WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:56 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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.
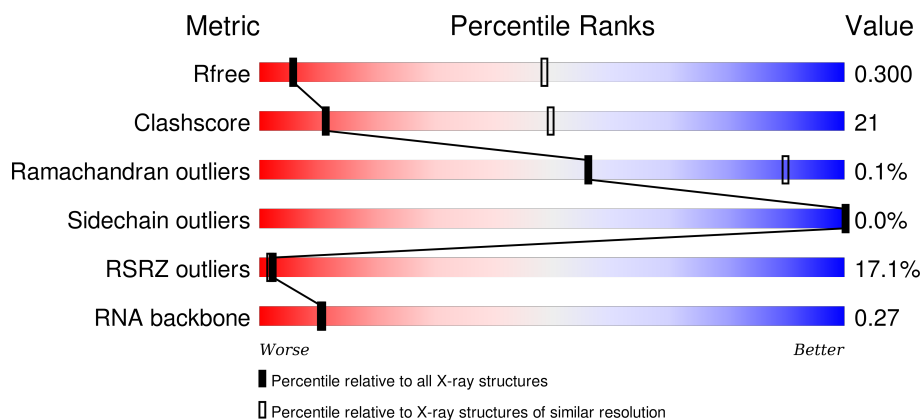
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1324 (4.14-3.50)
Clashscore	102246	1028 (4.12-3.52)
Ramachandran outliers	100387	1404 (4.14-3.50)
Sidechain outliers	100360	1399 (4.14-3.50)
RSRZ outliers	91569	1332 (4.14-3.50)
RNA backbone	2183	1071 (4.84-2.80)

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. 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%

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	267	7% / 81% / 19%
6	F	250	3% / 63% / 23% / 14%
7	G	243	3% / 61% / 36%
8	H	361	3% / 52% / 30% / 19%
9	I	295	14% / 49% / 26% / 25%
10	J	1003	27% / 69% / 25% / 6%
11	K	695	24% / 44% / 6% / 50%
12	R	45	27% / 13% / 42% / 13% / 31%

2 Entry composition (i)

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
			Total	C	N	O	S			
5	E	267	2050	1308	338	399	5	0	1	0

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
			Total	C	N	O	S			
6	F	215	1638	1023	273	332	10	0	0	0

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
			Total	C	N	O	S			
7	G	237	1792	1143	295	344	10	0	0	0

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
			Total	C	N	O	S			
8	H	293	2236	1393	403	428	12	0	0	0

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
			Total	C	N	O	S			
9	I	222	1653	1034	287	325	7	0	0	0

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 7427	C 4693	N 1304	O 1395	S 35	0	1	0

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 1982	C 1212	N 379	O 389	S 2	0	0	0

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 557	C 244	N 71	O 211	P 31	0	0	0

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

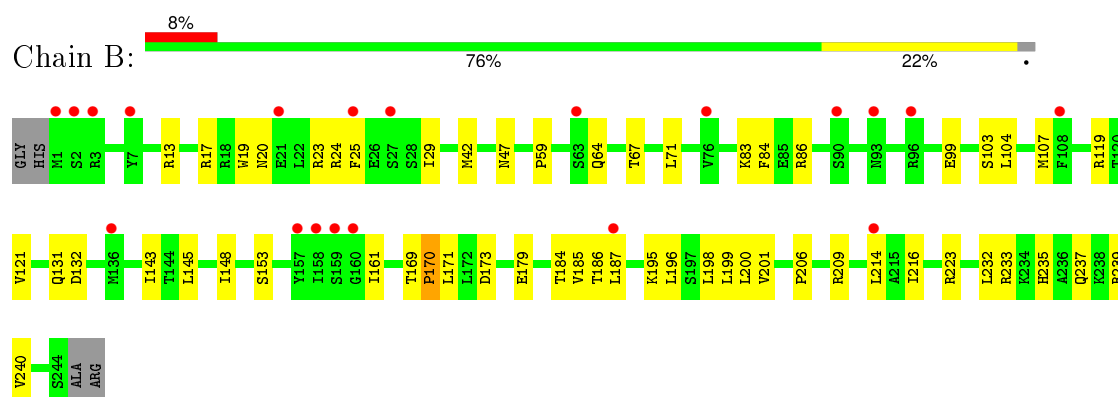| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total 1	Zn 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
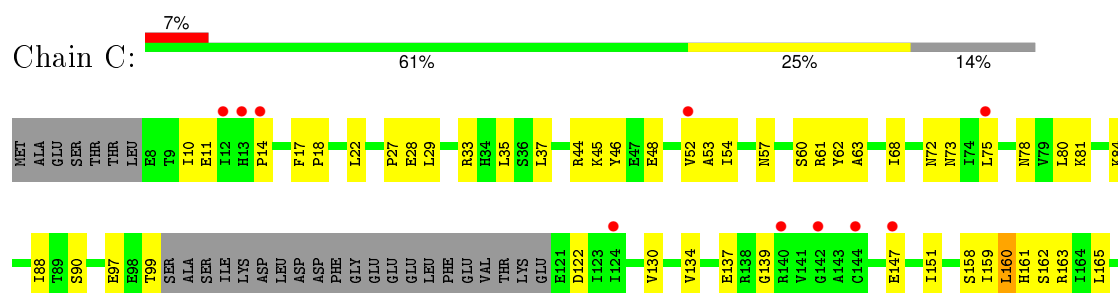
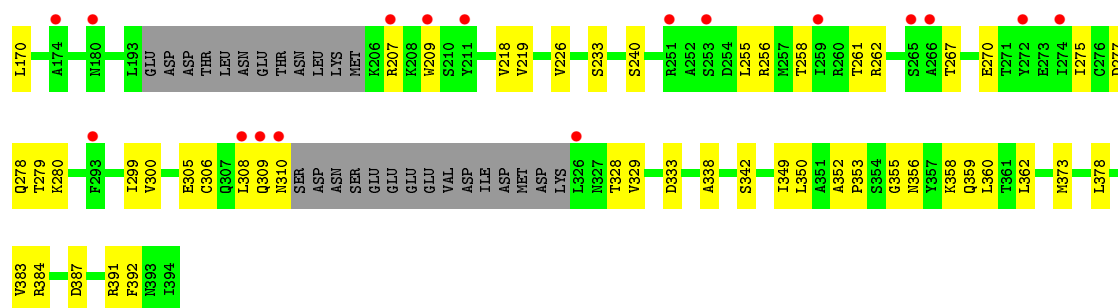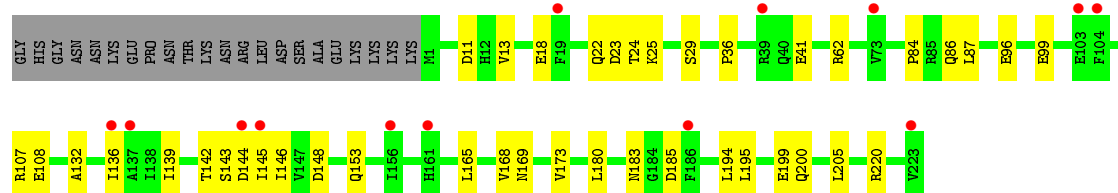- Molecule 1: Exosome complex component RRP45
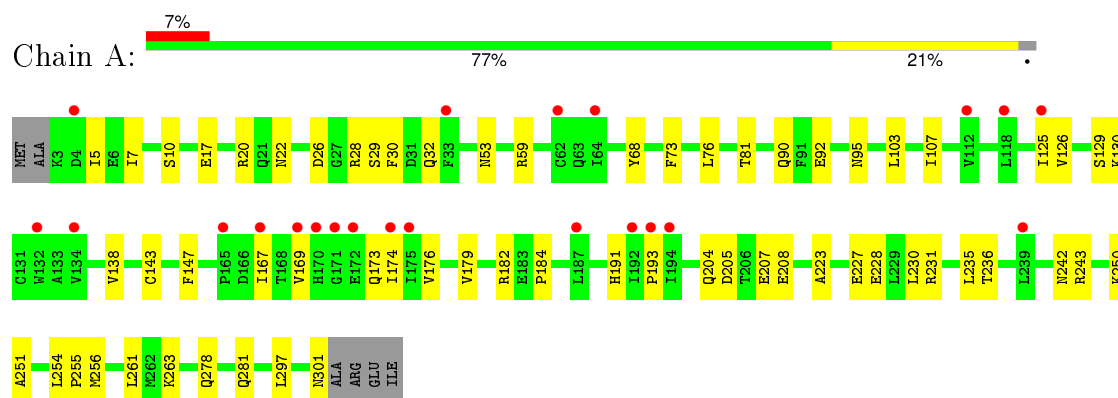
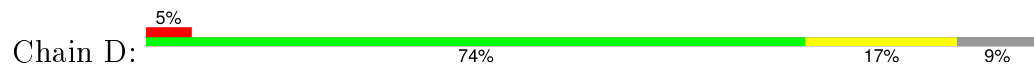- Molecule 2: Exosome complex component SKI6

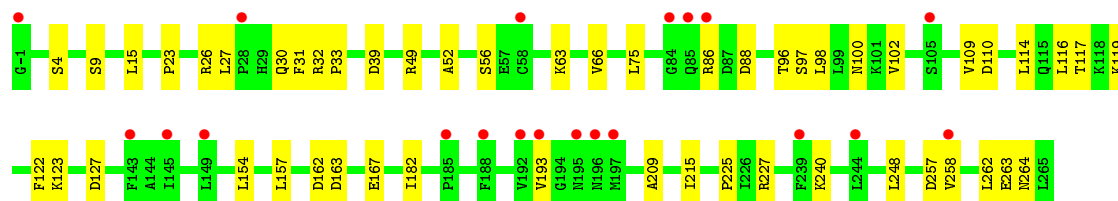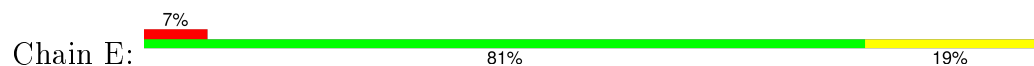- Molecule 3: Exosome complex component RRP43

L170 A174 N180 L193 GLU ASP ASP THR LEU ASN GLU THR ASN LEU LYS MET K206 R207 K208 W209 S210 Y211 V218 V219 V226 S233 S240 R251 A252 S253 D254 L255 R256 M257 T258 I259 R260 T261 R262 S265 A266 T267 E270 T271 Y272 E273 I274 I275 C276 D277

Q278 T279 K280 F293 I299 V300 E305 C306 Q307 L308 Q309 N310 SER ASP ASN SER GLU GLU GLU VAL ASP ILE ASP MET ASP LYS L326 N327 T328 V329 D333 A338 S342 I349 L350 A351 A352 P353 S354 G355 N356 Y357 K358 Q359 L360 T361 L362 M373 L378

V383 R384 D387 R391 F392 N393 I394

• **Molecule 4: Exosome complex component RRP46**

Chain D:

GLY HIS GLY ASN ASN LYS GLU PRO ASN THR LYS ASN ARG LEU ASP SER ALA GLU LYS LYS LYS M1 D11 H12 V13 E18 F19 Q22 D23 T24 K25 S29 P36 R39 Q40 E41 R62 V73 P84 R85 Q86 L87 E96 E99 E103 F104

R107 E108 A132 I136 A137 I138 I139 T142 S143 D144 I145 I146 V147 D148 Q153 I156 H161 L165 V168 N169 V173 L180 M183 G184 D185 F186 L194 L195 E199 Q200 L205 R220 V223

• **Molecule 5: Exosome complex component RRP42**

Chain E:

G-1 S4 S9 L15 P23 R26 L27 P28 H29 Q30 F31 R32 P33 D39 R49 A52 S56 E57 C58 K63 V66 L75 G84 Q85 R86 D87 D88 T96 S97 L98 L99 N100 K101 V102 S105 V109 D110 L114 Q115 L116 T117 K118 K119

F122 K123 D127 F143 A144 I145 I149 L154 L157 D162 D163 E167 I182 P185 F188 V192 V193 G194 N195 N196 M197 A209 I215 P225 I226 R227 F239 K240 I244 L248 D257 V258 E262 E263 N264 L265

• **Molecule 6: Exosome complex component MTR3**

Chain F:

MET ASN VAL Q4 K16 P17 M18 A19 F20 S21 N22 T23 THR THR HIS VAL PRO GLU LYS LYS SER THR ASP LEU THR PRO LYS GLY ASN E41 S47 F52 I53 E54 N55 C56 L61 L67 G68 I74 Y78 G79 P80 R81 S82 I83 R84 G85 S86 F87 T88 I93

S94 I95 Q96 L97 L101 L102 E103 K104 N108 E112 M118 V124 L127 K132 I137 F138 V139 Y140 Y143 D144 K145 D146 L147 T148 N149 ASN PRO GLN ASP ASP ASP SER GLN SER LYS MET THR SER S163 I176 E186 L187 V188 D189 M190 V200 V201

K205 E209 F213 W214 R229 D239 I242 S243 M246 N247 Q248 GLU THR

• **Molecule 7: Exosome complex component RRP40**

Chain G:

• Molecule 8: Exosome complex component RRP4

Chain H:

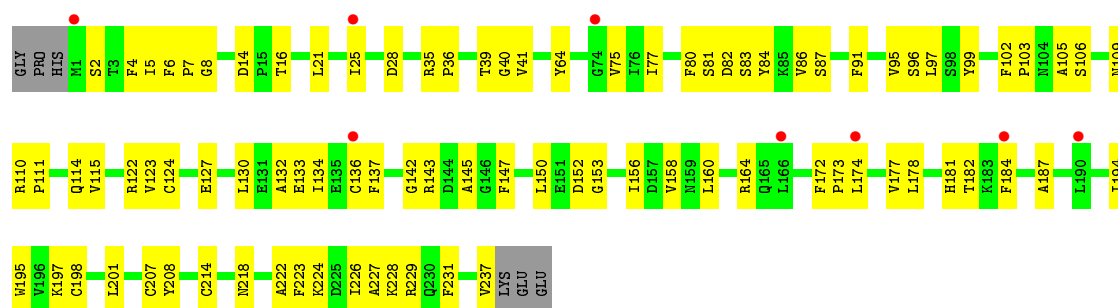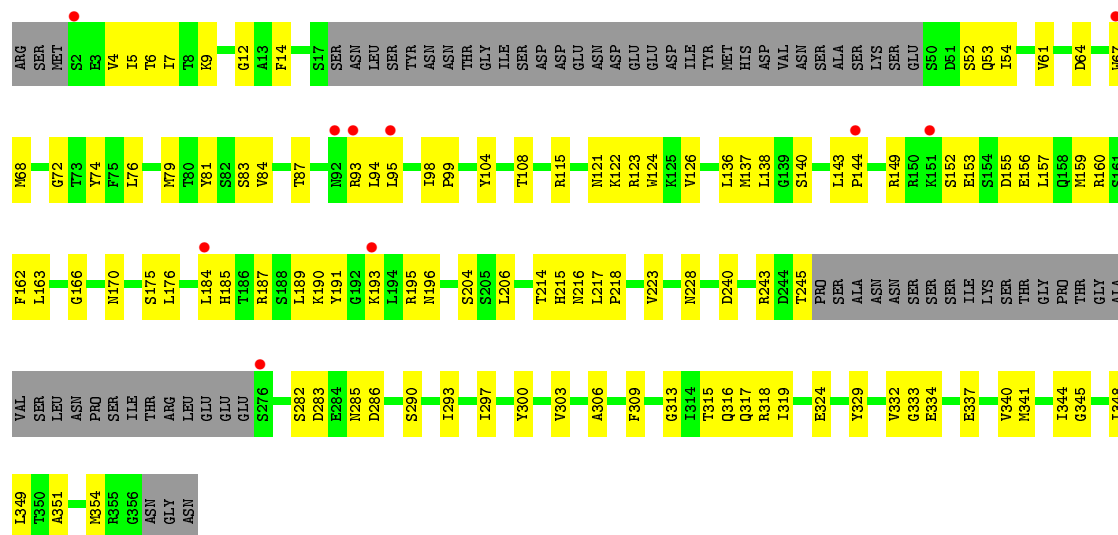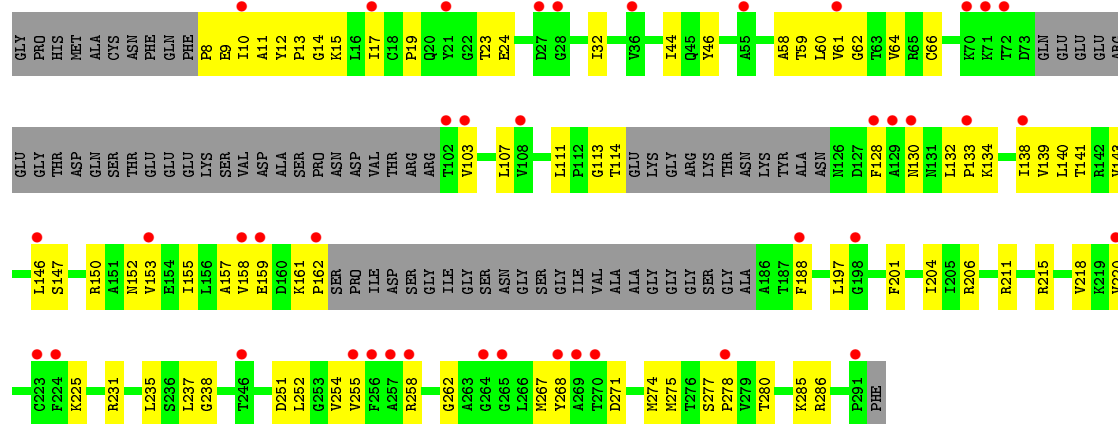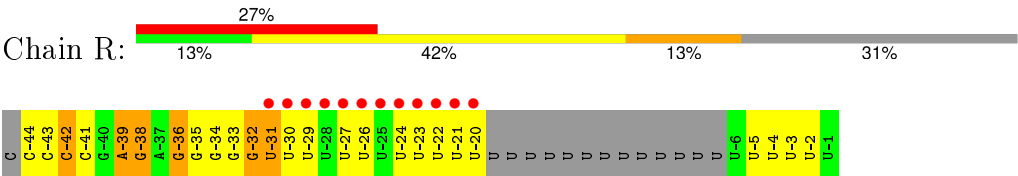• Molecule 9: Exosome complex component CSL4

Chain I:

• Molecule 10: Exosome complex exonuclease DIS3

Chain J:

• Molecule 11: Exosome complex exonuclease RRP6

Chain K:
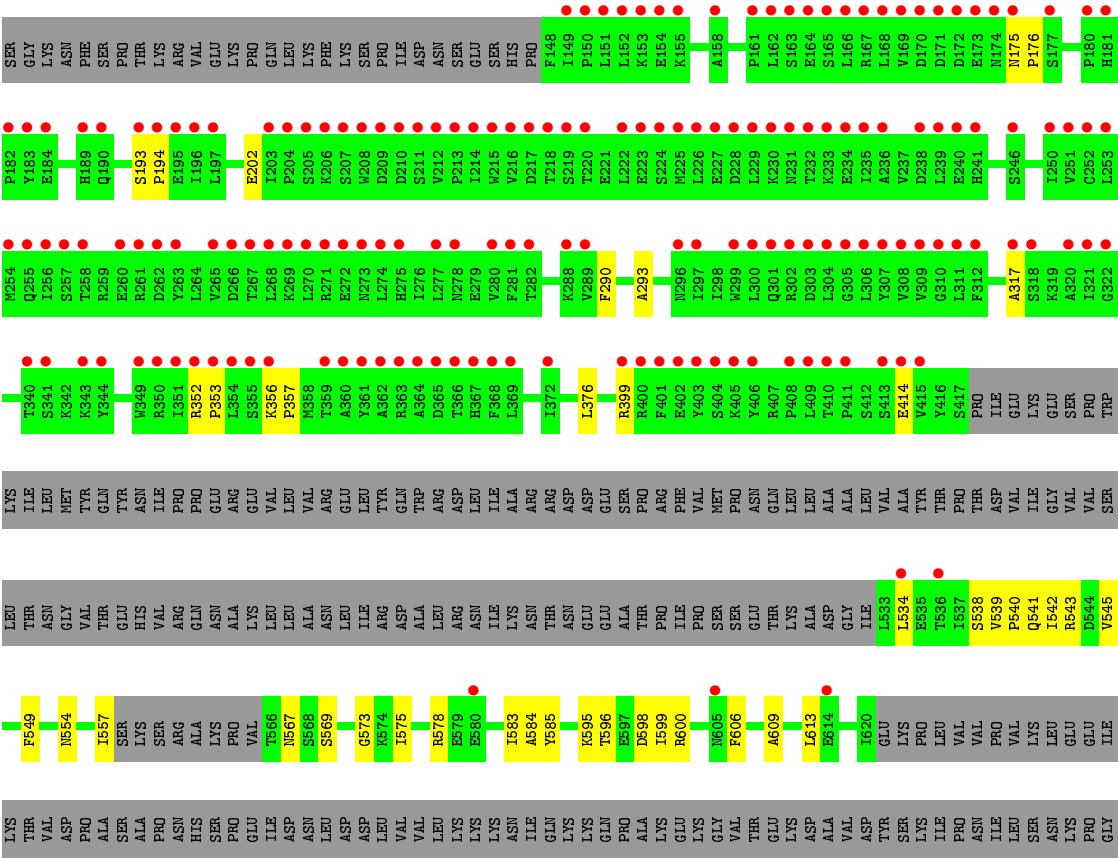
• Molecule 12: RNA synthetic

Chain R:

27%

13%   42%   13%   31%

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	2286 reflections (5.00%)	DCC
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 , 182.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.22$	Xtriage
Outliers	0 of 45806 reflections	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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 (i)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:467:PHE:HZ	10:J:469:ARG:C	1.42	1.12
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
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
5:E:116:LEU:HD11	5:E:157:LEU:CB	1.79	1.09
3:C:57:ASN:OD1	3:C:60:SER:HB3	1.52	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
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
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
1:A:90:GLN:NE2	7:G:91:PHE:HZ	1.62	0.97
6:F:41:GLU:OE2	6:F:229:ARG:NE	1.97	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
10:J:449:ILE:HB	10:J:467:PHE:HE1	1.28	0.90
9:I:139:VAL:HG13	9:I:157:ALA:O	1.71	0.90
12:R:-32:G:O2'	12:R:-31:U:C5	2.24	0.90
3:C:299:ILE:CG2	3:C:328:THR:HG23	2.02	0.90
3:C:88:ILE:HB	3:C:218:VAL:CG2	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
12:R:-33:G:H2'	12:R:-32:G:H5"	1.56	0.88
6:F:187:LEU:HB2	9:I:13:PRO:HB3	1.55	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
10:J:694:LEU:HD21	10:J:696:LEU:HG	1.58	0.86
7:G:102:PHE:HB3	7:G:103:PRO:HD2	1.53	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
10:J:425:ILE:HG21	10:J:990:ILE:O	1.76	0.84
5:E:66:VAL:HG21	10:J:30:GLY:O	1.77	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
9:I:225:LYS:HG3	9:I:286:ARG:CZ	2.08	0.83
4:D:144:ASP:OD1	4:D:145:ILE:N	2.12	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
10:J:236:PRO:HA	10:J:466:HIS:ND1	1.94	0.82
7:G:110:ARG:CD	12:R:-44:C:C4	2.62	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
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
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

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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
9:I:128:PHE:HE2	9:I:158:VAL:HG23	1.46	0.79
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
5:E:97:SER:HB2	6:F:108:ASN:HB3	1.62	0.79
8:H:315:THR:CB	8:H:318:ARG:HG3	2.09	0.79
5:E:116:LEU:HD11	5:E:157:LEU:CD2	2.12	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
9:I:143:VAL:HA	9:I:153:VAL:HG12	1.66	0.77
8:H:72:GLY:O	8:H:83:SER:N	2.13	0.77
2:B:233:ARG:O	2:B:237:GLN:HG2	1.84	0.77
9:I:132:LEU:HD12	9:I:133:PRO:CD	2.15	0.77
7:G:227:ALA:O	7:G:231:PHE:CD2	2.37	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
9:I:13:PRO:HD3	9:I:61:VAL:HG22	1.66	0.76
7:G:214:CYS:SG	7:G:223:PHE:CG	2.78	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
12:R:-31:U:OP1	12:R:-31:U:H4'	1.86	0.76
9:I:277:SER:HB3	9:I:280:THR:OG1	1.83	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)
10:J:945:THR:OG1	10:J:963:VAL:C	2.24	0.76
9:I:271:ASP:HB2	9:I:274:MET:HB2	1.67	0.76
11:K:554:ASN:O	11:K:557:ILE:HG22	1.85	0.76
10:J:126:TYR:N	10:J:127:PRO:HD2	2.01	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
10:J:253:PHE:O	10:J:254:THR:HG23	1.84	0.76
10:J:194:LEU:HB3	10:J:215:THR:HG22	1.66	0.76
5:E:119:LYS:HB3	5:E:163:ASP:OD2	1.86	0.76
1:A:278:GLN:O	1:A:281:GLN:HG2	1.85	0.75
8:H:309:PHE:HB3	8:H:341:MET:HE2	1.67	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
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
7:G:95:VAL:HG22	7:G:132:ALA:HB3	1.67	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
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
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
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
8:H:152:SER:HB3	8:H:155:ASP:OD2	1.88	0.73
6:F:67:LEU:HG	6:F:68:GLY:N	2.04	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
11:K:538:SER:OG	11:K:541:GLN:CG	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:258:TYR:CZ	10:J:309:ARG:NH2	2.56	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
12:R:-32:G:O2'	12:R:-31:U:H5	1.68	0.73
10:J:635:ASN:OD1	10:J:687:LYS:NZ	2.20	0.73
10:J:811:ARG:NH2	10:J:936:GLU:OE2	2.22	0.72
12:R:-36:G:H2'	12:R:-35:G:C8	2.23	0.72
10:J:589:ALA:O	10:J:887:LYS:HD2	1.90	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
7:G:95:VAL:CG1	7:G:134:ILE:HG23	2.20	0.72
2:B:83:LYS:HE3	2:B:131:GLN:OE1	1.90	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
12:R:-43:C:H2'	12:R:-42:C:C6	2.24	0.71
8:H:216:ASN:HD21	8:H:240:ASP:HB3	1.54	0.71
10:J:624:PHE:HZ	10:J:858:LEU:HG	1.54	0.71
8:H:160:ARG:HA	8:H:163:LEU:O	1.90	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
10:J:945:THR:HB	10:J:962:PHE:CD1	2.25	0.71
4:D:136:ILE:HG21	4:D:194:LEU:HD11	1.73	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
10:J:594:VAL:HG12	10:J:891:ALA:HA	1.73	0.70
8:H:215:HIS:HB3	8:H:316:GLN:NE2	2.06	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
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
4:D:195:LEU:O	4:D:199:GLU:HG3	1.92	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
10:J:253:PHE:O	10:J:254:THR:CG2	2.40	0.69
2:B:23:ARG:O	2:B:24:ARG:C	2.26	0.69
11:K:569:SER:CB	11:K:573:GLY:HA3	2.22	0.69
10:J:72:LEU:CD1	10:J:146:ILE:HG21	2.23	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
3:C:72:ASN:CG	6:F:102:LEU:CD2	2.61	0.69
3:C:61:ARG:HG3	3:C:62:TYR:CD2	2.28	0.69
2:B:148:ILE:HG21	2:B:232:LEU:HD21	1.73	0.69
9:I:132:LEU:CD1	9:I:133:PRO:HD2	2.21	0.69
8:H:315:THR:HB	8:H:318:ARG:CG	2.15	0.69
10:J:449:ILE:HB	10:J:467:PHE:CD1	2.26	0.68
3:C:299:ILE:HG23	3:C:328:THR:CG2	2.23	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
9:I:60:LEU:HD11	9:I:130:ASN:OD1	1.93	0.68
6:F:246:MET:HE1	9:I:10:ILE:CG1	2.24	0.68
8:H:149:ARG:HH12	8:H:152:SER:HB3	1.58	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
9:I:11:ALA:CB	9:I:62:GLY:O	2.37	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
6:F:187:LEU:HB2	9:I:13:PRO:CB	2.23	0.68
2:B:19:TRP:CZ3	2:B:216:ILE:HD12	2.28	0.68
8:H:315:THR:HG22	8:H:317:GLN:H	1.59	0.68
11:K:539:VAL:HB	11:K:540:PRO:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:LEU:HD11	5:E:122:PHE:C	2.14	0.68
10:J:571:ALA:O	10:J:845:PRO:HG3	1.93	0.68
7:G:97:LEU:HB2	7:G:134:ILE:HG13	1.77	0.67
10:J:633:SER:HB3	10:J:635:ASN:HD21	1.59	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
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
7:G:97:LEU:HB2	7:G:134:ILE:CG1	2.25	0.67
4:D:142:THR:HG22	4:D:144:ASP:HB2	1.76	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
10:J:574:THR:CG2	10:J:856:ARG:HG2	2.26	0.66
8:H:332:VAL:C	8:H:334:GLU:H	1.99	0.66
1:A:90:GLN:CD	7:G:91:PHE:HZ	1.98	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
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
11:K:596:THR:O	11:K:599:ILE:HG12	1.96	0.66
10:J:255:PHE:HB2	10:J:458:THR:HA	1.78	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
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
5:E:26:ARG:NH1	5:E:32:ARG:HG3	2.11	0.65
8:H:309:PHE:CB	8:H:341:MET:CE	2.73	0.65
2:B:17:ARG:HH12	2:B:173:ASP:HB3	1.61	0.65
1:A:167:ILE:HD11	1:A:176:VAL:HG23	1.79	0.65
8:H:126:VAL:HG11	8:H:184:LEU:HD12	1.77	0.65
9:I:128:PHE:CE2	9:I:158:VAL:HG23	2.30	0.65
9:I:141:THR:HG22	9:I:155:ILE:CA	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ARG:HD2	3:C:62:TYR:CZ	2.31	0.65
10:J:115:GLN:HB2	10:J:149:HIS:HA	1.78	0.65
7:G:7:PRO:HD3	7:G:39:THR:HG22	1.77	0.65
6:F:67:LEU:HG	6:F:68:GLY:H	1.60	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
7:G:227:ALA:O	7:G:231:PHE:HD2	1.77	0.65
3:C:391:ARG:HD2	3:C:392:PHE:CZ	2.32	0.65
1:A:68:TYR:CE2	1:A:76:LEU:HD22	2.32	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
10:J:440:ARG:HG3	10:J:443:GLU:HB2	1.77	0.64
3:C:255:LEU:HD12	3:C:256:ARG:N	2.12	0.64
5:E:264:ASN:HB3	8:H:9:LYS:HE3	1.80	0.64
8:H:140:SER:O	8:H:187:ARG:CD	2.45	0.64
6:F:188:VAL:CG1	9:I:44:ILE:HD13	2.26	0.64
6:F:93:ILE:HD11	6:F:127:LEU:HD21	1.79	0.64
5:E:109:VAL:HG13	5:E:182:ILE:HD11	1.80	0.64
1:A:26:ASP:OD2	1:A:28:ARG:NE	2.29	0.64
1:A:22:ASN:ND2	1:A:30:PHE:HE2	1.95	0.64
11:K:538:SER:HB2	11:K:540:PRO:HD2	1.79	0.64
3:C:352:ALA:O	3:C:355:GLY:N	2.29	0.64
1:A:5:ILE:CD1	1:A:90:GLN:HG2	2.28	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
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.79	0.64
9:I:141:THR:OG1	9:I:153:VAL:HG21	1.98	0.64
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
2:B:13:ARG:HD3	2:B:171:LEU:HD22	1.78	0.63
10:J:285:PHE:CZ	10:J:430:CYS:HA	2.33	0.63
12:R:-43:C:O5'	12:R:-43:C:H6	1.80	0.63
8:H:149:ARG:NH1	8:H:155:ASP:OD1	2.31	0.63
10:J:467:PHE:HZ	10:J:470:ASP:N	1.94	0.63
7:G:123:VAL:HG22	7:G:134:ILE:HG22	1.81	0.63
5:E:116:LEU:CD1	5:E:157:LEU:CD2	2.69	0.63
2:B:64:GLN:O	2:B:64:GLN:HG3	1.99	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: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
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
8:H:108:THR:HB	8:H:176:LEU:HD13	1.81	0.62
10:J:762:ASN:HB3	10:J:812:CYS:HB2	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:945:THR:HG1	10:J:963:VAL:C	2.01	0.62
6:F:87:PHE:CZ	8:H:160:ARG:NE	2.67	0.62
5:E:257:ASP:CG	8:H:4:VAL:HG21	2.15	0.62
12:R:-39:A:O2'	12:R:-38:G:O5'	2.18	0.62
10:J:921:VAL:O	10:J:922:PHE:CD1	2.53	0.62
10:J:484:LEU:HD11	10:J:897:ALA:C	2.20	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
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:263:GLU:O	5:E:263:GLU:HG3	1.99	0.62
5:E:33:PRO:HG3	8:H:337:GLU:OE2	1.98	0.62
8:H:215:HIS:HB3	8:H:316:GLN:CD	2.20	0.62
8:H:115:ARG:C	8:H:126:VAL:HG23	2.20	0.62
10:J:449:ILE:CB	10:J:467:PHE:CE1	2.75	0.62
3:C:134:VAL:HG11	3:C:151:ILE:HB	1.81	0.62
8:H:309:PHE:CB	8:H:341:MET:HE2	2.30	0.61
4:D:146:ILE:HD13	4:D:153:GLN:HE22	1.64	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
10:J:633:SER:HB3	10:J:635:ASN:ND2	2.15	0.61
1:A:167:ILE:HD13	1:A:176:VAL:HA	1.82	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
3:C:75:LEU:HD11	6:F:18:MET:HE1	1.81	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
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
2:B:179:GLU:HG2	2:B:184:THR:HG21	1.82	0.60
10:J:101:LEU:HD13	10:J:234:SER:CB	2.30	0.60
9:I:128:PHE:CE1	9:I:133:PRO:HD3	2.36	0.60
10:J:259:TYR:CD2	10:J:263:ARG:CD	2.85	0.60
3:C:258:THR:HG22	3:C:267:THR:HG22	1.82	0.60
10:J:440:ARG:CG	10:J:443:GLU:CB	2.69	0.59
7:G:184:PHE:CB	7:G:198:CYS:SG	2.88	0.59
4:D:22:GLN:HG2	4:D:23:ASP:N	2.16	0.59
3:C:61:ARG:NH1	6:F:20:PHE:CE1	2.70	0.59
3:C:17:PHE:HZ	9:I:255:VAL:CG1	2.13	0.59
7:G:152:ASP:CG	7:G:153:GLY:H	2.05	0.59
7:G:222:ALA:HB1	7:G:226:ILE:CG1	2.33	0.59
1:A:130:LYS:HD3	1:A:174:ILE:HG13	1.84	0.59
1:A:68:TYR:HE2	1:A:76:LEU:HD22	1.68	0.59
1:A:243:ARG:HG2	1:A:243:ARG:O	2.01	0.59
10:J:624:PHE:CE2	10:J:858:LEU:HD21	2.34	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
6:F:41:GLU:OE2	6:F:229:ARG:CZ	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:193:LYS:CE	8:H:283:ASP:OD1	2.51	0.59
1:A:173:GLN:HA	3:C:99:THR:CG2	2.32	0.59
3:C:122:ASP:O	3:C:163:ARG:NH2	2.36	0.59
8:H:67:TRP:CZ3	8:H:93:ARG:C	2.76	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
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
5:E:262:LEU:HD13	8:H:7:ILE:HD13	1.85	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
10:J:694:LEU:HD21	10:J:696:LEU:CD1	2.33	0.58
2:B:86:ARG:NH1	5:E:127:ASP:OD2	2.36	0.58
10:J:217:SER:O	10:J:220:GLN:N	2.37	0.58
9:I:128:PHE:O	9:I:128:PHE:CD1	2.57	0.58
7:G:4:PHE:CZ	7:G:40:GLY:HA2	2.38	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
3:C:45:LYS:HG2	3:C:46:TYR:H	1.69	0.57
1:A:7:ILE:HG21	1:A:230:LEU:HD21	1.86	0.57
10:J:440:ARG:O	10:J:440:ARG:HG2	2.03	0.57
7:G:110:ARG:CG	7:G:111:PRO:CD	2.82	0.57
2:B:23:ARG:NE	2:B:173:ASP:OD1	2.37	0.57
8:H:149:ARG:NH1	8:H:152:SER:CB	2.67	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
10:J:120:GLU:OE2	10:J:170:ASN:ND2	2.31	0.57
9:I:8:PRO:HB2	9:I:64:VAL:HB	1.87	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
6:F:87:PHE:HE1	8:H:160:ARG:HD3	1.64	0.57
2:B:23:ARG:NH2	2:B:173:ASP:OD1	2.37	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
10:J:574:THR:HG23	10:J:856:ARG:HG2	1.87	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
1:A:125:ILE:CG2	1:A:169:VAL:HG21	2.35	0.56
10:J:574:THR:HG21	10:J:856:ARG:HG2	1.88	0.56
3:C:255:LEU:HD12	3:C:256:ARG:O	2.05	0.56
8:H:309:PHE:CB	8:H:341:MET:HE1	2.35	0.56
6:F:41:GLU:OE2	6:F:229:ARG:NH2	2.37	0.56
10:J:309:ARG:HD2	10:J:456:TRP:O	2.05	0.56
10:J:196:THR:O	10:J:217:SER:HA	2.05	0.56
8:H:140:SER:HB2	8:H:185:HIS:HB2	1.87	0.56
10:J:309:ARG:CD	10:J:456:TRP:O	2.53	0.56
10:J:104:ASN:O	10:J:143:LYS:NZ	2.25	0.56
12:R:-36:G:O2'	12:R:-35:G:H5'	2.06	0.56
5:E:9:SER:HB3	8:H:285:ASN:HD22	1.70	0.56
7:G:156:ILE:CD1	7:G:208:TYR:HA	2.33	0.56
2:B:13:ARG:NH1	2:B:171:LEU:HB3	2.21	0.56
7:G:82:ASP:O	7:G:83:SER:HB3	2.06	0.56
3:C:207:ARG:NH1	3:C:270:GLU:O	2.39	0.56
9:I:23:THR:HG22	9:I:24:GLU:N	2.21	0.56
9:I:13:PRO:HD3	9:I:61:VAL:HG23	1.88	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
10:J:308:ASN:HB3	10:J:392:VAL:HG22	1.87	0.55
9:I:159:GLU:HG2	9:I:188:PHE:CE2	2.41	0.55
3:C:45:LYS:HG2	3:C:46:TYR:N	2.20	0.55
9:I:13:PRO:CD	9:I:61:VAL:HG22	2.36	0.55
2:B:29:ILE:HD11	2:B:145:LEU:HD22	1.87	0.55
10:J:539:ILE:HG23	10:J:553:ALA:HB1	1.89	0.55
8:H:300:TYR:O	8:H:303:VAL:HG22	2.06	0.55
9:I:231:ARG:HH11	9:I:252:LEU:HD23	1.71	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
3:C:299:ILE:CG2	3:C:328:THR:CG2	2.79	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
7:G:110:ARG:HD3	12:R:-44:C:C4	2.33	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
10:J:467:PHE:CZ	10:J:469:ARG:CA	2.89	0.55
7:G:222:ALA:HB1	7:G:226:ILE:HG13	1.88	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
10:J:539:ILE:HG22	10:J:648:SER:HA	1.89	0.55
8:H:104:TYR:CD1	8:H:228:ASN:HA	2.42	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
3:C:165[B]:LEU:HD21	3:C:170:LEU:HD11	1.89	0.55
5:E:257:ASP:HB3	8:H:4:VAL:CB	2.34	0.54
10:J:309:ARG:HB3	10:J:456:TRP:CD2	2.42	0.54
9:I:9:GLU:O	9:I:10:ILE:HD13	2.06	0.54
8:H:315:THR:O	8:H:319:ILE:HG13	2.07	0.54
7:G:127:GLU:HB2	7:G:130:LEU:HB3	1.88	0.54
4:D:84:PRO:O	4:D:86:GLN:HG2	2.06	0.54
3:C:147:GLU:O	3:C:151:ILE:HG13	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
3:C:160:LEU:HD12	3:C:160:LEU:O	2.06	0.54
10:J:309:ARG:NE	10:J:456:TRP:O	2.40	0.54
9:I:138:ILE:HG21	9:I:159:GLU:OE1	2.08	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
5:E:96:THR:O	5:E:100:ASN:ND2	2.36	0.54
5:E:15:LEU:HD11	5:E:23:PRO:HD3	1.90	0.54
7:G:142:GLY:O	7:G:143:ARG:CB	2.56	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
7:G:5:ILE:HD11	7:G:36:PRO:HG3	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:107:ARG:NH2	4:D:148:ASP:OD1	2.41	0.54
9:I:285:LYS:O	9:I:286:ARG:HD3	2.08	0.53
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
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
10:J:193:VAL:HG11	10:J:221:TYR:CD1	2.42	0.53
10:J:160:ARG:NH1	10:J:164:GLU:O	2.41	0.53
9:I:103:VAL:HG21	11:K:534:LEU:HD13	1.83	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
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
10:J:641:PHE:CE1	10:J:741:LYS:HB2	2.42	0.53
3:C:350:LEU:HD12	3:C:359:GLN:CG	2.37	0.53
11:K:599:ILE:HG13	11:K:600:ARG:N	2.24	0.53
3:C:349:ILE:HD13	3:C:378:LEU:HD23	1.90	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
3:C:28:GLU:HG2	3:C:342:SER:HB3	1.89	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
12:R:-39:A:HO2'	12:R:-38:G:C5'	2.22	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
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
9:I:103:VAL:HG11	11:K:534:LEU:HD13	1.92	0.52
7:G:214:CYS:HB3	7:G:223:PHE:CE2	2.44	0.52
6:F:88:THR:OG1	6:F:132:LYS:CA	2.57	0.52
10:J:661:ILE:HG23	10:J:675:ARG:HG2	1.92	0.52
3:C:391:ARG:HD2	3:C:392:PHE:CE2	2.44	0.52
2:B:187:LEU:HD22	2:B:196:LEU:HD13	1.91	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
3:C:88:ILE:HB	3:C:218:VAL:HG23	1.87	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)
5:E:116:LEU:CD1	5:E:157:LEU:CB	2.68	0.52
1:A:103:LEU:HD23	2:B:99:GLU:HG3	1.91	0.52
7:G:237:VAL:HG22	7:G:237:VAL:O	2.10	0.52
8:H:345:GLY:O	8:H:349:LEU:HG	2.10	0.52
7:G:28:ASP:OD2	7:G:35:ARG:NH1	2.43	0.52
7:G:99:TYR:O	7:G:102:PHE:CE2	2.63	0.52
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
8:H:121:ASN:CG	8:H:122:LYS:H	2.13	0.51
3:C:68:ILE:HD12	3:C:279:THR:HG23	1.92	0.51
1:A:22:ASN:ND2	1:A:30:PHE:CE2	2.68	0.51
10:J:530:LYS:HB2	10:J:864:TYR:CE1	2.45	0.51
3:C:75:LEU:HD21	6:F:18:MET:HE1	1.93	0.51
10:J:480:GLU:HG3	10:J:901:TYR:CE1	2.45	0.51
1:A:17:GLU:HG3	7:G:201:LEU:HD13	1.92	0.51
3:C:22:LEU:HD11	3:C:29:LEU:HD23	1.93	0.51
7:G:156:ILE:CG1	7:G:208:TYR:CD2	2.91	0.51
8:H:309:PHE:HB3	8:H:341:MET:CE	2.33	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
10:J:18:SER:O	10:J:41:LEU:N	2.40	0.51
7:G:99:TYR:O	7:G:102:PHE:CD2	2.63	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:12:ARG:NH1	10:J:154:GLU:CD	2.61	0.51
10:J:125:SER:C	10:J:127:PRO:HD2	2.31	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
9:I:13:PRO:CD	9:I:61:VAL:CG2	2.87	0.51
7:G:214:CYS:CA	7:G:223:PHE:CE1	2.94	0.51
4:D:22:GLN:CG	4:D:23:ASP:H	2.17	0.51
10:J:839:TYR:OH	12:R:-3:U:OP1	2.24	0.51
6:F:47:SER:HA	11:K:567:ASN:OD1	2.11	0.51
2:B:153:SER:HB3	8:H:83:SER:HG	1.75	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
2:B:67:THR:HB	2:B:119:ARG:CZ	2.41	0.51
9:I:103:VAL:CG2	11:K:534:LEU:HD12	2.29	0.50
8:H:124:TRP:HB2	8:H:136:LEU:HB3	1.94	0.50
7:G:227:ALA:HB1	7:G:231:PHE:CE2	2.40	0.50
10:J:573:VAL:HG21	10:J:845:PRO:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:309:GLN:O	3:C:310:ASN:CB	2.59	0.50
10:J:628:TRP:CH2	10:J:734:ALA:HA	2.46	0.50
10:J:963:VAL:HG23	10:J:963:VAL:O	2.10	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:440:ARG:CD	10:J:443:GLU:HB2	2.41	0.50
7:G:214:CYS:CB	7:G:223:PHE:CE1	2.95	0.50
10:J:285:PHE:CE1	10:J:430:CYS:O	2.64	0.50
6:F:148:THR:O	6:F:149:ASN:C	2.48	0.50
3:C:219:VAL:HG11	3:C:226:VAL:HG21	1.93	0.50
10:J:264:VAL:HA	10:J:273:LEU:HD12	1.92	0.50
6:F:242:ILE:HG13	6:F:243:SER:N	2.25	0.50
4:D:142:THR:CG2	4:D:144:ASP:CB	2.90	0.50
8:H:126:VAL:CG1	8:H:184:LEU:HD12	2.39	0.50
3:C:387:ASP:OD2	3:C:391:ARG:NH2	2.39	0.50
6:F:137:ILE:HG21	6:F:176:ILE:HG23	1.92	0.50
10:J:694:LEU:HD21	10:J:696:LEU:HD11	1.93	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
9:I:197:LEU:O	9:I:197:LEU:HG	2.10	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:77:ILE:HD13	7:G:87:SER:HB2	1.93	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
12:R:-31:U:O4'	12:R:-31:U:P	2.70	0.50
6:F:148:THR:O	6:F:149:ASN:O	2.30	0.50
1:A:179:VAL:O	1:A:182:ARG:O	2.30	0.50
9:I:12:TYR:CE2	9:I:15:LYS:CD	2.87	0.50
1:A:10:SER:HB3	7:G:152:ASP:O	2.12	0.50
2:B:67:THR:HB	2:B:119:ARG:NH2	2.27	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
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
9:I:19:PRO:HB3	11:K:545:VAL:CG1	2.42	0.49
10:J:217:SER:O	10:J:218:LEU:C	2.49	0.49
5:E:66:VAL:CG2	10:J:31:GLY:HA2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:152:SER:HB3	8:H:155:ASP:CG	2.32	0.49
8:H:318:ARG:HD3	8:H:348:ILE:HG21	1.95	0.49
6:F:201:VAL:CG2	6:F:213:PHE:CE1	2.96	0.49
10:J:285:PHE:HZ	10:J:429:LYS:O	1.95	0.49
9:I:146:LEU:HD22	9:I:220:VAL:CG1	2.29	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
1:A:103:LEU:O	1:A:107:ILE:HG12	2.12	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
3:C:255:LEU:HD11	10:J:294:ARG:NE	2.28	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
10:J:311:PHE:HE2	10:J:431:LEU:CD2	2.26	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
8:H:206:LEU:HB3	8:H:313:GLY:HA2	1.94	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
8:H:157:LEU:HD13	9:I:235:LEU:HD13	1.92	0.48
7:G:181:HIS:ND1	7:G:231:PHE:CZ	2.81	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
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
10:J:311:PHE:CE2	10:J:431:LEU:CG	2.93	0.48
8:H:126:VAL:HG11	8:H:184:LEU:CD1	2.42	0.48
10:J:842:PHE:HE1	10:J:855:HIS:HA	1.78	0.48
3:C:81:LYS:HD3	11:K:578:ARG:HB3	1.96	0.48
1:A:92:GLU:HB2	1:A:95:ASN:HB2	1.95	0.48
10:J:98:ALA:HB2	10:J:236:PRO:CD	2.43	0.48
3:C:275:ILE:HG21	6:F:21:SER:HB3	1.95	0.48
2:B:83:LYS:HE3	2:B:131:GLN:CD	2.33	0.48
11:K:352:ARG:HA	11:K:353:PRO:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:97:LEU:HB2	7:G:134:ILE:CD1	2.44	0.48
12:R:-43:C:O5'	12:R:-43:C:C6	2.65	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
5:E:31:PHE:CB	8:H:5:ILE:HD12	2.44	0.48
3:C:161:HIS:ND1	4:D:183:ASN:HB3	2.29	0.48
9:I:139:VAL:HG11	9:I:155:ILE:CG2	2.39	0.48
3:C:278:GLN:NE2	6:F:20:PHE:HB3	2.29	0.48
10:J:158:VAL:O	10:J:169:ARG:NH1	2.47	0.48
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
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
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:384:ARG:NH1	11:K:583:ILE:HD11	2.29	0.47
3:C:37:LEU:HD12	11:K:606:PHE:HD1	1.79	0.47
11:K:539:VAL:N	11:K:540:PRO:HD2	2.29	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
12:R:-39:A:O2'	12:R:-38:G:C4'	2.63	0.47
8:H:175:SER:C	8:H:176:LEU:HD12	2.34	0.47
10:J:12:ARG:NH2	10:J:16:GLY:O	2.48	0.47
1:A:126:VAL:HG23	1:A:130:LYS:H	1.80	0.47
10:J:668:ASP:OD1	10:J:671:THR:OG1	2.31	0.47
2:B:235:HIS:O	2:B:239:ARG:HG2	2.14	0.47
9:I:161:LYS:O	9:I:162:PRO:C	2.52	0.47
6:F:16:LYS:HB3	6:F:16:LYS:NZ	2.29	0.47
4:D:139:ILE:CD1	4:D:146:ILE:HD12	2.44	0.47
1:A:208:GLU:HA	8:H:76:LEU:HD22	1.96	0.47
8:H:340:VAL:HG12	8:H:344:ILE:CD1	2.45	0.47
10:J:79:LEU:HD22	10:J:226:PRO:HD3	1.97	0.47
1:A:126:VAL:HG23	1:A:129:SER:HB2	1.97	0.47
11:K:542:ILE:O	11:K:545:VAL:HB	2.15	0.47
1:A:191:HIS:CE1	1:A:193:PRO:HG3	2.50	0.47
5:E:27:LEU:HB2	5:E:30:GLN:HG2	1.96	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
3:C:10:ILE:HG22	3:C:11:GLU:N	2.29	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
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
10:J:694:LEU:CG	10:J:696:LEU:HG	2.44	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
12:R:-31:U:OP1	12:R:-31:U:O4'	2.32	0.47
9:I:128:PHE:CZ	9:I:133:PRO:CD	2.97	0.46
3:C:139:GLY:HA3	6:F:78:TYR:CD2	2.50	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
8:H:293:ILE:O	8:H:297:ILE:HG12	2.15	0.46
5:E:33:PRO:CG	8:H:337:GLU:OE2	2.63	0.46
2:B:23:ARG:O	2:B:25:PHE:N	2.49	0.46
7:G:99:TYR:C	7:G:102:PHE:CE2	2.87	0.46
10:J:841:HIS:HB3	10:J:851:ASP:OD1	2.16	0.46
10:J:72:LEU:HD13	10:J:146:ILE:HG21	1.95	0.46
3:C:387:ASP:OD2	11:K:585:TYR:OH	2.22	0.46
9:I:150:ARG:NE	9:I:204:ILE:HD13	2.30	0.46
8:H:140:SER:O	8:H:187:ARG:NE	2.48	0.46
8:H:64:ASP:OD2	8:H:93:ARG:NH1	2.47	0.46
10:J:845:PRO:HA	10:J:851:ASP:HB2	1.98	0.46
8:H:218:PRO:HG2	8:H:300:TYR:OH	2.16	0.46
10:J:473:THR:HG22	10:J:474:ILE:N	2.30	0.46
1:A:261:LEU:HD12	2:B:196:LEU:HD12	1.97	0.46
9:I:150:ARG:HD2	9:I:204:ILE:HD13	1.98	0.46
3:C:28:GLU:HG2	3:C:342:SER:CB	2.45	0.46
2:B:71:LEU:HB2	2:B:121:VAL:HG22	1.97	0.46
6:F:239:ASP:O	6:F:242:ILE:HG12	2.15	0.46
3:C:10:ILE:CG2	3:C:11:GLU:N	2.78	0.46
10:J:770:LEU:O	10:J:775:ASN:N	2.49	0.46
3:C:280:LYS:NZ	3:C:280:LYS:HB3	2.30	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
3:C:57:ASN:O	3:C:63:ALA:HB2	2.16	0.46
10:J:641:PHE:CD1	10:J:741:LYS:HG2	2.49	0.46
6:F:205:LYS:HG2	9:I:46:TYR:CE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:86:VAL:CG1	7:G:134:ILE:HD11	2.38	0.46
5:E:75:LEU:O	5:E:75:LEU:HG	2.16	0.46
5:E:163:ASP:HA	5:E:167:GLU:HA	1.98	0.46
11:K:317:ALA:CB	11:K:376:LEU:CB	2.92	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
10:J:467:PHE:CE2	10:J:469:ARG:C	2.80	0.46
7:G:84:TYR:HB2	7:G:97:LEU:HB3	1.98	0.46
10:J:18:SER:N	10:J:41:LEU:O	2.38	0.46
5:E:75:LEU:HD23	5:E:114:LEU:HD12	1.98	0.46
10:J:663:ASP:O	10:J:664:LYS:CB	2.64	0.46
3:C:308:LEU:HD22	11:K:613:LEU:CB	2.46	0.46
3:C:255:LEU:CD1	3:C:256:ARG:N	2.77	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
9:I:211:ARG:CZ	9:I:218:VAL:HG22	2.46	0.46
3:C:54:ILE:HB	3:C:78:ASN:HD21	1.81	0.46
7:G:75:VAL:O	7:G:75:VAL:HG13	2.15	0.46
3:C:73:ASN:H	6:F:102:LEU:HD11	1.81	0.45
12:R:-32:G:O2'	12:R:-31:U:C6	2.59	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
5:E:86:ARG:HG2	5:E:88:ASP:H	1.81	0.45
2:B:206:PRO:HB2	2:B:209:ARG:HD3	1.99	0.45
9:I:23:THR:CG2	9:I:24:GLU:N	2.79	0.45
6:F:246:MET:CE	9:I:10:ILE:CG1	2.89	0.45
4:D:165:LEU:HD11	4:D:199:GLU:HG2	1.99	0.45
3:C:261:THR:CG2	3:C:262:ARG:N	2.52	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
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
1:A:207:GLU:HG3	8:H:74:TYR:HD2	1.82	0.45
12:R:-39:A:C2'	12:R:-38:G:O5'	2.64	0.45
3:C:45:LYS:CG	3:C:46:TYR:H	2.29	0.45
5:E:215:ILE:HD13	5:E:248:LEU:HD23	1.99	0.45
4:D:168:VAL:HB	7:G:8:GLY:O	2.16	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

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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
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
10:J:98:ALA:HB2	10:J:236:PRO:HD3	1.99	0.45
9:I:12:TYR:CZ	9:I:15:LYS:CB	2.93	0.45
10:J:660:ARG:NE	10:J:666:GLN:OE1	2.49	0.45
10:J:302:VAL:O	10:J:306:ASN:ND2	2.43	0.45
10:J:229:ASP:HA	10:J:232:ARG:HE	1.80	0.45
10:J:440:ARG:HG3	10:J:443:GLU:CG	2.47	0.45
10:J:224:LEU:HG	10:J:224:LEU:O	2.16	0.45
6:F:201:VAL:HG21	6:F:213:PHE:CE1	2.51	0.45
10:J:285:PHE:CE1	10:J:430:CYS:C	2.90	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:143:TYR:HE2	6:F:145:LYS:HE2	1.82	0.45
3:C:14:PRO:HG3	9:I:268:TYR:CE2	2.52	0.45
10:J:739:ALA:HB2	10:J:840:THR:HG22	1.99	0.45
5:E:257:ASP:CG	8:H:4:VAL:HG23	2.36	0.45
7:G:134:ILE:O	7:G:134:ILE:HG13	2.17	0.45
11:K:538:SER:HG	11:K:541:GLN:H	1.63	0.45
10:J:311:PHE:CE2	10:J:431:LEU:CD2	2.99	0.45
2:B:187:LEU:CD2	2:B:199:LEU:HD13	2.47	0.45
10:J:387:GLN:HA	10:J:388:PRO:HD3	1.80	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
7:G:4:PHE:HD2	7:G:6:PHE:CZ	2.36	0.44
6:F:124:VAL:HG12	6:F:187:LEU:HD22	1.99	0.44
10:J:326:TRP:HZ3	10:J:380:ALA:HB2	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
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
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
10:J:440:ARG:HG3	10:J:443:GLU:CB	2.45	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:680:LEU:HB2	10:J:730:PHE:HZ	1.81	0.44
4:D:99:GLU:OE2	4:D:108:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:236:PRO:HA	10:J:466:HIS:CE1	2.51	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
8:H:67:TRP:CE3	8:H:93:ARG:C	2.91	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
8:H:195:ARG:NH1	8:H:282:SER:N	2.65	0.44
8:H:68:MET:O	8:H:94:LEU:HD12	2.18	0.44
2:B:169:THR:HA	2:B:170:PRO:HD3	1.67	0.44
3:C:134:VAL:HG11	3:C:151:ILE:CB	2.45	0.44
10:J:326:TRP:CZ3	10:J:380:ALA:CB	3.00	0.44
3:C:97:GLU:HG2	3:C:209:TRP:CD1	2.52	0.44
10:J:236:PRO:HA	10:J:466:HIS:CG	2.53	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
5:E:15:LEU:HD23	5:E:193:VAL:HG21	2.00	0.44
3:C:162:SER:HB3	3:C:358:LYS:CB	2.48	0.44
8:H:170:ASN:HB2	8:H:191:TYR:HA	2.00	0.44
1:A:5:ILE:CG1	1:A:90:GLN:HG2	2.47	0.44
7:G:106:SER:CB	7:G:109:ASN:HB3	2.44	0.44
6:F:186:GLU:HG2	9:I:60:LEU:HD21	2.00	0.44
3:C:139:GLY:HA3	6:F:78:TYR:CG	2.53	0.44
10:J:688:ARG:NH1	10:J:729:GLU:OE2	2.51	0.44
1:A:297:LEU:O	1:A:301:ASN:HB2	2.17	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
10:J:131:ARG:O	10:J:134:THR:OG1	2.34	0.43
9:I:66:CYS:HA	9:I:107:LEU:O	2.18	0.43
12:R:-35:G:C2'	12:R:-34:G:H5'	2.47	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
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:643:LYS:HD2	10:J:864:TYR:CE2	2.53	0.43
12:R:-39:A:O2'	12:R:-38:G:C5'	2.66	0.43
10:J:597:VAL:HB	10:J:902:TYR:HD2	1.84	0.43
10:J:873:ASP:HB3	10:J:876:LYS:HB2	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
3:C:27:PRO:HB3	3:C:338:ALA:HA	2.00	0.43
5:E:66:VAL:HG21	10:J:31:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:431:LEU:HA	10:J:432:PRO:HD3	1.88	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
1:A:176:VAL:CG1	1:A:176:VAL:O	2.65	0.43
9:I:258:ARG:HB2	9:I:262:GLY:HA2	2.00	0.43
10:J:959:LYS:HD3	10:J:972:ASP:OD2	2.19	0.43
3:C:277:ASP:OD1	3:C:280:LYS:N	2.45	0.43
1:A:254:LEU:HD12	1:A:255:PRO:HD2	2.01	0.43
1:A:204:GLN:HG3	1:A:205:ASP:OD1	2.18	0.43
2:B:17:ARG:HH11	2:B:23:ARG:HG3	1.78	0.43
10:J:606:MET:O	10:J:610:THR:OG1	2.24	0.43
7:G:214:CYS:HB3	7:G:223:PHE:CE1	2.53	0.43
1:A:169:VAL:HG22	1:A:174:ILE:CD1	2.49	0.43
10:J:579:PRO:HA	10:J:584:ASP:OD2	2.19	0.43
10:J:255:PHE:N	10:J:458:THR:HB	2.34	0.43
12:R:-3:U:H2'	12:R:-2:U:C6	2.54	0.43
1:A:228:GLU:HG3	1:A:231:ARG:CZ	2.49	0.43
10:J:213:ILE:HG12	10:J:215:THR:HG23	2.00	0.43
1:A:167:ILE:HD12	1:A:176:VAL:HA	1.99	0.43
6:F:87:PHE:CE1	8:H:160:ARG:CZ	3.02	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
9:I:138:ILE:CG2	9:I:159:GLU:OE1	2.66	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
3:C:33:ARG:NH1	3:C:306:CYS:HA	2.34	0.43
9:I:141:THR:HG21	9:I:155:ILE:HG13	2.00	0.43
10:J:17:LEU:CD1	10:J:42:ARG:HA	2.37	0.43
10:J:12:ARG:NH1	10:J:154:GLU:OE1	2.52	0.43
9:I:150:ARG:CD	9:I:204:ILE:HD13	2.49	0.43
8:H:190:LYS:HE3	8:H:191:TYR:CZ	2.53	0.43
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
8:H:121:ASN:CG	8:H:122:LYS:N	2.71	0.42
9:I:19:PRO:HG3	11:K:549:PHE:HB2	2.01	0.42
8:H:215:HIS:CD2	8:H:316:GLN:OE1	2.72	0.42
10:J:959:LYS:HE2	10:J:974:TYR:HE1	1.84	0.42
7:G:172:PHE:HA	7:G:173:PRO:HD3	1.78	0.42
10:J:113:VAL:HG11	10:J:132:LEU:HD21	2.02	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)
7:G:106:SER:HB3	7:G:109:ASN:H	1.83	0.42
8:H:84:VAL:HG21	8:H:99:PRO:HG3	2.01	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
1:A:250:LYS:O	2:B:198:LEU:HA	2.18	0.42
7:G:114:GLN:O	7:G:115:VAL:C	2.58	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
2:B:186:THR:HB	2:B:200:LEU:HB3	2.01	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: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:17:LEU:HD11	10:J:42:ARG:NH1	2.35	0.42
8:H:155:ASP:O	8:H:159:MET:CG	2.68	0.42
10:J:112[B]:ILE:CD1	10:J:181:TYR:CE1	2.97	0.42
3:C:309:GLN:HG3	3:C:310:ASN:N	2.34	0.42
3:C:352:ALA:O	3:C:355:GLY:CA	2.67	0.42
1:A:107:ILE:HG21	1:A:236:THR:HG21	2.02	0.42
7:G:64:TYR:HA	7:G:160:LEU:HD11	2.01	0.42
3:C:362:LEU:HD22	4:D:180:LEU:HD23	2.01	0.42
8:H:124:TRP:CH2	8:H:159:MET:HE3	2.54	0.42
1:A:278:GLN:O	1:A:281:GLN:CG	2.62	0.42
6:F:88:THR:OG1	6:F:132:LYS:N	2.52	0.42
6:F:67:LEU:CG	6:F:68:GLY:N	2.73	0.42
10:J:570:ILE:HG22	10:J:845:PRO:HD3	2.02	0.42
3:C:383:VAL:HG12	11:K:585:TYR:CD2	2.54	0.42
3:C:305:GLU:O	3:C:305:GLU:CG	2.67	0.42
3:C:130:VAL:HG22	3:C:159:ILE:HD12	2.01	0.42
12:R:-33:G:C3'	12:R:-32:G:C5'	2.94	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
10:J:641:PHE:HZ	10:J:737:SER:O	2.03	0.41
8:H:5:ILE:HG12	8:H:6:THR:N	2.35	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
10:J:98:ALA:HB2	10:J:236:PRO:CG	2.50	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
10:J:596:LEU:HB3	10:J:898:SER:OG	2.20	0.41
3:C:134:VAL:O	3:C:134:VAL:HG13	2.21	0.41
5:E:102:VAL:HG22	5:E:225:PRO:HD2	2.01	0.41
10:J:588:ALA:O	10:J:883:ASN:OD1	2.38	0.41
3:C:356:ASN:HB3	4:D:185:ASP:OD1	2.20	0.41
10:J:23:VAL:HB	10:J:36:VAL:HG22	2.01	0.41
1:A:223:ALA:HB1	1:A:227:GLU:HB2	2.02	0.41
7:G:95:VAL:CG1	7:G:132:ALA:O	2.68	0.41
2:B:240:VAL:HG21	8:H:54:ILE:CD1	2.47	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
3:C:137:GLU:CD	6:F:140:TYR:CE1	2.93	0.41
7:G:2:SER:OG	7:G:41:VAL:HG22	2.20	0.41
1:A:81:THR:HG22	1:A:138:VAL:HB	2.02	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:61:ARG:NH1	6:F:20:PHE:CE2	2.89	0.41
10:J:285:PHE:HE1	10:J:430:CYS:C	2.24	0.41
3:C:29:LEU:HB2	9:I:258:ARG:HH22	1.85	0.41
10:J:85:LYS:HE2	10:J:85:LYS:HB2	1.92	0.41
10:J:834:LEU:HD21	12:R:-4:U:H4'	2.03	0.41
8:H:189:LEU:HD12	8:H:190:LYS:N	2.35	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: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
8:H:123:ARG:HG2	8:H:137:MET:HA	2.03	0.41
9:I:143:VAL:HG22	9:I:153:VAL:HG12	2.03	0.41
7:G:178:LEU:HD13	7:G:184:PHE:HZ	1.85	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
9:I:277:SER:HA	9:I:278:PRO:HD3	1.84	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
10:J:19:VAL:HB	10:J:40:TYR:CD2	2.56	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:694:LEU:CD2	10:J:696:LEU:CD1	2.99	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
10:J:967:SER:OG	10:J:968:ASP:N	2.53	0.41
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
10:J:165:THR:HG22	10:J:166:ILE:N	2.36	0.40
4:D:168:VAL:HG23	4:D:173:VAL:HB	2.02	0.40
10:J:20:THR:OG1	10:J:21:GLN:N	2.54	0.40
9:I:17:ILE:HD11	9:I:58:ALA:HB2	2.03	0.40
8:H:309:PHE:HB2	8:H:341:MET:CE	2.39	0.40
7:G:110:ARG:HB2	12:R:-44:C:N4	2.36	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
2:B:104:LEU:HD13	2:B:143:ILE:HD11	2.03	0.40
3:C:80:LEU:HD23	3:C:233:SER:HB2	2.04	0.40
3:C:53:ALA:CB	11:K:575:ILE:HD11	2.51	0.40
1:A:263:LYS:HB3	1:A:263:LYS:HE2	1.97	0.40
2:B:161:ILE:HD12	2:B:161:ILE:HA	1.95	0.40
2:B:103:SER:O	2:B:107:MET:HG3	2.21	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:53:ASN:HB3	4:D:11:ASP:OD2	2.22	0.40
5:E:75:LEU:HD21	5:E:114:LEU:HB3	2.01	0.40
3:C:275:ILE:CG2	6:F:21:SER:HB3	2.51	0.40
10:J:255:PHE:O	10:J:458:THR:HG21	2.20	0.40
4:D:24:THR:OG1	4:D:107:ARG:NH1	2.54	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
8:H:67:TRP:CE3	8:H:95:LEU:HB2	2.56	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
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%)	39	80
3	C	332/394 (84%)	312 (94%)	19 (6%)	1 (0%)	46	83
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%)	46	83
9	I	214/295 (72%)	208 (97%)	6 (3%)	0	100	100
10	J	939/1003 (94%)	899 (96%)	39 (4%)	1 (0%)	56	90
11	K	344/695 (50%)	330 (96%)	14 (4%)	0	100	100
All	All	3587/4306 (83%)	3445 (96%)	138 (4%)	4 (0%)	56	90

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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%)	93	97
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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	299/305 (98%)	0.35	22 (7%)	17	11	168, 206, 270, 304	0
2	B	244/248 (98%)	0.58	20 (8%)	14	9	162, 209, 280, 314	0
3	C	339/394 (86%)	0.51	27 (7%)	15	9	205, 234, 301, 333	0
4	D	223/245 (91%)	0.44	13 (5%)	26	16	170, 206, 259, 300	0
5	E	267/267 (100%)	0.47	20 (7%)	17	11	179, 216, 267, 309	0
6	F	215/250 (86%)	0.34	8 (3%)	45	30	189, 221, 266, 308	0
7	G	237/243 (97%)	0.19	8 (3%)	49	34	167, 203, 253, 283	0
8	H	293/361 (81%)	0.21	10 (3%)	49	34	175, 209, 263, 286	0
9	I	222/295 (75%)	0.94	41 (18%)	2	1	205, 244, 291, 345	0
10	J	944/1003 (94%)	1.47	274 (29%)	1	1	238, 377, 429, 458	0
11	K	350/695 (50%)	2.51	170 (48%)	0	1	227, 378, 404, 428	0
12	R	31/45 (68%)	3.38	12 (38%)	0	1	265, 295, 398, 401	0
All	All	3664/4351 (84%)	0.93	625 (17%)	2	2	162, 242, 405, 458	0

All (625) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	270	LEU	16.0
10	J	553	ALA	15.3
12	R	-27	U	14.3
12	R	-26	U	13.5
10	J	698	SER	13.3
12	R	-28	U	13.2
10	J	699	PRO	13.1
10	J	554	LEU	13.1
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	11.3
10	J	697	ALA	10.7
11	K	216	VAL	10.6
11	K	217	ASP	10.4
12	R	-20	U	10.2
11	K	207	SER	10.1
11	K	267	THR	10.1
11	K	210	ASP	10.0
10	J	937	GLY	10.0
10	J	703	VAL	9.7
12	R	-25	U	9.7
11	K	151	LEU	9.6
11	K	308	VAL	9.4
11	K	171	ASP	9.4
11	K	209	ASP	9.2
12	R	-29	U	9.1
10	J	973	VAL	9.0
11	K	271	ARG	9.0
10	J	407	LEU	9.0
10	J	926	ILE	9.0
11	K	208	TRP	8.9
11	K	273	ASN	8.8
10	J	615	LEU	8.8
10	J	968	ASP	8.5
10	J	556	ALA	8.4
11	K	218	THR	8.4
11	K	205	SER	8.3
10	J	976	PHE	8.3
10	J	933	PHE	8.3
11	K	365	ASP	8.3
10	J	700	GLU	8.2
3	C	265	SER	8.2
11	K	252	CYS	8.2
11	K	274	LEU	8.1
3	C	309	GLN	8.0
11	K	206	LYS	8.0
12	R	-24	U	7.8
11	K	165	SER	7.7
11	K	195	GLU	7.7
10	J	1001	LYS	7.7
11	K	350	ARG	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	7.6
11	K	305	GLY	7.4
10	J	972	ASP	7.4
10	J	935	VAL	7.3
11	K	306	LEU	7.3
10	J	1000	LEU	7.2
9	I	269	ALA	7.2
11	K	353	PRO	7.2
11	K	196	ILE	7.2
11	K	219	SER	7.0
11	K	341	SER	6.9
10	J	932	LYS	6.9
10	J	934	GLY	6.8
10	J	903	VAL	6.8
11	K	266	ASP	6.8
11	K	253	LEU	6.7
10	J	507	GLY	6.7
10	J	998	LEU	6.7
11	K	213	PRO	6.7
10	J	730	PHE	6.7
10	J	990	ILE	6.6
11	K	163	SER	6.6
11	K	238	ASP	6.6
10	J	971	ARG	6.6
10	J	569	HIS	6.5
10	J	320	LEU	6.5
11	K	260	GLU	6.5
10	J	980	GLU	6.4
11	K	254	MET	6.4
12	R	-30	U	6.4
10	J	970	PRO	6.4
12	R	-23	U	6.3
10	J	837	ASP	6.3
11	K	173	GLU	6.1
11	K	150	PRO	6.1
10	J	634	ALA	6.1
10	J	540	CYS	6.1
10	J	979	VAL	6.1
11	K	230	LYS	6.1
10	J	996	ALA	6.0
11	K	368	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
10	J	632	ASP	6.0
10	J	950	SER	6.0
11	K	304	LEU	6.0
11	K	152	LEU	6.0
11	K	309	VAL	6.0
11	K	153	LYS	6.0
3	C	142	GLY	5.9
10	J	529	THR	5.9
11	K	227	GLU	5.9
10	J	710	SER	5.9
10	J	696	LEU	5.9
10	J	969	LYS	5.9
9	I	291	PRO	5.9
11	K	268	LEU	5.8
10	J	422	VAL	5.8
11	K	272	GLU	5.8
11	K	231	ASN	5.8
10	J	931	PRO	5.8
12	R	-21	U	5.7
11	K	303	ASP	5.7
11	K	300	LEU	5.7
11	K	369	LEU	5.7
10	J	489	ASP	5.7
10	J	733	LEU	5.6
10	J	715	VAL	5.6
10	J	147	VAL	5.5
10	J	555	HIS	5.5
10	J	677	LEU	5.5
10	J	928	VAL	5.5
10	J	776	MET	5.5
10	J	633	SER	5.5
10	J	148	PHE	5.4
11	K	211	SER	5.4
11	K	194	PRO	5.4
11	K	312	PHE	5.4
10	J	408	ALA	5.4
11	K	166	LEU	5.3
12	R	-22	U	5.3
11	K	310	GLY	5.3
10	J	567	GLY	5.3
10	J	504	PRO	5.3
10	J	90	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
10	J	829	PHE	5.3
11	K	362	ALA	5.2
11	K	226	LEU	5.2
10	J	763	PHE	5.2
10	J	438	THR	5.2
10	J	149	HIS	5.2
11	K	182	PRO	5.1
11	K	212	VAL	5.1
9	I	28	GLY	5.1
8	H	2	SER	5.1
10	J	936	GLU	5.1
11	K	349	TRP	5.1
10	J	826	TYR	5.0
10	J	714	GLU	5.0
11	K	234	GLU	5.0
11	K	228	ASP	5.0
10	J	597	VAL	4.9
10	J	964	PRO	4.9
10	J	385	LYS	4.9
10	J	947	ASP	4.9
10	J	565	GLU	4.9
11	K	183	TYR	4.9
10	J	997	GLU	4.9
11	K	265	VAL	4.9
10	J	949	ASN	4.8
10	J	97	GLN	4.8
10	J	364	VAL	4.8
11	K	359	THR	4.8
10	J	409	PRO	4.8
10	J	944	LEU	4.8
11	K	261	ARG	4.8
11	K	281	PHE	4.8
10	J	919	ILE	4.8
9	I	268	TYR	4.7
11	K	400	ARG	4.7
10	J	98	ALA	4.7
11	K	257	SER	4.7
10	J	318	VAL	4.7
11	K	172	ASP	4.7
10	J	899	ILE	4.7
9	I	102	THR	4.7
11	K	256	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
10	J	807	ILE	4.7
11	K	229	LEU	4.6
7	G	74	GLY	4.6
10	J	405	GLY	4.6
1	A	165	PRO	4.6
10	J	777	SER	4.6
1	A	172	GLU	4.6
10	J	713	ASN	4.6
10	J	437	ARG	4.6
2	B	2	SER	4.5
11	K	174	ASN	4.5
5	E	86	ARG	4.5
9	I	162	PRO	4.5
3	C	266	ALA	4.5
10	J	636	ILE	4.5
11	K	402	GLU	4.5
10	J	449	ILE	4.5
5	E	84	GLY	4.4
9	I	103	VAL	4.4
11	K	301	GLN	4.4
10	J	101	LEU	4.4
2	B	63	SER	4.4
10	J	918	VAL	4.4
10	J	992	SER	4.4
3	C	308	LEU	4.4
11	K	414	GLU	4.4
10	J	966	ASN	4.3
10	J	513	PRO	4.3
10	J	927	VAL	4.3
3	C	251	ARG	4.3
10	J	628	TRP	4.3
10	J	808	MET	4.3
10	J	938	LEU	4.3
10	J	376	ASP	4.3
10	J	952	ALA	4.3
11	K	204	PRO	4.3
10	J	517	ASP	4.3
1	A	62	CYS	4.2
11	K	161	PRO	4.2
11	K	189	HIS	4.2
4	D	145	ILE	4.2
10	J	712	PRO	4.2

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

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Mol	Chain	Res	Type	RSRZ
4	D	19	PHE	3.6
10	J	967	SER	3.6
3	C	180	ASN	3.6
11	K	352	ARG	3.6
10	J	571	ALA	3.6
10	J	929	LEU	3.6
10	J	210	GLU	3.6
10	J	542	ILE	3.6
10	J	508	HIS	3.6
10	J	608	LEU	3.6
11	K	311	LEU	3.6
11	K	408	PRO	3.6
5	E	193	VAL	3.6
11	K	223	GLU	3.6
4	D	223	VAL	3.5
4	D	136	ILE	3.5
10	J	766	LEU	3.5
10	J	813	MET	3.5
10	J	423	PHE	3.5
10	J	695	ASN	3.5
10	J	898	SER	3.5
10	J	709	THR	3.5
10	J	915	THR	3.5
4	D	137	ALA	3.5
10	J	380	ALA	3.5
10	J	894	ALA	3.5
11	K	241	HIS	3.5
11	K	410	THR	3.5
10	J	418	SER	3.5
2	B	7	TYR	3.5
10	J	650	GLU	3.5
1	A	194	ILE	3.4
10	J	774	LYS	3.4
10	J	113	VAL	3.4
9	I	27	ASP	3.4
9	I	264	GLY	3.4
10	J	87	TYR	3.4
10	J	412	VAL	3.4
10	J	974	TYR	3.3
11	K	162	LEU	3.3
10	J	387	GLN	3.3
10	J	88	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
11	K	251	VAL	3.3
5	E	145	ILE	3.3
11	K	149	ILE	3.3
11	K	415	VAL	3.3
10	J	862	ILE	3.3
11	K	175	ASN	3.3
11	K	372	ILE	3.3
10	J	420	GLN	3.3
11	K	222	LEU	3.3
3	C	272	TYR	3.3
10	J	326	TRP	3.3
11	K	258	THR	3.3
10	J	702	LYS	3.3
11	K	169	VAL	3.3
10	J	708	GLU	3.3
1	A	239	LEU	3.2
10	J	417	SER	3.2
6	F	85	GLY	3.2
2	B	93	ASN	3.2
2	B	159	SER	3.2
11	K	180	PRO	3.2
11	K	167	ARG	3.2
11	K	278	ASN	3.2
2	B	160	GLY	3.2
9	I	128	PHE	3.2
11	K	220	THR	3.2
10	J	726	LEU	3.2
11	K	158	ALA	3.2
1	A	125	ILE	3.2
2	B	3	ARG	3.1
11	K	255	GLN	3.1
11	K	168	LEU	3.1
11	K	262	ASP	3.1
10	J	154	GLU	3.1
10	J	917	TYR	3.1
1	A	169	VAL	3.1
10	J	295	PHE	3.1
1	A	64	ILE	3.1
10	J	155	HIS	3.1
9	I	159	GLU	3.1
11	K	299	TRP	3.1
3	C	274	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
10	J	613	CYS	3.1
9	I	130	ASN	3.1
10	J	519	PRO	3.1
10	J	259	TYR	3.1
11	K	240	GLU	3.1
11	K	366	THR	3.1
10	J	580	GLY	3.1
10	J	413	ASP	3.1
11	K	235	ILE	3.1
3	C	207	ARG	3.1
10	J	114	PRO	3.1
10	J	961	THR	3.1
10	J	635	ASN	3.0
10	J	108	PHE	3.0
10	J	41	LEU	3.0
10	J	514	THR	3.0
10	J	651	ALA	3.0
10	J	762	ASN	3.0
10	J	15	ASP	3.0
9	I	258	ARG	3.0
11	K	233	LYS	3.0
6	F	82	SER	3.0
11	K	250	ILE	3.0
5	E	185	PRO	3.0
9	I	133	PRO	3.0
5	E	188	PHE	3.0
10	J	674	MET	3.0
11	K	215	TRP	3.0
11	K	317	ALA	3.0
10	J	652	PHE	2.9
10	J	977	ASP	2.9
6	F	213	PHE	2.9
8	H	67	TRP	2.9
10	J	598	ASP	2.9
10	J	46	PRO	2.9
11	K	340	THR	2.9
10	J	541	SER	2.9
3	C	52	VAL	2.9
4	D	161	HIS	2.9
10	J	218	LEU	2.9
10	J	102	LEU	2.9
11	K	280	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
11	K	405	LYS	2.8
9	I	198	GLY	2.8
10	J	227	ASN	2.8
10	J	156	THR	2.8
10	J	963	VAL	2.8
11	K	320	ALA	2.8
10	J	111	VAL	2.8
10	J	779	SER	2.8
11	K	318	SER	2.8
6	F	143	TYR	2.8
10	J	415	GLN	2.8
10	J	221	TYR	2.8
10	J	624	PHE	2.8
6	F	80	PRO	2.8
11	K	288	LYS	2.8
10	J	770	LEU	2.8
11	K	401	PHE	2.8
9	I	158	VAL	2.8
10	J	419	THR	2.8
11	K	177	SER	2.8
11	K	344	TYR	2.8
10	J	383	SER	2.8
10	J	72	LEU	2.8
8	H	93	ARG	2.8
10	J	436	ILE	2.8
1	A	33	PHE	2.8
11	K	224	SER	2.7
10	J	573	VAL	2.7
10	J	400	TRP	2.7
10	J	630	LEU	2.7
10	J	717	ILE	2.7
11	K	154	GLU	2.7
11	K	275	HIS	2.7
9	I	70	LYS	2.7
10	J	537	LYS	2.7
11	K	302	ARG	2.7
7	G	190	LEU	2.7
10	J	631	ASP	2.7
10	J	812	CYS	2.7
2	B	25	PHE	2.7
10	J	491	GLU	2.7
10	J	384	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
11	K	184	GLU	2.7
3	C	124	ILE	2.7
4	D	156	ILE	2.7
9	I	36	VAL	2.7
11	K	282	THR	2.7
10	J	617	PRO	2.6
9	I	256	PHE	2.6
10	J	444	LEU	2.6
10	J	876	LYS	2.6
9	I	278	PRO	2.6
10	J	751	MET	2.6
10	J	374	ALA	2.6
9	I	17	ILE	2.6
5	E	244	LEU	2.6
11	K	354	LEU	2.6
2	B	1	MET	2.6
9	I	71	LYS	2.6
10	J	923	ASN	2.6
10	J	994	ARG	2.6
3	C	211	TYR	2.6
11	K	155	LYS	2.6
3	C	144	CYS	2.6
10	J	621	ARG	2.6
2	B	187	LEU	2.6
10	J	742	ILE	2.6
10	J	299	VAL	2.6
11	K	614	GLU	2.6
5	E	28	PRO	2.6
9	I	72	THR	2.6
10	J	181	TYR	2.6
10	J	477	ALA	2.6
10	J	68	PRO	2.5
11	K	409	LEU	2.5
9	I	61	VAL	2.5
10	J	464	LEU	2.5
10	J	145	PHE	2.5
10	J	694	LEU	2.5
11	K	355	SER	2.5
10	J	209	VAL	2.5
1	A	132	TRP	2.5
11	K	232	THR	2.5
1	A	192	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	356	LYS	2.5
10	J	95	VAL	2.5
3	C	14	PRO	2.5
10	J	568	VAL	2.5
11	K	399	ARG	2.5
11	K	406	TYR	2.5
2	B	90	SER	2.5
8	H	276	SER	2.5
11	K	343	LYS	2.5
10	J	711	ASP	2.5
10	J	954	ASP	2.5
10	J	214	ILE	2.5
4	D	144	ASP	2.5
10	J	760	SER	2.5
11	K	411	PRO	2.5
10	J	799	PRO	2.5
7	G	166	LEU	2.5
10	J	373	LEU	2.4
9	I	265	GLY	2.4
11	K	351	ILE	2.4
8	H	184	LEU	2.4
1	A	171	GLY	2.4
9	I	10	ILE	2.4
10	J	679	LYS	2.4
10	J	152	PHE	2.4
10	J	744	ASP	2.4
11	K	193	SER	2.4
11	K	197	LEU	2.4
5	E	239	PHE	2.4
10	J	793	CYS	2.4
11	K	404	SER	2.4
1	A	174	ILE	2.4
10	J	195	VAL	2.4
1	A	167	ILE	2.4
5	E	143	PHE	2.4
5	E	192	VAL	2.4
10	J	193	VAL	2.4
10	J	897	ALA	2.4
6	F	4	GLN	2.4
3	C	174	ALA	2.4
9	I	255	VAL	2.4
3	C	12	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
11	K	203	ILE	2.3
1	A	170	HIS	2.3
9	I	129	ALA	2.3
11	K	367	HIS	2.3
1	A	193	PRO	2.3
11	K	605	ASN	2.3
7	G	174	LEU	2.3
5	E	196	ASN	2.3
10	J	512	ALA	2.3
10	J	39	HIS	2.3
10	J	40	TYR	2.3
11	K	534	LEU	2.3
10	J	42	ARG	2.3
9	I	220	VAL	2.3
3	C	326	LEU	2.3
9	I	146	LEU	2.3
10	J	375	LYS	2.3
3	C	259	ILE	2.3
3	C	253	SER	2.3
10	J	637	VAL	2.3
12	R	-31	U	2.3
10	J	948	PRO	2.3
10	J	518	ASP	2.3
10	J	71	ILE	2.3
10	J	305	LYS	2.3
7	G	184	PHE	2.3
10	J	22	LYS	2.2
9	I	224	PHE	2.2
9	I	246	THR	2.2
7	G	136	CYS	2.2
10	J	716	GLU	2.2
2	B	108	PHE	2.2
10	J	539	ILE	2.2
9	I	223	CYS	2.2
5	E	85	GLN	2.2
11	K	190	GLN	2.2
10	J	203	GLU	2.2
3	C	209	TRP	2.2
10	J	490	VAL	2.2
11	K	297	ILE	2.2
4	D	39	ARG	2.2
11	K	360	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
11	K	536	THR	2.2
8	H	151	LYS	2.2
6	F	93	ILE	2.2
11	K	246	SER	2.2
11	K	296	ASN	2.2
5	E	258	VAL	2.2
8	H	92	ASN	2.2
6	F	188	VAL	2.2
10	J	773	ARG	2.2
8	H	144	PRO	2.2
10	J	612	LEU	2.2
3	C	147	GLU	2.1
4	D	103	GLU	2.1
9	I	153	VAL	2.1
4	D	186	PHE	2.1
1	A	112	VAL	2.1
1	A	118	LEU	2.1
2	B	96	ARG	2.1
3	C	13	HIS	2.1
10	J	59	VAL	2.1
2	B	214	LEU	2.1
10	J	800	TYR	2.1
2	B	21	GLU	2.1
8	H	193	LYS	2.1
10	J	99	ILE	2.1
11	K	321	ILE	2.1
1	A	187	LEU	2.1
2	B	136	MET	2.1
1	A	134	VAL	2.1
3	C	75	LEU	2.1
5	E	149	LEU	2.1
9	I	257	ALA	2.1
10	J	63	ALA	2.1
10	J	440	ARG	2.1
10	J	828	ASP	2.1
10	J	941	LEU	2.1
4	D	104	PHE	2.1
11	K	263	TYR	2.1
10	J	392	VAL	2.1
1	A	175	ILE	2.1
7	G	25	ILE	2.1
9	I	55	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
10	J	435	ARG	2.1
5	E	-1	GLY	2.1
11	K	580	GLU	2.1
10	J	201	ASN	2.1
11	K	403	TYR	2.1
10	J	914	GLU	2.1
2	B	76	VAL	2.0
5	E	195	ASN	2.0
10	J	939	ILE	2.0
4	D	73	VAL	2.0
11	K	277	LEU	2.0
10	J	34	LYS	2.0
2	B	27	SER	2.0
10	J	676	ALA	2.0
11	K	289	VAL	2.0
1	A	4	ASP	2.0
10	J	827	PRO	2.0
10	J	882	ARG	2.0
11	K	236	ALA	2.0
10	J	960	LEU	2.0
5	E	58	CYS	2.0
11	K	322	GLY	2.0
10	J	738	VAL	2.0
7	G	1	MET	2.0
9	I	108	VAL	2.0
10	J	538	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	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.