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
1:A:204:GLN:HG3	1:A:205:ASP:H	1.15	1.10
7:G:86:VAL:HG11	7:G:134:ILE:HD13	1.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:116:LEU:CD1	5:E:157:LEU:HD22	1.90	1.01
10:J:945:THR:OG1	10:J:963:VAL:O	1.78	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
1:A:90:GLN:NE2	7:G:91:PHE:HZ	1.62	0.97
5:E:116:LEU:CD1	5:E:157:LEU:HB2	1.95	0.97
6:F:41:GLU:OE2	6:F:229:ARG:NE	1.97	0.97
6:F:205:LYS:HE3	9:I:46:TYR:CE1	2.00	0.97
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
3:C:261:THR:HG22	3:C:262:ARG:N	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O5'	12:R:-42:C:H6	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:351:ALA:HA	8:H:354:MET:HE3	1.61	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
10:J:945:THR:OG1	10:J:963:VAL:C	2.24	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
9:I:23:THR:HG21	11:K:539:VAL:CG1	2.11	0.80
10:J:694:LEU:HD21	10:J:696:LEU:CG	2.11	0.80
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:C4'	12:R:-31:U:OP1	2.30	0.80
10:J:624:PHE:CZ	10:J:858:LEU:HD23	2.15	0.80
7:G:99:TYR:HA	7:G:102:PHE:HE2	1.46	0.79
7:G:136:CYS:O	7:G:147:PHE:CB	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:72:ASN:CG	6:F:102:LEU:HD22	2.09	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
3:C:72:ASN:CA	6:F:102:LEU:HD21	2.12	0.78
5:E:116:LEU:HD11	5:E:157:LEU:CG	2.12	0.78
12:R:-41:C:H6	12:R:-41:C:O5'	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
6:F:246:MET:HE3	9:I:10:ILE:CD1	2.14	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
7:G:95:VAL:HG13	7:G:132:ALA:C	2.10	0.76
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:246:MET:HE3	9:I:10:ILE:HD11	1.68	0.75
1:A:278:GLN:O	1:A:281:GLN:HG2	1.85	0.75
6:F:88:THR:OG1	6:F:132:LYS:HA	1.84	0.75
6:F:201:VAL:CG2	6:F:213:PHE:HD1	1.99	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
9:I:275:MET:HE3	9:I:288:CYS:SG	2.28	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
7:G:110:ARG:CD	12:R:-44:C:C5	2.71	0.74
9:I:267:MET:HG2	9:I:277:SER:HB2	1.70	0.74
6:F:201:VAL:HG22	6:F:213:PHE:HD1	1.45	0.74
2:B:23:ARG:O	2:B:24:ARG:C	2.26	0.73
3:C:72:ASN:OD1	6:F:102:LEU:CD2	2.34	0.73
10:J:610:THR:O	10:J:616:LYS:CE	2.36	0.73
8:H:83:SER:O	8:H:84:VAL:CG1	2.37	0.73
6:F:67:LEU:HG	6:F:68:GLY:N	2.04	0.73
6:F:205:LYS:HE3	9:I:46:TYR:CD1	2.22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:75:LEU:HD11	5:E:122:PHE:C	2.14	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
3:C:72:ASN:CG	6:F:102:LEU:CD2	2.61	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
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
10:J:945:THR:HG1	10:J:963:VAL:C	1.96	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
7:G:222:ALA:C	7:G:226:ILE:HG12	2.15	0.71
10:J:404:VAL:CG2	10:J:486:LEU:HD11	2.20	0.71
1:A:90:GLN:CD	7:G:91:PHE:HZ	1.98	0.71
4:D:136:ILE:HG21	4:D:194:LEU:HD11	1.73	0.71
10:J:12:ARG:HH12	10:J:154:GLU:CD	1.99	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
8:H:332:VAL:C	8:H:334:GLU:H	1.99	0.71
5:E:257:ASP:CG	8:H:4:VAL:CG2	2.63	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:262:MET:HE2	2:B:211:GLU:HB2	1.73	0.70
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
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
8:H:309:PHE:HB2	8:H:341:MET:HE1	1.73	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
5:E:9:SER:HB3	8:H:285:ASN:ND2	2.08	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
10:J:253:PHE:O	10:J:254:THR:CG2	2.40	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
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
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
8:H:315:THR:HG22	8:H:317:GLN:H	1.59	0.68
10:J:571:ALA:O	10:J:845:PRO:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:257:ASP:CG	8:H:4:VAL:HG21	2.15	0.67
8:H:215:HIS:HB3	8:H:316:GLN:CD	2.20	0.67
7:G:99:TYR:HA	7:G:102:PHE:CE2	2.29	0.67
9:I:254:VAL:HG12	9:I:275:MET:HE1	1.75	0.67
3:C:88:ILE:HB	3:C:218:VAL:HG22	1.74	0.67
10:J:484:LEU:HD11	10:J:897:ALA:C	2.20	0.67
7:G:214:CYS:HB3	7:G:223:PHE:CZ	2.31	0.66
8:H:115:ARG:C	8:H:126:VAL:HG23	2.20	0.66
10:J:72:LEU:HD11	10:J:146:ILE:HG23	1.77	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
6:F:188:VAL:O	9:I:14:GLY:HA2	1.95	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
6:F:95:ILE:H	6:F:118:MET:HE2	1.61	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:113:GLY:C	9:I:114:THR:HG23	2.22	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
7:G:152:ASP:CG	7:G:153:GLY:H	2.05	0.64
10:J:556:ALA:HB2	10:J:677:LEU:HD21	1.78	0.64
3:C:75:LEU:HD21	6:F:18:MET:HE1	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:H6	12:R:-43:C:O5'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:67:TRP:CZ3	8:H:93:ARG:C	2.76	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
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:467:PHE:HZ	10:J:470:ASP:N	1.94	0.62
10:J:556:ALA:HB2	10:J:677:LEU:CD2	2.30	0.62
3:C:61:ARG:NH2	6:F:20:PHE:CE1	2.67	0.62
5:E:75:LEU:CD1	5:E:122:PHE:O	2.45	0.62
5:E:257:ASP:OD2	8:H:4:VAL:CG2	2.47	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
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: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
7:G:99:TYR:C	7:G:102:PHE:HE2	2.08	0.62
10:J:259:TYR:CD2	10:J:263:ARG:NE	2.67	0.62
5:E:263:GLU:HG3	5:E:263:GLU:O	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
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
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
3:C:48:GLU:HG2	11:K:584:ALA:HB2	1.82	0.60
5:E:75:LEU:HD21	5:E:114:LEU:CB	2.31	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
9:I:254:VAL:CG1	9:I:275:MET:HE1	2.32	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
10:J:253:PHE:C	10:J:254:THR:HG23	2.26	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
8:H:83:SER:C	8:H:84:VAL:HG13	2.25	0.59
10:J:440:ARG:CG	10:J:443:GLU:CB	2.69	0.59
2:B:23:ARG:HE	2:B:173:ASP:CG	2.10	0.59
3:C:17:PHE:HZ	9:I:255:VAL:CG1	2.13	0.59
3:C:61:ARG:NH1	6:F:20:PHE:CE1	2.70	0.59
1:A:68:TYR:HE2	1:A:76:LEU:HD22	1.68	0.59
1:A:130:LYS:HD3	1:A:174:ILE:HG13	1.84	0.59
1:A:243:ARG:O	1:A:243:ARG:HG2	2.01	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:617:PRO:HA	10:J:648:SER:HB3	1.85	0.59
10:J:624:PHE:CE2	10:J:858:LEU:HD21	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:HA	3:C:99:THR:CG2	2.32	0.59
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
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
6:F:186:GLU:HA	9:I:59:THR:O	2.02	0.58
9:I:146:LEU:CD2	9:I:220:VAL:HG11	2.33	0.58
10:J:106:ASN:O	10:J:227:ASN:ND2	2.36	0.58
6:F:147:LEU:C	6:F:149:ASN:H	2.12	0.58
10:J:81:ALA:HB1	10:J:82:PRO:HA	1.84	0.58
10:J:100:ASP:HB3	10:J:468:VAL:HG13	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:HG2	10:J:440:ARG:O	2.03	0.57
6:F:187:LEU:O	9:I:59:THR:HA	2.04	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
3:C:387:ASP:OD2	11:K:585:TYR:OH	2.22	0.56
8:H:121:ASN:CG	8:H:122:LYS:H	2.13	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
10:J:527:LEU:HD11	10:J:865:GLU:CD	2.31	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:12:ARG:NH1	10:J:154:GLU:CD	2.61	0.56
10:J:125:SER:C	10:J:127:PRO:HD2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:539:ILE:HG23	10:J:553:ALA:HB1	1.89	0.55
6:F:148:THR:O	6:F:149:ASN:C	2.48	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
8:H:290:SER:HG	8:H:293:ILE:HG13	1.71	0.55
1:A:242:ASN:HB3	10:J:872:ARG:HH21	1.58	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
10:J:72:LEU:CD1	10:J:146:ILE:HG23	2.36	0.55
10:J:527:LEU:CD1	10:J:865:GLU:CD	2.80	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
1:A:90:GLN:CD	7:G:91:PHE:CZ	2.83	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:O	3:C:160:LEU:HD12	2.06	0.54
7:G:97:LEU:HD13	7:G:134:ILE:O	2.07	0.54
7:G:102:PHE:O	7:G:105:ALA:HB2	2.08	0.54
8:H:156:GLU:O	8:H:159:MET:HG3	2.07	0.54
10:J:217:SER:O	10:J:218:LEU:C	2.49	0.54
8:H:152:SER:HB3	8:H:155:ASP:CG	2.32	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
2:B:145:LEU:HG	2:B:228:MET:HE3	1.88	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
11:K:569:SER:HB3	11:K:573:GLY:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:GLU:O	6:F:104:LYS:HD2	2.07	0.54
7:G:5:ILE:HD11	7:G:36:PRO:HG3	1.88	0.54
9:I:12:TYR:CE2	9:I:15:LYS:HB2	2.43	0.54
9:I:139:VAL:HG12	9:I:140:LEU:N	2.23	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
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:349:ILE:HD13	3:C:378:LEU:HD23	1.90	0.53
3:C:350:LEU:HD12	3:C:359:GLN:CG	2.37	0.53
10:J:641:PHE:CE1	10:J:741:LYS:HB2	2.42	0.53
11:K:352:ARG:HA	11:K:353:PRO:C	2.34	0.53
2:B:83:LYS:HE3	2:B:131:GLN:CD	2.33	0.53
3:C:28:GLU:HG2	3:C:342:SER:HB3	1.89	0.53
5:E:192:VAL:HG22	5:E:197:MET:HE3	1.91	0.53
8:H:193:LYS:HE2	8:H:283:ASP:OD1	2.09	0.53
10:J:98:ALA:HB2	10:J:236:PRO:HG3	1.90	0.53
10:J:467:PHE:CE2	10:J:469:ARG:C	2.80	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
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
11:K:599:ILE:HG13	11:K:600:ARG:N	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:175:SER:C	8:H:176:LEU:HD12	2.34	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
9:I:161:LYS:O	9:I:162:PRO:C	2.52	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
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:28:ASP:OD2	7:G:35:ARG:NH1	2.43	0.52
7:G:237:VAL:O	7:G:237:VAL:HG22	2.10	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: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
10:J:480:GLU:HG3	10:J:901:TYR:CE1	2.45	0.51
10:J:530:LYS:HB2	10:J:864:TYR:CE1	2.45	0.51
7:G:156:ILE:CG1	7:G:208:TYR:CD2	2.91	0.51
1:A:5:ILE:HD11	1:A:90:GLN:CG	2.37	0.51
1:A:125:ILE:HG22	1:A:169:VAL:HG21	1.92	0.51
2:B:153:SER:HB3	8:H:83:SER:HG	1.74	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
7:G:99:TYR:C	7:G:102:PHE:CE2	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:103:VAL:CG2	11:K:534:LEU:HD12	2.29	0.50
10:J:375:LYS:HA	10:J:378:MET:HE2	1.91	0.50
10:J:573:VAL:HG21	10:J:845:PRO:HB2	1.92	0.50
10:J:628:TRP:CH2	10:J:734:ALA:HA	2.46	0.50
2:B:59:PRO:HG3	2:B:121:VAL:HG23	1.93	0.50
9:I:159:GLU:CD	9:I:231:ARG:HE	2.17	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:O	10:J:963:VAL:HG23	2.10	0.50
3:C:219:VAL:HG11	3:C:226:VAL:HG21	1.93	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
7:G:152:ASP:CG	7:G:153:GLY:N	2.65	0.50
8:H:126:VAL:CG1	8:H:184:LEU:HD12	2.39	0.50
9:I:285:LYS:C	9:I:286:ARG:HG2	2.37	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
5:E:197:MET:HE1	5:E:213:LEU:HD12	1.93	0.50
7:G:77:ILE:HD13	7:G:87:SER:HB2	1.93	0.50
9:I:197:LEU:HG	9:I:197:LEU:O	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:160:ARG:O	8:H:163:LEU:O	2.30	0.49
10:J:285:PHE:CE1	10:J:430:CYS:C	2.90	0.49
10:J:309:ARG:HD2	10:J:456:TRP:CG	2.46	0.49
10:J:668:ASP:OD1	10:J:668:ASP:O	2.30	0.49
6:F:41:GLU:CD	6:F:229:ARG:HE	2.12	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:628:TRP:CZ2	10:J:734:ALA:HA	2.47	0.49
10:J:663:ASP:HB2	10:J:665:THR:OG1	2.11	0.49
5:E:66:VAL:CG2	10:J:31:GLY:HA2	2.43	0.49
5:E:257:ASP:CG	8:H:4:VAL:HG23	2.36	0.49
3:C:387:ASP:CG	3:C:391:ARG:HH21	2.20	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
1:A:143:CYS:SG	1:A:147:PHE:CE2	3.05	0.49
3:C:350:LEU:CD1	3:C:359:GLN:HG2	2.38	0.49
9:I:146:LEU:HD22	9:I:220:VAL:CG1	2.29	0.49
3:C:57:ASN:HB2	3:C:240:SER:OG	2.13	0.49
3:C:255:LEU:HD11	10:J:294:ARG:NE	2.28	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:67:TRP:CE3	8:H:93:ARG:C	2.91	0.49
6:F:87:PHE:CE1	8:H:160:ARG:NH1	2.81	0.49
8:H:140:SER:HA	8:H:187:ARG:HD2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:33:PRO:HG3	8:H:337:GLU:CD	2.38	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
3:C:275:ILE:HG21	6:F:21:SER:HB3	1.95	0.48
10:J:98:ALA:HB2	10:J:236:PRO:CD	2.43	0.48
10:J:920:LYS:HB2	10:J:927:VAL:HB	1.96	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
8:H:332:VAL:C	8:H:334:GLU:N	2.62	0.48
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:37:LEU:HD12	11:K:606:PHE:HD1	1.79	0.47
3:C:384:ARG:NH1	11:K:583:ILE:HD11	2.29	0.47
6:F:246:MET:CE	9:I:10:ILE:CG1	2.89	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
8:H:162:PHE:CD2	8:H:163:LEU:HG	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:121:ASN:CG	8:H:122:LYS:N	2.71	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
7:G:114:GLN:O	7:G:115:VAL:C	2.58	0.47
10:J:774:LYS:HB3	10:J:776:MET:HE2	1.95	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
2:B:25:PHE:CZ	2:B:42:MET:HE1	2.49	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
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
11:K:542:ILE:O	11:K:545:VAL:HB	2.15	0.47
6:F:87:PHE:HE2	9:I:238:GLY:O	1.93	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
3:C:353:PRO:C	3:C:355:GLY:N	2.70	0.47
8:H:195:ARG:NE	8:H:282:SER:O	2.39	0.47
8:H:217:LEU:HD11	8:H:223:VAL:HG12	1.96	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
9:I:139:VAL:CG1	9:I:140:LEU:N	2.78	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:353:PRO:C	3:C:355:GLY:H	2.23	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
1:A:207:GLU:N	1:A:207:GLU:CD	2.73	0.46
8:H:64:ASP:OD2	8:H:93:ARG:NH1	2.47	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
10:J:845:PRO:HA	10:J:851:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:GLU:HG2	3:C:342:SER:CB	2.45	0.46
3:C:137:GLU:CD	6:F:140:TYR:CE1	2.93	0.46
3:C:280:LYS:NZ	3:C:280:LYS:HB3	2.30	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
10:J:285:PHE:HE1	10:J:430:CYS:C	2.24	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
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:75:LEU:HG	5:E:75:LEU:O	2.16	0.46
5:E:163:ASP:HA	5:E:167:GLU:HA	1.98	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:54:ILE:HB	3:C:78:ASN:HD21	1.81	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
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:663:ASP:O	10:J:664:LYS:CB	2.64	0.46
10:J:762:ASN:HD21	10:J:814:MET:HE3	1.80	0.46
2:B:84:PHE:O	5:E:63:LYS:NZ	2.38	0.45
3:C:73:ASN:H	6:F:102:LEU:HD11	1.81	0.45
5:E:86:ARG:HG2	5:E:88:ASP:H	1.81	0.45
10:J:473:THR:HG22	10:J:474:ILE:N	2.30	0.45
10:J:566:VAL:HG21	10:J:680:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:23:THR:CG2	9:I:24:GLU:N	2.79	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
8:H:67:TRP:HZ3	8:H:93:ARG:C	2.21	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
8:H:138:LEU:HD22	8:H:159:MET:SD	2.57	0.45
12:R:-42:C:O5'	12:R:-42:C:C6	2.54	0.45
12:R:-42:C:H2'	12:R:-41:C:C6	2.51	0.45
9:I:12:TYR:CZ	9:I:15:LYS:CB	2.93	0.45
10:J:98:ALA:HB2	10:J:236:PRO:HD3	1.99	0.45
10:J:229:ASP:HA	10:J:232:ARG:HE	1.80	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:52:PHE:CE2	6:F:61:LEU:HB2	2.52	0.45
6:F:201:VAL:HG21	6:F:213:PHE:CE1	2.51	0.45
10:J:224:LEU:HG	10:J:224:LEU:O	2.16	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
6:F:190:MET:HE3	9:I:13:PRO:HB2	1.98	0.45
10:J:311:PHE:CE2	10:J:431:LEU:CD2	2.99	0.45
10:J:387:GLN:HA	10:J:388:PRO:HD3	1.80	0.45
11:K:538:SER:HG	11:K:541:GLN:H	1.63	0.45
1:A:208:GLU:HA	8:H:76:LEU:CD2	2.46	0.45
5:E:75:LEU:CD2	5:E:114:LEU:HD12	2.46	0.45
8:H:79:MET:HB3	8:H:81:TYR:CE1	2.51	0.45
3:C:125:ALA:O	3:C:167:LYS:NZ	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:212:MET:HE3	7:G:212:MET:HB3	1.76	0.44
10:J:234:SER:C	10:J:466:HIS:CD2	2.95	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
7:G:236:THR:C	7:G:237:VAL:HG12	2.42	0.44
10:J:79:LEU:HD13	10:J:224:LEU:HG	1.98	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
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
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:68:MET:O	8:H:94:LEU:HD12	2.18	0.44
8:H:195:ARG:NH1	8:H:282:SER:N	2.65	0.44
8:H:216:ASN:OD1	8:H:243:ARG:NH1	2.50	0.44
9:I:150:ARG:HD2	9:I:204:ILE:HG23	1.99	0.44
3:C:97:GLU:HG2	3:C:209:TRP:CD1	2.52	0.44
3:C:134:VAL:HG11	3:C:151:ILE:CB	2.45	0.44
7:G:134:ILE:HG13	7:G:134:ILE:O	2.17	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
6:F:87:PHE:CZ	8:H:160:ARG:CZ	3.00	0.44
7:G:95:VAL:HG11	7:G:134:ILE:CG2	2.38	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:5:ILE:CG1	1:A:90:GLN:HG2	2.47	0.44
1:A:297:LEU:O	1:A:301:ASN:HB2	2.17	0.44
2:B:86:ARG:NH1	5:E:127:ASP:CG	2.76	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:351:ALA:HA	8:H:354:MET:HE2	1.98	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
11:K:326:HIS:O	11:K:327:SER:C	2.61	0.43
1:A:176:VAL:O	1:A:176:VAL:CG1	2.65	0.43
5:E:66:VAL:HG21	10:J:31:GLY:HA2	2.00	0.43
6:F:246:MET:HE1	9:I:10:ILE:HG13	1.97	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:112[B]:ILE:HD13	10:J:181:TYR:CD1	2.54	0.43
3:C:158:SER:OG	3:C:359:GLN:CD	2.58	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
10:J:921:VAL:C	10:J:922:PHE:CD1	2.97	0.43
9:I:19:PRO:HG3	11:K:549:PHE:HB2	2.01	0.42
9:I:32:ILE:HB	9:I:103:VAL:HG12	2.01	0.42
10:J:216:LYS:HD2	10:J:220:GLN:HG2	2.00	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
1:A:250:LYS:O	2:B:198:LEU:HA	2.18	0.42
2:B:23:ARG:CZ	2:B:173:ASP:OD1	2.67	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:157:ASP:C	7:G:158:VAL:HG13	2.45	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
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
6:F:246:MET:HE3	9:I:10:ILE:CG1	2.49	0.42
7:G:81:SER:OG	12:R:-31:U:OP2	2.23	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:75:LEU:HD11	6:F:18:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:J:751:MET:HE2	10:J:877:MET:HE1	2.02	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
8:H:189:LEU:HD12	8:H:189:LEU:C	2.45	0.42
10:J:570:ILE:HG22	10:J:845:PRO:HD3	2.02	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
5:E:250:MET:HE3	5:E:250:MET:HB2	1.98	0.41
10:J:62:ASP:O	10:J:63:ALA:C	2.63	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
1:A:242:ASN:HB3	10:J:872:ARG:HH22	1.66	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:98:ALA:HB2	10:J:236:PRO:CG	2.50	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
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
7:G:2:SER:OG	7:G:41:VAL:HG22	2.20	0.41
7:G:95:VAL:CG1	7:G:132:ALA:O	2.68	0.41
11:K:356:LYS:N	11:K:357:PRO:CD	2.83	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
3:C:61:ARG:NH1	6:F:20:PHE:CE2	2.89	0.41
3:C:134:VAL:O	3:C:134:VAL:HG13	2.21	0.41
10:J:85:LYS:HB2	10:J:85:LYS:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:174:LEU:O	7:G:177:VAL:HG22	2.20	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
10:J:19:VAL:HB	10:J:40:TYR:CD2	2.56	0.41
3:C:17:PHE:CZ	9:I:255:VAL:CG1	2.98	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
7:G:110:ARG:HD2	12:R:-44:C:N3	2.34	0.41
8:H:83:SER:C	8:H:84:VAL:CG1	2.91	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:17:ILE:HD11	9:I:58:ALA:HB2	2.03	0.40
9:I:152:ASN:OD1	9:I:204:ILE:HG12	2.22	0.40
10:J:20:THR:OG1	10:J:21:GLN:N	2.54	0.40
10:J:165:THR:HG22	10:J:166:ILE:N	2.36	0.40
1:A:263:LYS:HE2	1:A:263:LYS:HB3	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:53:ALA:CB	11:K:575:ILE:HD11	2.51	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
7:G:110:ARG:HB2	12:R:-44:C:N4	2.36	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
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:HD1	10:J:902:TYR:HA	1.81	0.40
11:K:399:ARG:CB	11:K:414:GLU:O	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/305 (97%)	290 (98%)	7 (2%)	0	100	100
2	B	242/248 (98%)	237 (98%)	4 (2%)	1 (0%)	30	63
3	C	332/394 (84%)	312 (94%)	19 (6%)	1 (0%)	36	68
4	D	222/245 (91%)	218 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	68
9	I	214/295 (72%)	208 (97%)	6 (3%)	0	100	100
10	J	939/1003 (94%)	899 (96%)	39 (4%)	1 (0%)	48	79
11	K	344/695 (50%)	330 (96%)	14 (4%)	0	100	100
All	All	3587/4306 (83%)	3445 (96%)	138 (4%)	4 (0%)	48	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	333	GLY
2	B	170	PRO
10	J	598	ASP
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%)	253 (99%)	2 (1%)	73	75
2	B	210/219 (96%)	210 (100%)	0	100	100
3	C	282/350 (81%)	280 (99%)	2 (1%)	76	77
4	D	196/216 (91%)	195 (100%)	1 (0%)	81	81
5	E	238/241 (99%)	235 (99%)	3 (1%)	61	71
6	F	181/219 (83%)	179 (99%)	2 (1%)	65	73
7	G	194/211 (92%)	194 (100%)	0	100	100
8	H	243/313 (78%)	241 (99%)	2 (1%)	73	75
9	I	174/242 (72%)	173 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	816/901 (91%)	806 (99%)	10 (1%)	63	71
11	K	81/636 (13%)	81 (100%)	0	100	100
All	All	2870/3814 (75%)	2847 (99%)	23 (1%)	73	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	234	VAL
3	C	160	LEU
3	C	362	LEU
4	D	177	VAL
5	E	109	VAL
5	E	178	VAL
5	E	222	ILE
6	F	61	LEU
6	F	83	ILE
8	H	155	ASP
8	H	221	ILE
9	I	275	MET
10	J	23	VAL
10	J	176	LYS
10	J	213	ILE
10	J	392	VAL
10	J	412	VAL
10	J	539	ILE
10	J	630	LEU
10	J	645	VAL
10	J	981	VAL
10	J	986	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	177	HIS
2	B	212	ASN
2	B	237	GLN
3	C	156	HIS
3	C	239	GLN

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Mol	Chain	Res	Type
3	C	278	GLN
4	D	86	GLN
4	D	183	ASN
5	E	183	ASN
6	F	49	HIS
6	F	70	GLN
6	F	122	ASN
6	F	206	ASN
6	F	247	ASN
7	G	218	ASN
10	J	167	ASN
10	J	771	ASN
10	J	855	HIS
10	J	883	ASN
10	J	909	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/305 (98%)	-0.36	6 (2%) 65 45	168, 206, 270, 304	0
2	B	244/248 (98%)	-0.38	4 (1%) 70 49	162, 209, 280, 314	0
3	C	339/394 (86%)	-0.49	4 (1%) 76 55	141, 234, 301, 333	1 (0%)
4	D	223/245 (91%)	-0.44	0 100 100	131, 206, 259, 300	1 (0%)
5	E	267/267 (100%)	-0.35	5 (1%) 66 46	135, 216, 267, 309	1 (0%)
6	F	215/250 (86%)	-0.35	3 (1%) 73 52	189, 221, 266, 308	0
7	G	237/243 (97%)	-0.44	0 100 100	167, 203, 253, 283	0
8	H	293/361 (81%)	-0.47	1 (0%) 90 78	175, 209, 263, 286	0
9	I	222/295 (75%)	-0.29	2 (0%) 81 61	205, 244, 291, 345	0
10	J	944/1003 (94%)	-0.51	0 100 100	190, 377, 429, 458	1 (0%)
11	K	350/695 (50%)	-0.48	0 100 100	227, 378, 404, 428	0
12	R	31/45 (68%)	-0.23	0 100 100	265, 295, 398, 401	0
All	All	3664/4351 (84%)	-0.43	25 (0%) 84 66	131, 242, 405, 458	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	VAL	5.0
5	E	145	ILE	3.7
5	E	244	LEU	3.6
2	B	76	VAL	3.0
1	A	194	ILE	2.8
2	B	139	LEU	2.8
3	C	230	CYS	2.8
8	H	184	LEU	2.8
9	I	143	VAL	2.8
6	F	213	PHE	2.7
3	C	52	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	243	LEU	2.6
1	A	192	ILE	2.5
5	E	193	VAL	2.4
1	A	108	ILE	2.4
1	A	62	CYS	2.3
1	A	150	ALA	2.2
2	B	3	ARG	2.2
5	E	149	LEU	2.1
3	C	220	LEU	2.1
9	I	269	ALA	2.1
2	B	108	PHE	2.1
6	F	80	PRO	2.1
6	F	137	ILE	2.0
3	C	140	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	J	1101	1/1	0.95	0.05	298,298,298,298	0

6.5 Other polymers [i](#)

There are no such residues in this entry.