Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 08:12 PM JST

PDB ID	:	7XPN
Title	:	Structure of the Spring Viraemia of Carp Virus Nucleoprotein
Authors	:	Wang, Z.X.; Liu, B.; Zhang, Y.A.; Ouyang, S.Y.
Deposited on	:	2022-05-04
Resolution	:	3.98 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

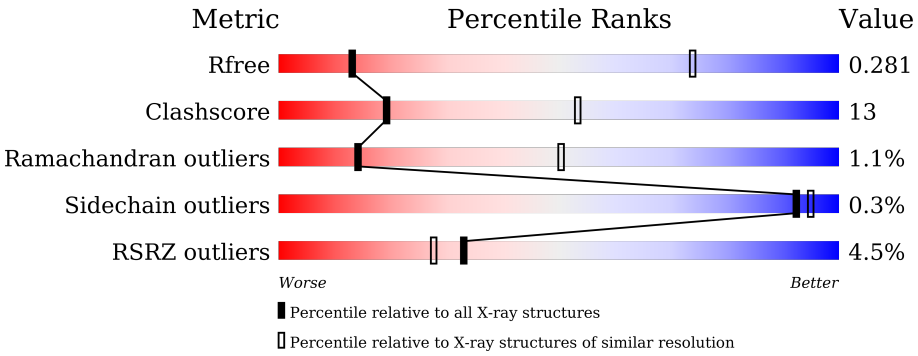
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	418	3% 68% 31%
1	B	418	7% 70% 29%
1	C	418	4% 74% 25%
1	D	418	5% 67% 32%
1	E	418	3% 64% 35%
1	F	418	2% 71% 29%

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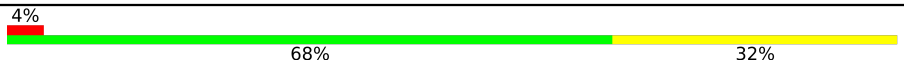
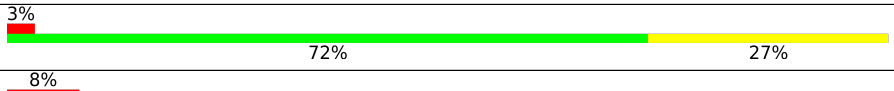
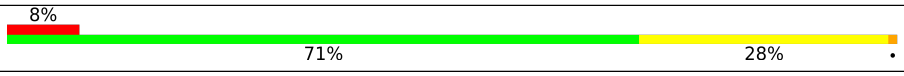
Mol	Chain	Length	Quality of chain
1	G	418	
1	H	418	
1	I	418	
1	J	418	
1	K	418	
1	L	418	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 39588 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 Nucleoprotein.

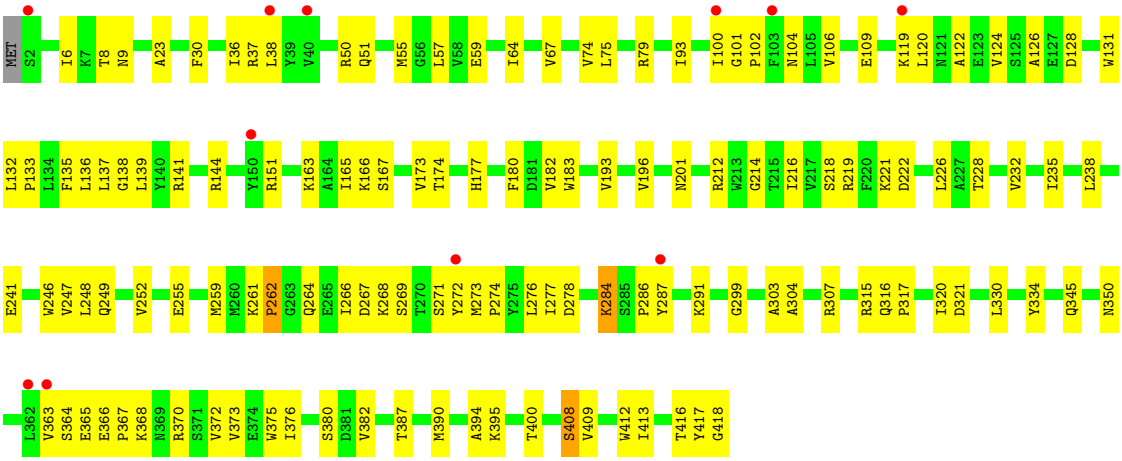
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	E	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	F	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	I	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	K	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	B	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	C	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	G	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	H	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	D	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	J	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			
1	L	417	Total	C	N	O	S	0	0	0
			3299	2108	556	618	17			

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.

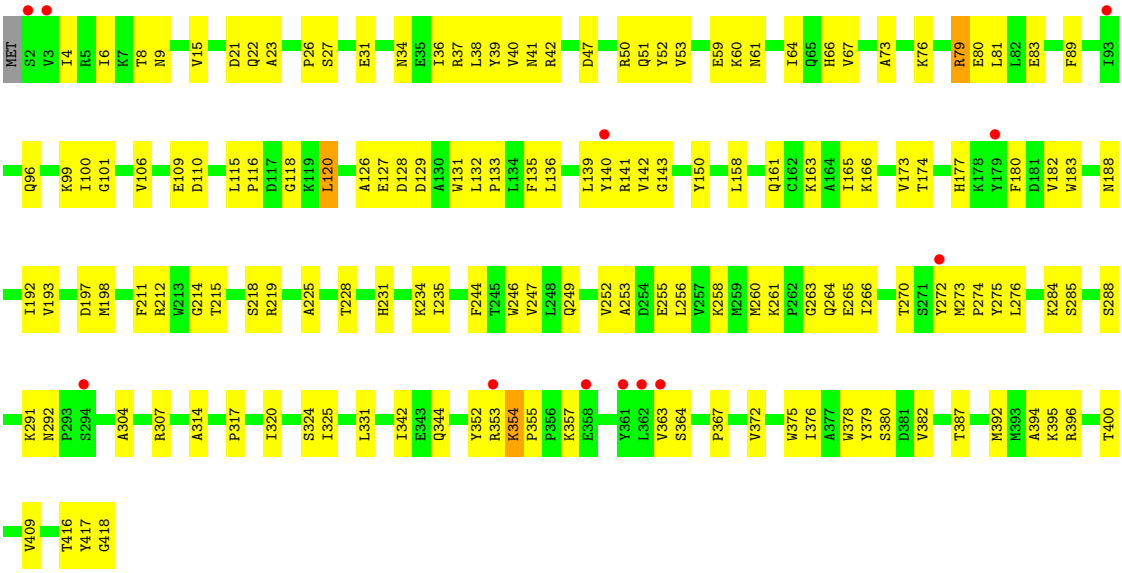
• Molecule 1: Nucleoprotein

Chain A:



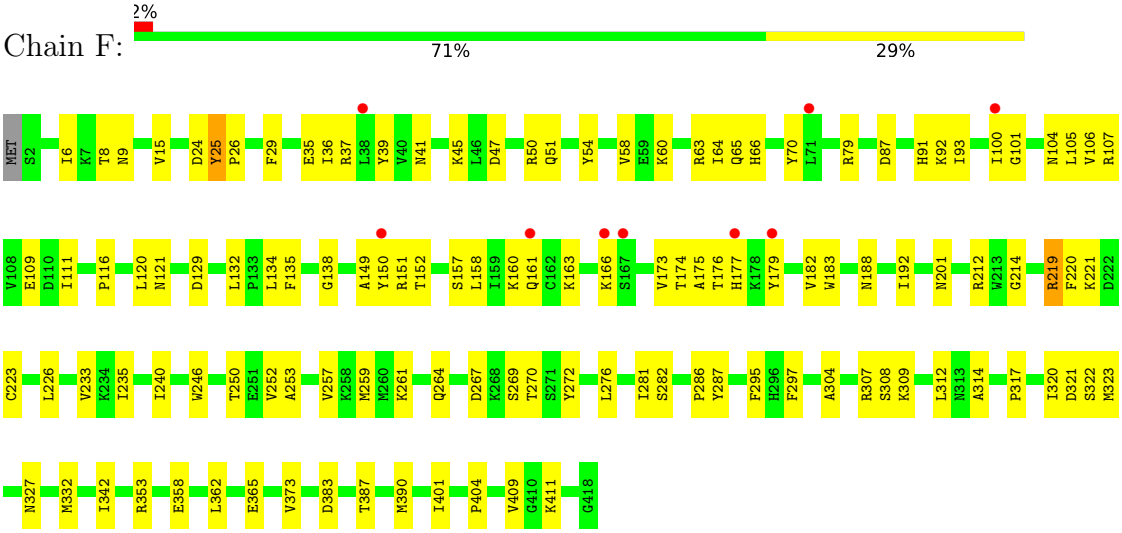
• Molecule 1: Nucleoprotein

Chain E:



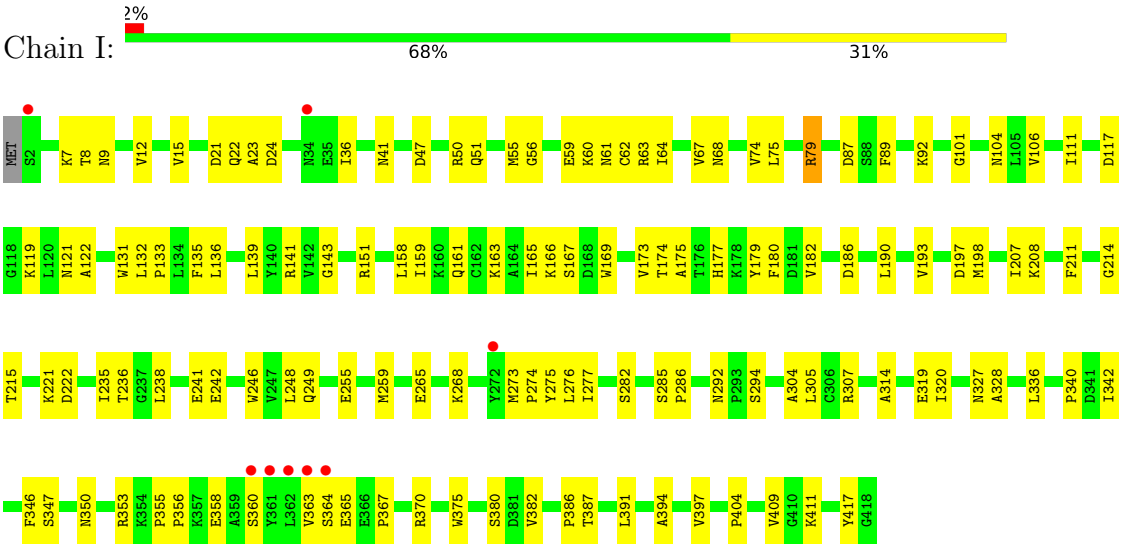
• Molecule 1: Nucleoprotein

Chain F:



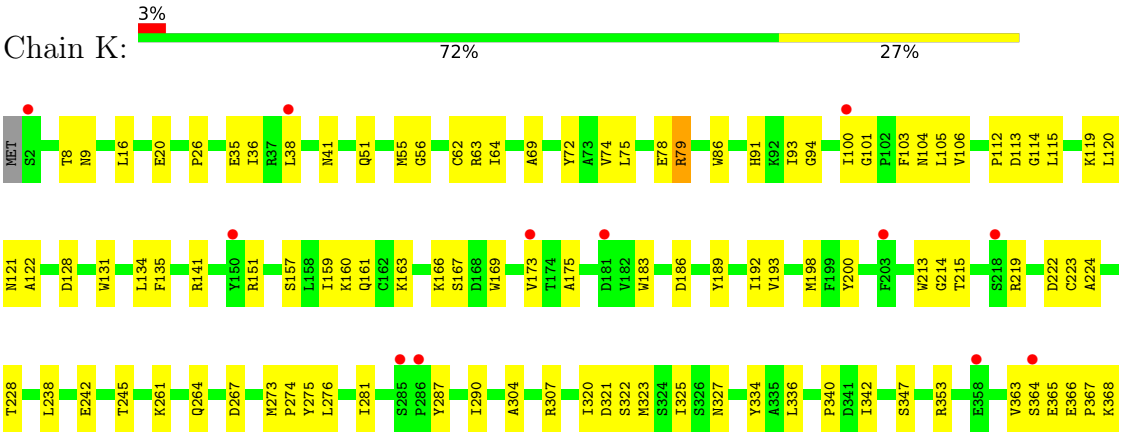
• Molecule 1: Nucleoprotein

Chain I:



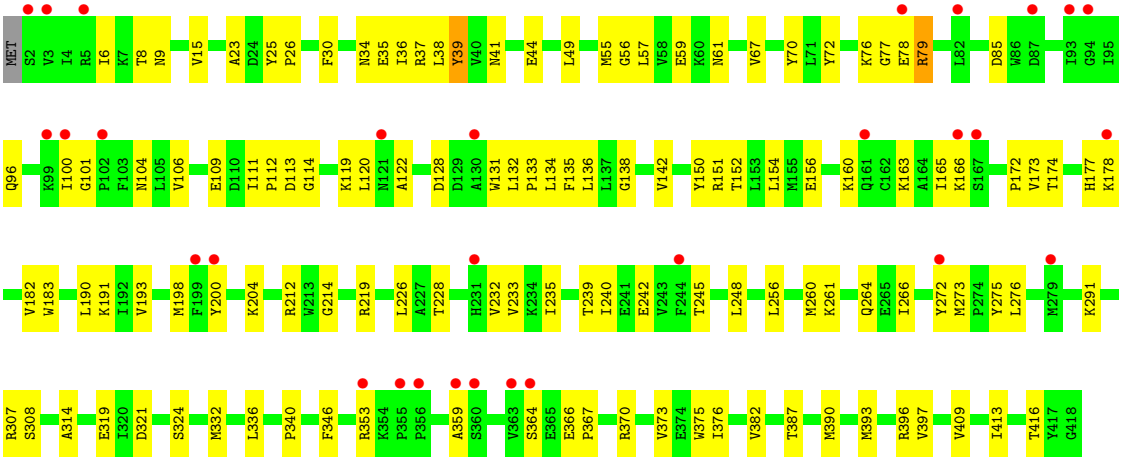
• Molecule 1: Nucleoprotein

Chain K:



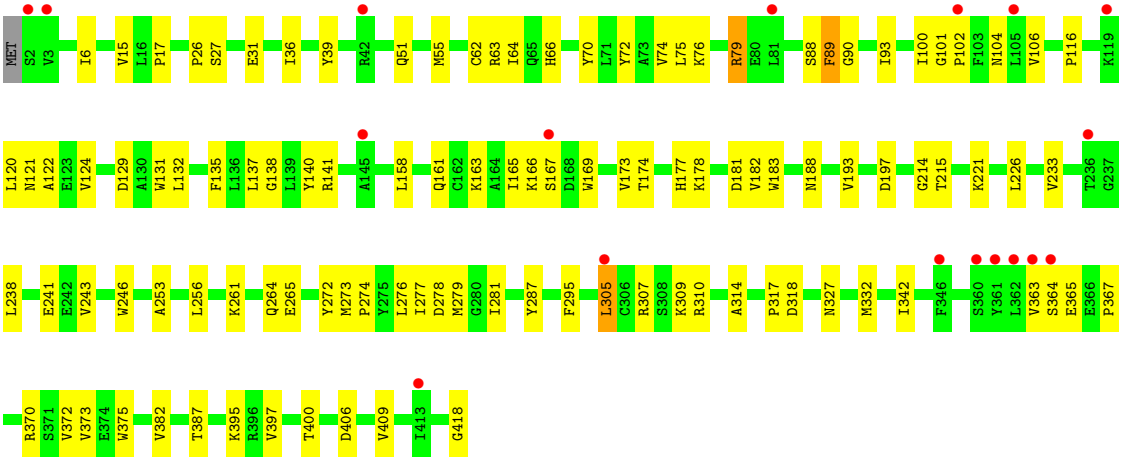
• Molecule 1: Nucleoprotein

Chain B:



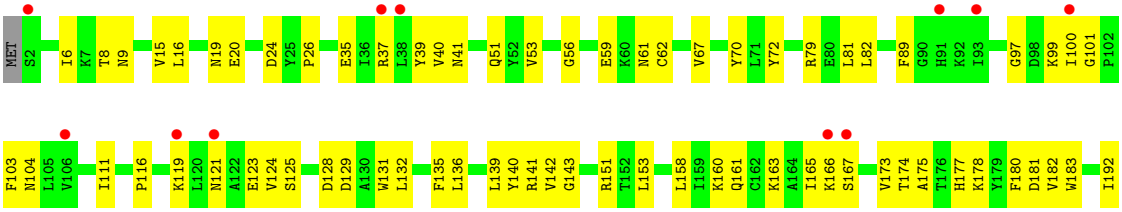
• Molecule 1: Nucleoprotein

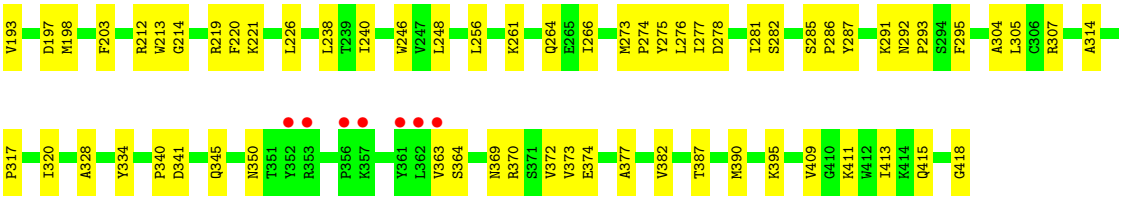
Chain C:



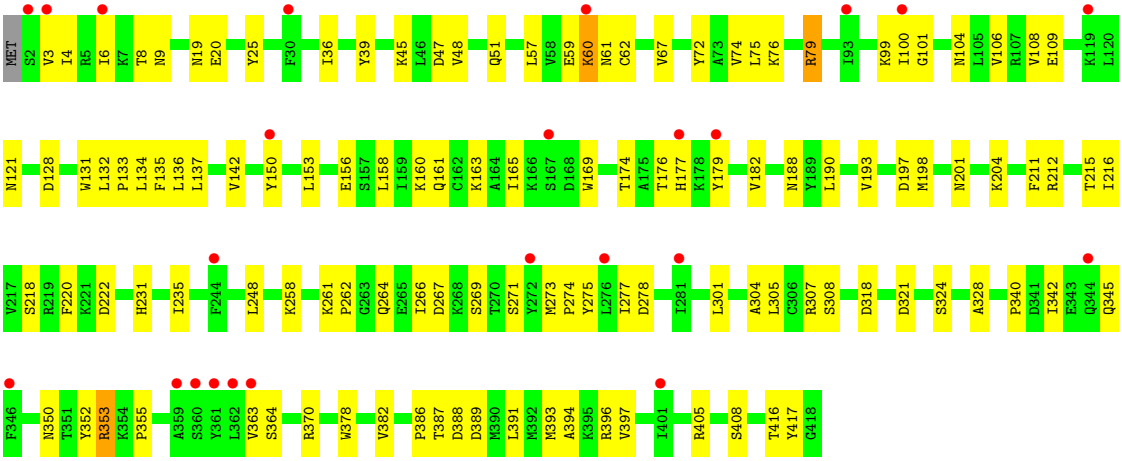
• Molecule 1: Nucleoprotein

Chain G:

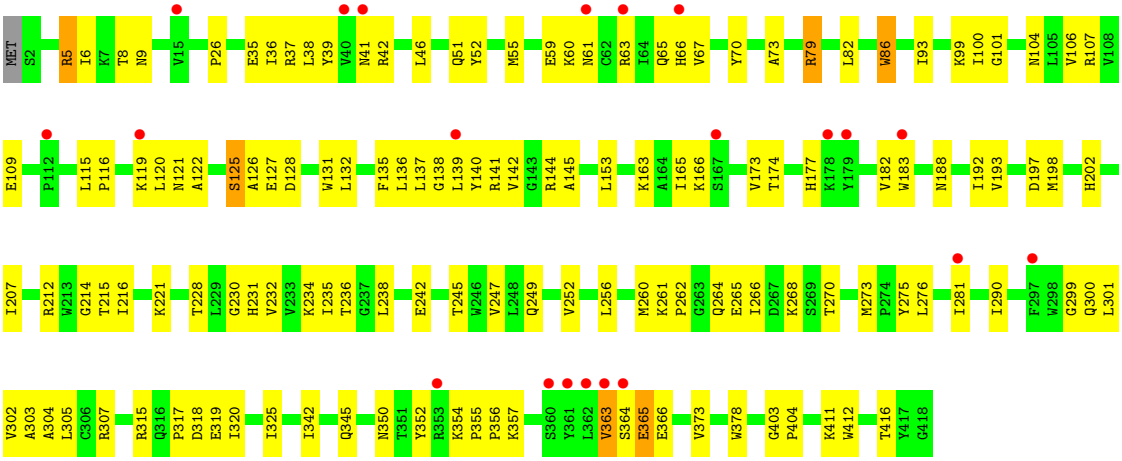




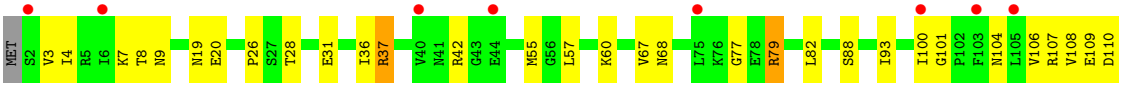
• Molecule 1: Nucleoprotein

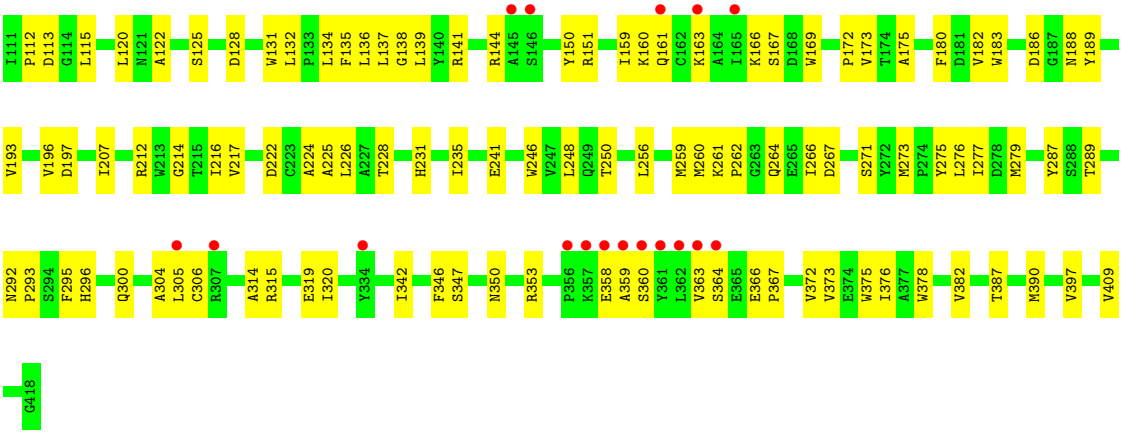


• Molecule 1: Nucleoprotein



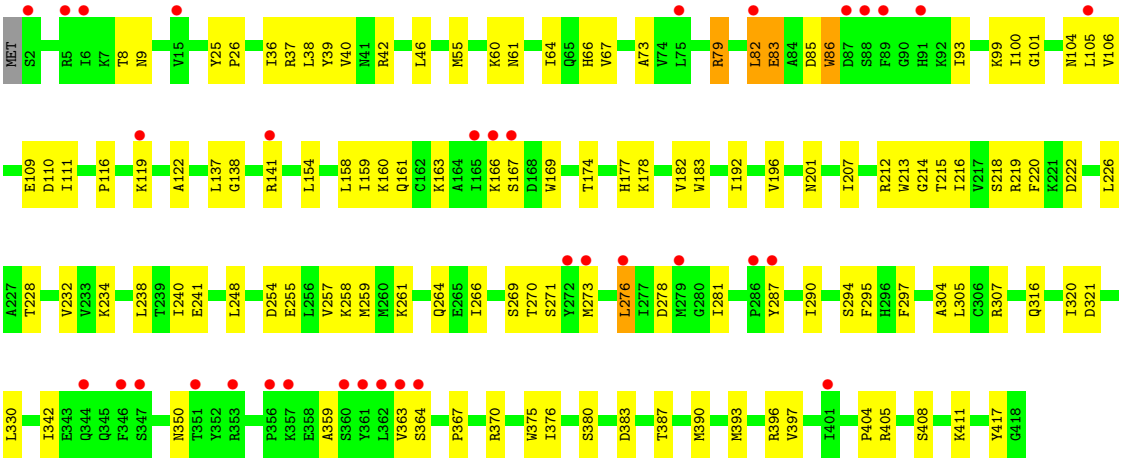
• Molecule 1: Nucleoprotein





• Molecule 1: Nucleoprotein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	174.25Å 298.70Å 332.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.86 – 3.98 75.26 – 3.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.86-3.98) 91.4 (75.26-3.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.255 , 0.284 0.252 , 0.281	Depositor DCC
R_{free} test set	1986 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å^2)	135.7	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 100.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	39588	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0/3375	0.53	0/4575
1	B	0.25	0/3375	0.53	0/4575
1	C	0.25	0/3375	0.52	0/4575
1	D	0.25	0/3375	0.54	0/4575
1	E	0.25	0/3375	0.53	1/4575 (0.0%)
1	F	0.26	0/3375	0.51	0/4575
1	G	0.25	0/3375	0.53	0/4575
1	H	0.25	0/3375	0.51	0/4575
1	I	0.24	0/3375	0.52	0/4575
1	J	0.25	0/3375	0.52	0/4575
1	K	0.25	0/3375	0.52	0/4575
1	L	0.25	0/3375	0.53	1/4575 (0.0%)
All	All	0.25	0/40500	0.52	2/54900 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	120	LEU	CA-CB-CG	5.81	128.66	115.30
1	L	276	LEU	CA-CB-CG	5.72	128.46	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	125	SER	Peptide
1	J	112	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3299	0	3279	97	0
1	B	3299	0	3279	87	0
1	C	3299	0	3279	83	0
1	D	3299	0	3279	100	0
1	E	3299	0	3279	112	0
1	F	3299	0	3279	90	0
1	G	3299	0	3279	98	0
1	H	3299	0	3279	84	0
1	I	3299	0	3279	88	0
1	J	3299	0	3279	104	0
1	K	3299	0	3279	74	0
1	L	3299	0	3279	83	0
All	All	39588	0	39348	1017	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1017) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ARG:HB2	1:E:214:GLY:HA2	1.49	0.93
1:J:305:LEU:HA	1:J:397:VAL:HG11	1.56	0.86
1:E:61:ASN:HD21	1:B:166:LYS:HE2	1.39	0.85
1:B:138:GLY:HA2	1:B:214:GLY:HA3	1.58	0.84
1:F:35:GLU:HG2	1:F:107:ARG:HG2	1.60	0.84
1:C:163:LYS:HG3	1:H:182:VAL:HG22	1.60	0.83
1:J:387:THR:HG22	1:J:390:MET:HG3	1.59	0.83
1:E:307:ARG:HH12	1:E:400:THR:HG21	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HG3	1:A:418:GLY:HA2	1.62	0.81
1:I:141:ARG:HB2	1:I:214:GLY:HA2	1.62	0.81
1:D:41:ASN:HD21	1:D:115:LEU:HD13	1.46	0.80
1:K:51:GLN:OE1	1:K:121:ASN:ND2	2.15	0.79
1:D:247:VAL:HG13	1:D:252:VAL:HG23	1.65	0.79
1:C:166:LYS:HG3	1:C:167:SER:H	1.47	0.79
1:L:158:LEU:HD23	1:L:161:GLN:HE21	1.48	0.78
1:L:55:MET:HB2	1:L:122:ALA:HB2	1.63	0.78
1:A:163:LYS:HG3	1:F:182:VAL:HG22	1.65	0.77
1:L:166:LYS:HG3	1:L:167:SER:H	1.50	0.76
1:B:77:GLY:HA2	1:B:79:ARG:HH11	1.51	0.76
1:D:165:ILE:HG13	1:D:166:LYS:H	1.49	0.76
1:J:166:LYS:HG3	1:J:167:SER:H	1.52	0.75
1:D:261:LYS:HD3	1:D:262:PRO:HD2	1.68	0.75
1:B:128:ASP:HB2	1:B:131:TRP:HE1	1.52	0.75
1:E:249:GLN:HB2	1:E:252:VAL:HG22	1.67	0.75
1:B:6:ILE:HD12	1:B:15:VAL:HG11	1.68	0.75
1:A:307:ARG:HH12	1:A:400:THR:HG21	1.52	0.75
1:L:393:MET:HA	1:L:396:ARG:HD2	1.67	0.75
1:D:141:ARG:HB2	1:D:214:GLY:HA2	1.69	0.74
1:K:55:MET:HG2	1:K:122:ALA:HB2	1.67	0.74
1:F:39:TYR:O	1:F:188:ASN:ND2	2.20	0.74
1:A:141:ARG:HB2	1:A:214:GLY:HA2	1.70	0.74
1:L:64:ILE:HD12	1:L:183:TRP:HA	1.71	0.73
1:G:166:LYS:HG3	1:G:167:SER:H	1.54	0.73
1:G:51:GLN:NE2	1:G:123:GLU:O	2.22	0.72
1:E:165:ILE:HG13	1:E:166:LYS:H	1.54	0.72
1:H:39:TYR:O	1:H:188:ASN:ND2	2.22	0.72
1:A:100:ILE:HG23	1:A:101:GLY:H	1.55	0.72
1:A:387:THR:H	1:A:390:MET:HE3	1.54	0.72
1:K:36:ILE:HB	1:K:106:VAL:HG23	1.69	0.72
1:I:259:MET:SD	1:I:292:ASN:ND2	2.63	0.72
1:H:51:GLN:HG2	1:H:121:ASN:HB3	1.71	0.71
1:A:317:PRO:HG2	1:A:320:ILE:HD13	1.72	0.71
1:J:100:ILE:HG23	1:J:101:GLY:H	1.55	0.71
1:I:174:THR:HG21	1:I:177:HIS:HB3	1.73	0.71
1:C:100:ILE:HG13	1:C:104:ASN:HD21	1.55	0.71
1:F:362:LEU:HB2	1:F:365:GLU:HB2	1.71	0.71
1:A:37:ARG:HG2	1:A:109:GLU:HG3	1.71	0.71
1:J:82:LEU:HD11	1:J:100:ILE:HD12	1.72	0.71
1:F:36:ILE:HG13	1:F:106:VAL:HG23	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:LEU:HD11	1:K:160:LYS:HE3	1.73	0.70
1:J:259:MET:SD	1:J:292:ASN:ND2	2.64	0.70
1:I:158:LEU:HD22	1:I:169:TRP:HE1	1.57	0.70
1:H:198:MET:HB2	1:H:275:TYR:HE2	1.57	0.70
1:K:353:ARG:NH1	1:L:380:SER:OG	2.25	0.70
1:J:141:ARG:HB2	1:J:214:GLY:HA2	1.75	0.69
1:G:395:LYS:HG2	1:G:418:GLY:HA2	1.73	0.69
1:F:51:GLN:HB3	1:F:121:ASN:HB3	1.74	0.69
1:B:239:THR:OG1	1:B:242:GLU:OE1	2.06	0.69
1:F:100:ILE:HG23	1:F:101:GLY:H	1.57	0.69
1:E:67:VAL:HG13	1:E:136:LEU:HD13	1.74	0.69
1:B:100:ILE:HG23	1:B:101:GLY:H	1.58	0.69
1:H:100:ILE:HG23	1:H:101:GLY:H	1.58	0.69
1:L:100:ILE:HG23	1:L:101:GLY:H	1.56	0.69
1:D:238:LEU:HD12	1:D:242:GLU:HG2	1.75	0.69
1:I:166:LYS:HG3	1:I:167:SER:H	1.58	0.68
1:D:100:ILE:HG23	1:D:101:GLY:H	1.57	0.68
1:D:319:GLU:HB3	1:L:234:LYS:HE2	1.75	0.68
1:I:7:LYS:O	1:B:346:PHE:HA	1.93	0.68
1:E:50:ARG:NH1	1:E:129:ASP:OD2	2.27	0.68
1:F:219:ARG:O	1:F:221:LYS:N	2.26	0.68
1:H:174:THR:HG21	1:H:177:HIS:HB3	1.75	0.68
1:L:36:ILE:HB	1:L:106:VAL:HG23	1.75	0.68
1:G:100:ILE:HG13	1:G:104:ASN:HD21	1.58	0.68
1:H:364:SER:O	1:H:378:TRP:NE1	2.26	0.68
1:K:364:SER:HB2	1:K:366:GLU:HG3	1.74	0.68
1:C:158:LEU:HD23	1:C:161:GLN:HE21	1.58	0.67
1:D:365:GLU:HB2	1:D:378:TRP:HD1	1.59	0.67
1:A:36:ILE:HB	1:A:106:VAL:HG23	1.77	0.67
1:G:6:ILE:HD11	1:J:241:GLU:HA	1.75	0.67
1:G:277:ILE:HD11	1:G:285:SER:HB2	1.77	0.67
1:D:174:THR:HG21	1:D:177:HIS:HB3	1.76	0.67
1:B:416:THR:OG1	1:H:307:ARG:NH2	2.28	0.67
1:C:174:THR:HG21	1:C:177:HIS:HB3	1.76	0.67
1:H:100:ILE:HG13	1:H:104:ASN:HD21	1.60	0.67
1:F:100:ILE:HG13	1:F:104:ASN:HD21	1.59	0.67
1:B:67:VAL:HG13	1:B:136:LEU:HD13	1.75	0.67
1:B:321:ASP:OD2	1:B:324:SER:OG	2.09	0.67
1:K:395:LYS:HG3	1:K:418:GLY:HA2	1.76	0.66
1:F:226:LEU:HD13	1:F:287:TYR:HB3	1.77	0.66
1:K:273:MET:HG3	1:K:274:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:HB3	1:B:37:ARG:HH12	1.58	0.66
1:G:266:ILE:HA	1:G:273:MET:HG2	1.77	0.66
1:L:141:ARG:HB2	1:L:214:GLY:HA2	1.77	0.66
1:K:223:CYS:HB2	1:K:287:TYR:HB2	1.78	0.66
1:J:3:VAL:HG13	1:J:4:ILE:HG13	1.77	0.66
1:I:131:TRP:HD1	1:I:165:ILE:HD11	1.61	0.65
1:G:51:GLN:OE1	1:G:121:ASN:HB2	1.95	0.65
1:F:65:GLN:HB3	1:F:116:PRO:HG3	1.78	0.65
1:A:368:LYS:NZ	1:F:383:ASP:OD1	2.30	0.65
1:I:36:ILE:HB	1:I:106:VAL:HG23	1.78	0.65
1:B:36:ILE:HG12	1:B:106:VAL:HG23	1.79	0.65
1:H:36:ILE:HB	1:H:106:VAL:HG23	1.79	0.64
1:L:82:LEU:HD11	1:L:86:TRP:HB2	1.80	0.64
1:L:405:ARG:HB2	1:L:408:SER:HB3	1.79	0.64
1:B:182:VAL:HG13	1:H:163:LYS:HG3	1.79	0.64
1:D:100:ILE:HG13	1:D:104:ASN:HD21	1.61	0.64
1:B:61:ASN:O	1:B:119:LYS:NZ	2.26	0.64
1:G:174:THR:HG21	1:G:177:HIS:HB3	1.80	0.64
1:A:364:SER:HB2	1:A:366:GLU:HG3	1.81	0.63
1:K:100:ILE:HG23	1:K:101:GLY:H	1.63	0.63
1:A:138:GLY:HA2	1:A:214:GLY:HA3	1.81	0.63
1:A:394:ALA:HB1	1:A:417:TYR:HB3	1.80	0.63
1:B:382:VAL:HG11	1:B:387:THR:HG22	1.81	0.63
1:C:141:ARG:HB2	1:C:214:GLY:HA2	1.79	0.63
1:D:363:VAL:HG22	1:D:364:SER:H	1.63	0.63
1:B:373:VAL:HG21	1:H:350:ASN:HB3	1.80	0.63
1:A:182:VAL:HG22	1:I:163:LYS:HG3	1.79	0.63
1:A:350:ASN:HB3	1:F:373:VAL:HG21	1.81	0.63
1:C:135:PHE:HZ	1:C:173:VAL:HB	1.62	0.63
1:D:5:ARG:H	1:D:5:ARG:HD3	1.63	0.63
1:L:226:LEU:HD13	1:L:287:TYR:HB3	1.81	0.63
1:F:37:ARG:HD2	1:F:109:GLU:HG3	1.80	0.62
1:J:128:ASP:OD1	1:J:131:TRP:NE1	2.32	0.62
1:A:363:VAL:HG13	1:A:364:SER:H	1.63	0.62
1:A:144:ARG:HH22	1:A:221:LYS:HE2	1.64	0.62
1:E:394:ALA:HB1	1:E:417:TYR:HB3	1.81	0.62
1:J:42:ARG:NE	1:J:110:ASP:OD1	2.19	0.62
1:K:163:LYS:HG3	1:L:182:VAL:HG22	1.81	0.62
1:C:193:VAL:HG13	1:C:215:THR:HG23	1.81	0.62
1:H:197:ASP:OD1	1:H:215:THR:OG1	2.16	0.62
1:E:73:ALA:HA	1:E:76:LYS:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:382:VAL:HG11	1:I:387:THR:HG22	1.80	0.62
1:C:89:PHE:HE1	1:C:265:GLU:HB2	1.65	0.62
1:C:197:ASP:HB2	1:C:215:THR:HG22	1.82	0.62
1:H:3:VAL:HG22	1:H:4:ILE:HG13	1.82	0.62
1:H:8:THR:HG22	1:H:9:ASN:H	1.64	0.62
1:D:265:GLU:HG2	1:D:268:LYS:HD2	1.81	0.62
1:C:131:TRP:HD1	1:C:165:ILE:HD11	1.65	0.62
1:B:30:PHE:HA	1:B:34:ASN:HB3	1.81	0.61
1:D:39:TYR:O	1:D:188:ASN:ND2	2.33	0.61
1:L:266:ILE:HA	1:L:273:MET:HG2	1.82	0.61
1:B:266:ILE:HA	1:B:273:MET:SD	2.40	0.61
1:E:416:THR:OG1	1:B:307:ARG:NH2	2.32	0.61
1:B:174:THR:HG21	1:B:177:HIS:HB3	1.82	0.61
1:C:36:ILE:HB	1:C:106:VAL:HG23	1.83	0.61
1:A:166:LYS:HG3	1:A:167:SER:H	1.65	0.61
1:A:201:ASN:OD1	1:A:219:ARG:NH1	2.34	0.61
1:F:41:ASN:HB3	1:F:111:ILE:HG21	1.83	0.61
1:C:373:VAL:HG11	1:G:350:ASN:HB3	1.82	0.61
1:G:363:VAL:HG13	1:G:364:SER:H	1.66	0.61
1:I:151:ARG:NH2	1:I:175:ALA:O	2.34	0.60
1:K:141:ARG:HB2	1:K:214:GLY:HA2	1.83	0.60
1:G:135:PHE:HZ	1:G:173:VAL:HB	1.65	0.60
1:J:8:THR:HG22	1:J:9:ASN:H	1.65	0.60
1:F:63:ARG:HD2	1:F:66:HIS:CE1	2.37	0.60
1:C:158:LEU:HD22	1:C:169:TRP:HE1	1.66	0.60
1:H:382:VAL:HG11	1:H:387:THR:HG22	1.83	0.60
1:G:100:ILE:HG23	1:G:101:GLY:H	1.65	0.60
1:D:51:GLN:HB3	1:D:121:ASN:HA	1.83	0.60
1:H:363:VAL:HG13	1:H:364:SER:H	1.66	0.60
1:K:363:VAL:HG13	1:K:364:SER:H	1.67	0.60
1:B:128:ASP:HB2	1:B:131:TRP:NE1	2.16	0.60
1:D:65:GLN:N	1:D:65:GLN:OE1	2.35	0.60
1:D:82:LEU:HD11	1:D:100:ILE:HD12	1.82	0.60
1:D:373:VAL:HG21	1:L:350:ASN:HB3	1.83	0.60
1:A:226:LEU:HD13	1:A:287:TYR:HB3	1.84	0.59
1:E:174:THR:HG21	1:E:177:HIS:HB3	1.84	0.59
1:I:22:GLN:HG2	1:I:23:ALA:H	1.67	0.59
1:C:182:VAL:HG22	1:G:163:LYS:HG3	1.84	0.59
1:D:137:LEU:HD22	1:D:193:VAL:HG23	1.85	0.59
1:E:100:ILE:HG23	1:E:101:GLY:H	1.66	0.59
1:L:93:ILE:HD12	1:L:105:LEU:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:363:VAL:HG13	1:L:364:SER:H	1.66	0.59
1:I:8:THR:HG22	1:I:9:ASN:H	1.68	0.59
1:G:197:ASP:OD1	1:G:275:TYR:OH	2.12	0.59
1:F:47:ASP:OD1	1:F:50:ARG:NH1	2.29	0.59
1:I:131:TRP:CD1	1:I:165:ILE:HD11	2.37	0.59
1:C:39:TYR:O	1:C:188:ASN:ND2	2.36	0.59
1:D:131:TRP:HD1	1:D:165:ILE:HG21	1.67	0.59
1:F:174:THR:HG21	1:F:177:HIS:HB3	1.84	0.59
1:I:67:VAL:HG13	1:I:136:LEU:HD13	1.85	0.59
1:D:212:ARG:O	1:D:216:ILE:HG13	2.03	0.59
1:E:8:THR:HG22	1:E:9:ASN:H	1.67	0.58
1:C:6:ILE:HD12	1:C:15:VAL:HG11	1.85	0.58
1:G:317:PRO:HG2	1:G:320:ILE:HD13	1.85	0.58
1:D:125:SER:O	1:D:127:GLU:N	2.36	0.58
1:A:174:THR:HG21	1:A:177:HIS:HB3	1.85	0.58
1:G:221:LYS:NZ	1:G:278:ASP:OD1	2.36	0.58
1:J:139:LEU:HB3	1:J:180:PHE:CD2	2.39	0.58
1:F:6:ILE:HD12	1:F:15:VAL:HG11	1.84	0.58
1:K:151:ARG:NH2	1:K:175:ALA:O	2.36	0.58
1:B:56:GLY:HA2	1:B:59:GLU:HB2	1.86	0.58
1:D:266:ILE:HA	1:D:273:MET:SD	2.43	0.58
1:J:67:VAL:HG13	1:J:136:LEU:HD13	1.85	0.58
1:A:38:LEU:HD12	1:A:106:VAL:HG11	1.86	0.58
1:J:137:LEU:HD22	1:J:193:VAL:HG23	1.85	0.58
1:F:50:ARG:NH2	1:F:129:ASP:OD2	2.34	0.58
1:K:38:LEU:HD11	1:K:192:ILE:HG13	1.85	0.58
1:J:125:SER:HB2	1:J:128:ASP:HB2	1.85	0.58
1:B:134:LEU:HD21	1:B:160:LYS:HB3	1.86	0.58
1:H:352:TYR:CD1	1:H:355:PRO:HD3	2.39	0.58
1:F:138:GLY:HA2	1:F:214:GLY:HA3	1.86	0.57
1:G:182:VAL:HA	1:J:163:LYS:HG3	1.85	0.57
1:H:79:ARG:HD3	1:H:99:LYS:HB3	1.86	0.57
1:B:261:LYS:O	1:B:264:GLN:NE2	2.37	0.57
1:L:79:ARG:HD2	1:L:99:LYS:HB3	1.85	0.57
1:L:174:THR:HG21	1:L:177:HIS:HB3	1.86	0.57
1:E:22:GLN:OE1	1:E:258:LYS:NZ	2.37	0.57
1:H:131:TRP:HD1	1:H:165:ILE:HD11	1.70	0.57
1:D:8:THR:HG22	1:D:9:ASN:H	1.69	0.57
1:F:39:TYR:HB2	1:F:188:ASN:HD21	1.69	0.57
1:K:8:THR:HG22	1:K:9:ASN:H	1.67	0.57
1:C:72:TYR:O	1:C:76:LYS:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:MET:O	1:C:276:LEU:HG	2.05	0.57
1:D:182:VAL:HA	1:L:163:LYS:HG3	1.86	0.57
1:J:135:PHE:HZ	1:J:173:VAL:HB	1.69	0.57
1:G:141:ARG:HB2	1:G:214:GLY:HA2	1.85	0.57
1:I:394:ALA:HB1	1:I:417:TYR:HB3	1.87	0.57
1:D:273:MET:O	1:D:276:LEU:HG	2.05	0.57
1:A:8:THR:HG22	1:A:9:ASN:H	1.68	0.57
1:D:345:GLN:HG3	1:J:250:THR:HA	1.87	0.57
1:B:393:MET:HA	1:B:396:ARG:HD2	1.86	0.57
1:B:26:PRO:HB3	1:B:276:LEU:HD21	1.86	0.56
1:D:128:ASP:HB2	1:D:131:TRP:HE1	1.71	0.56
1:D:163:LYS:HG3	1:J:182:VAL:HG22	1.87	0.56
1:L:219:ARG:HD3	1:L:220:PHE:HD1	1.70	0.56
1:B:200:TYR:HB2	1:B:212:ARG:HD3	1.86	0.56
1:C:88:SER:O	1:C:90:GLY:N	2.36	0.56
1:G:131:TRP:CD1	1:G:165:ILE:HD11	2.40	0.56
1:D:304:ALA:O	1:D:307:ARG:N	2.35	0.56
1:G:382:VAL:HG21	1:G:387:THR:HG22	1.86	0.56
1:E:128:ASP:HB2	1:E:131:TRP:HE1	1.70	0.56
1:E:163:LYS:HG3	1:I:182:VAL:HG22	1.87	0.56
1:J:26:PRO:HG2	1:J:264:GLN:HG3	1.88	0.56
1:L:100:ILE:HG13	1:L:104:ASN:HD21	1.70	0.56
1:E:135:PHE:CZ	1:E:173:VAL:HB	2.41	0.56
1:B:150:TYR:HE2	1:B:178:LYS:HG2	1.71	0.56
1:H:62:CYS:HB3	1:H:179:TYR:HE1	1.70	0.56
1:A:238:LEU:HD21	1:A:370:ARG:HD3	1.87	0.56
1:H:25:TYR:OH	1:H:258:LYS:O	2.19	0.56
1:A:55:MET:SD	1:A:122:ALA:HB2	2.46	0.56
1:E:26:PRO:HB2	1:E:89:PHE:CE2	2.41	0.56
1:E:324:SER:HB2	1:B:340:PRO:O	2.06	0.55
1:A:128:ASP:HB2	1:A:131:TRP:HE1	1.70	0.55
1:H:134:LEU:HD11	1:H:160:LYS:HE3	1.87	0.55
1:H:198:MET:HB2	1:H:275:TYR:CE2	2.41	0.55
1:L:138:GLY:HA2	1:L:214:GLY:HA3	1.89	0.55
1:E:21:ASP:OD2	1:B:204:LYS:NZ	2.26	0.55
1:K:342:ILE:HG23	1:L:248:LEU:HD13	1.87	0.55
1:C:241:GLU:HB3	1:H:6:ILE:HD11	1.87	0.55
1:A:273:MET:HG3	1:A:274:PRO:HD3	1.88	0.55
1:K:26:PRO:HB3	1:K:276:LEU:HD13	1.89	0.55
1:L:8:THR:HG22	1:L:9:ASN:H	1.71	0.55
1:L:36:ILE:HD12	1:L:36:ILE:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:ARG:HH11	1:E:355:PRO:HB3	1.71	0.55
1:E:363:VAL:HG13	1:E:364:SER:H	1.71	0.55
1:F:276:LEU:HD21	1:F:286:PRO:HD2	1.88	0.55
1:K:79:ARG:H	1:K:79:ARG:HD2	1.71	0.55
1:H:128:ASP:HB2	1:H:131:TRP:HE1	1.71	0.55
1:J:150:TYR:HH	1:J:180:PHE:HE1	1.54	0.55
1:D:352:TYR:O	1:D:354:LYS:HG2	2.07	0.55
1:J:107:ARG:HG2	1:J:109:GLU:HG3	1.87	0.55
1:E:304:ALA:O	1:E:307:ARG:N	2.37	0.55
1:F:64:ILE:HD13	1:F:183:TRP:CG	2.41	0.55
1:I:238:LEU:HD21	1:I:370:ARG:HD3	1.89	0.55
1:H:158:LEU:HD23	1:H:161:GLN:HE21	1.71	0.55
1:D:228:THR:HG23	1:D:300:GLN:HG2	1.88	0.55
1:C:363:VAL:HG13	1:C:364:SER:H	1.71	0.54
1:J:363:VAL:HG13	1:J:364:SER:H	1.71	0.54
1:D:142:VAL:HG22	1:D:153:LEU:HB3	1.89	0.54
1:A:57:LEU:HD11	1:A:135:PHE:HE2	1.73	0.54
1:K:93:ILE:HD13	1:K:105:LEU:HG	1.90	0.54
1:E:364:SER:O	1:E:378:TRP:NE1	2.38	0.54
1:B:240:ILE:HD12	1:B:240:ILE:H	1.73	0.54
1:A:299:GLY:O	1:A:303:ALA:N	2.34	0.54
1:E:31:GLU:O	1:E:34:ASN:ND2	2.38	0.54
1:E:38:LEU:HG	1:E:40:VAL:HG13	1.88	0.54
1:G:131:TRP:HD1	1:G:165:ILE:HD11	1.72	0.54
1:I:305:LEU:HA	1:I:397:VAL:HG11	1.90	0.54
1:G:51:GLN:HE22	1:G:123:GLU:C	2.10	0.54
1:L:159:ILE:O	1:L:163:LYS:HD3	2.08	0.54
1:A:75:LEU:O	1:A:102:PRO:HG2	2.07	0.54
1:G:26:PRO:HB3	1:G:276:LEU:HD22	1.90	0.54
1:L:82:LEU:HD22	1:L:100:ILE:HD12	1.89	0.54
1:E:79:ARG:H	1:E:79:ARG:HD2	1.73	0.54
1:B:248:LEU:HD21	1:B:376:ILE:HD11	1.90	0.54
1:C:166:LYS:HD3	1:H:61:ASN:HD21	1.73	0.54
1:D:299:GLY:O	1:D:303:ALA:N	2.35	0.54
1:L:160:LYS:HE2	1:L:213:TRP:HB2	1.90	0.54
1:E:158:LEU:HD23	1:E:161:GLN:HE21	1.72	0.53
1:F:317:PRO:O	1:F:320:ILE:HG12	2.07	0.53
1:D:67:VAL:HG13	1:D:136:LEU:HD13	1.89	0.53
1:E:81:LEU:HD21	1:E:99:LYS:HE3	1.90	0.53
1:E:140:TYR:HE2	1:E:218:SER:HB2	1.74	0.53
1:E:354:LYS:HD2	1:E:354:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:TYR:OH	1:D:144:ARG:NH2	2.41	0.53
1:E:139:LEU:HA	1:E:142:VAL:HG12	1.91	0.53
1:I:158:LEU:HD23	1:I:161:GLN:HE21	1.72	0.53
1:J:159:ILE:O	1:J:163:LYS:HD3	2.09	0.53
1:A:412:TRP:O	1:A:416:THR:HG22	2.09	0.53
1:A:139:LEU:HG	1:A:180:PHE:CD2	2.44	0.53
1:K:304:ALA:O	1:K:307:ARG:N	2.39	0.53
1:I:51:GLN:OE1	1:I:121:ASN:HB2	2.09	0.53
1:H:304:ALA:O	1:H:307:ARG:N	2.37	0.53
1:J:256:LEU:O	1:J:260:MET:HG2	2.08	0.53
1:A:30:PHE:HE2	1:A:272:TYR:HD2	1.57	0.53
1:A:212:ARG:O	1:A:216:ILE:HG13	2.09	0.53
1:F:223:CYS:HB2	1:F:287:TYR:HB2	1.90	0.53
1:F:321:ASP:O	1:F:323:MET:N	2.42	0.53
1:G:61:ASN:O	1:G:119:LYS:HE3	2.09	0.53
1:E:395:LYS:HG2	1:E:418:GLY:HA2	1.90	0.53
1:I:236:THR:HG22	1:I:238:LEU:HG	1.90	0.53
1:C:55:MET:HG2	1:C:122:ALA:HB2	1.91	0.53
1:E:142:VAL:HG13	1:E:180:PHE:HE2	1.75	0.52
1:F:134:LEU:HD21	1:F:160:LYS:HE3	1.90	0.52
1:B:23:ALA:HB2	1:B:291:LYS:HG2	1.91	0.52
1:B:44:GLU:HG3	1:B:49:LEU:HD21	1.90	0.52
1:B:55:MET:SD	1:B:122:ALA:HB2	2.49	0.52
1:H:3:VAL:HG13	1:H:4:ILE:H	1.73	0.52
1:B:35:GLU:HB3	1:B:37:ARG:NH1	2.24	0.52
1:G:8:THR:HG22	1:G:9:ASN:H	1.74	0.52
1:F:353:ARG:NH1	1:K:380:SER:OG	2.43	0.52
1:C:100:ILE:HG23	1:C:101:GLY:H	1.73	0.52
1:L:294:SER:HB2	1:L:320:ILE:HD11	1.92	0.52
1:E:128:ASP:HB2	1:E:131:TRP:NE1	2.24	0.52
1:E:135:PHE:HZ	1:E:173:VAL:HB	1.75	0.52
1:E:193:VAL:HG13	1:E:215:THR:HG22	1.90	0.52
1:E:249:GLN:NE2	1:E:325:ILE:HA	2.25	0.52
1:F:8:THR:HG22	1:F:9:ASN:H	1.74	0.52
1:C:305:LEU:HA	1:C:397:VAL:HG11	1.90	0.52
1:J:315:ARG:H	1:J:315:ARG:HD2	1.75	0.52
1:A:131:TRP:CD1	1:A:165:ILE:HD11	2.45	0.52
1:F:35:GLU:OE1	1:F:91:HIS:NE2	2.43	0.52
1:D:37:ARG:HE	1:D:107:ARG:HH22	1.56	0.52
1:J:7:LYS:HG2	1:J:8:THR:H	1.75	0.52
1:L:66:HIS:NE2	1:L:116:PRO:HB2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:GLY:HA2	1:E:150:TYR:HE1	1.75	0.52
1:K:135:PHE:HZ	1:K:173:VAL:HB	1.74	0.52
1:E:244:PHE:CZ	1:E:256:LEU:HD23	2.45	0.52
1:G:151:ARG:HH12	1:G:175:ALA:HB1	1.74	0.52
1:G:158:LEU:HD23	1:G:161:GLN:HE21	1.74	0.52
1:B:387:THR:H	1:B:390:MET:HE3	1.75	0.52
1:B:397:VAL:HG12	1:B:413:ILE:HG21	1.92	0.52
1:C:79:ARG:HA	1:C:101:GLY:HA2	1.92	0.52
1:D:138:GLY:HA2	1:D:214:GLY:HA3	1.92	0.52
1:L:158:LEU:HD22	1:L:169:TRP:HE1	1.75	0.52
1:E:52:TYR:CZ	1:E:118:GLY:HA2	2.45	0.51
1:F:63:ARG:HD2	1:F:66:HIS:HE1	1.74	0.51
1:K:321:ASP:O	1:K:323:MET:N	2.43	0.51
1:D:342:ILE:HD11	1:J:248:LEU:HD13	1.92	0.51
1:J:138:GLY:HA2	1:J:214:GLY:HA3	1.90	0.51
1:I:255:GLU:OE2	1:I:294:SER:HB2	2.10	0.51
1:I:363:VAL:HG13	1:I:364:SER:H	1.74	0.51
1:B:248:LEU:HD13	1:H:342:ILE:HG23	1.92	0.51
1:C:131:TRP:CE2	1:C:132:LEU:HD22	2.45	0.51
1:A:59:GLU:OE1	1:A:119:LYS:NZ	2.43	0.51
1:A:273:MET:O	1:A:276:LEU:HG	2.10	0.51
1:I:197:ASP:OD2	1:I:275:TYR:OH	2.16	0.51
1:B:319:GLU:HG2	1:H:231:HIS:CE1	2.46	0.51
1:G:59:GLU:OE1	1:G:119:LYS:NZ	2.36	0.51
1:H:231:HIS:CE1	1:H:235:ILE:HD11	2.46	0.51
1:D:403:GLY:H	1:D:404:PRO:HD3	1.76	0.51
1:L:240:ILE:H	1:L:240:ILE:HD12	1.76	0.51
1:A:36:ILE:HD12	1:A:36:ILE:H	1.75	0.51
1:A:382:VAL:HG11	1:A:387:THR:HG22	1.92	0.51
1:B:142:VAL:HG11	1:B:154:LEU:HG	1.92	0.51
1:G:41:ASN:HD22	1:G:116:PRO:HD3	1.74	0.51
1:E:234:LYS:HD2	1:I:319:GLU:HB3	1.91	0.51
1:B:57:LEU:HG	1:B:172:PRO:HB2	1.92	0.51
1:H:51:GLN:CG	1:H:121:ASN:HB3	2.39	0.51
1:K:186:ASP:OD1	1:K:189:TYR:N	2.36	0.51
1:C:273:MET:HG3	1:C:274:PRO:HD3	1.93	0.51
1:G:373:VAL:HG11	1:J:350:ASN:HB3	1.92	0.51
1:F:93:ILE:HD11	1:F:272:TYR:HE1	1.74	0.51
1:H:222:ASP:HB2	1:H:277:ILE:HD11	1.92	0.51
1:L:342:ILE:HG13	1:L:342:ILE:O	2.11	0.51
1:I:249:GLN:N	1:I:249:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:MET:O	1:B:336:LEU:HG	2.09	0.51
1:C:74:VAL:HG13	1:C:75:LEU:HG	1.93	0.51
1:G:377:ALA:HA	1:J:353:ARG:HD3	1.92	0.51
1:F:188:ASN:O	1:F:192:ILE:HD12	2.10	0.51
1:B:233:VAL:HG21	1:B:240:ILE:HG13	1.92	0.51
1:J:273:MET:O	1:J:276:LEU:HG	2.11	0.51
1:E:273:MET:O	1:E:276:LEU:HG	2.10	0.51
1:F:151:ARG:NH2	1:F:175:ALA:O	2.44	0.51
1:K:64:ILE:HD12	1:K:183:TRP:HA	1.92	0.51
1:C:93:ILE:HG22	1:C:100:ILE:HD11	1.92	0.51
1:H:394:ALA:HB1	1:H:417:TYR:HB3	1.93	0.51
1:E:41:ASN:ND2	1:E:116:PRO:HD3	2.26	0.50
1:G:182:VAL:HG22	1:J:163:LYS:HD2	1.92	0.50
1:J:364:SER:HB2	1:J:366:GLU:HG3	1.94	0.50
1:C:88:SER:OG	1:C:89:PHE:N	2.44	0.50
1:G:40:VAL:HG11	1:G:72:TYR:CD2	2.46	0.50
1:E:244:PHE:CE1	1:I:15:VAL:HG21	2.46	0.50
1:I:55:MET:SD	1:I:122:ALA:HB2	2.52	0.50
1:K:353:ARG:HB2	1:L:376:ILE:HG22	1.94	0.50
1:C:406:ASP:OD1	1:C:406:ASP:N	2.44	0.50
1:G:286:PRO:O	1:G:292:ASN:ND2	2.45	0.50
1:K:166:LYS:HG3	1:K:167:SER:H	1.76	0.50
1:B:85:ASP:OD1	1:B:96:GLN:N	2.45	0.50
1:C:238:LEU:HD21	1:C:370:ARG:HD3	1.93	0.50
1:G:317:PRO:O	1:G:320:ILE:HG12	2.12	0.50
1:D:249:GLN:HB2	1:D:252:VAL:HG22	1.92	0.50
1:A:304:ALA:O	1:A:307:ARG:N	2.40	0.50
1:E:256:LEU:O	1:E:260:MET:HG2	2.11	0.50
1:F:317:PRO:HG2	1:F:320:ILE:HD13	1.93	0.50
1:C:253:ALA:HB2	1:G:345:GLN:HG2	1.92	0.50
1:J:55:MET:SD	1:J:122:ALA:HB2	2.51	0.50
1:A:267:ASP:OD1	1:A:268:LYS:HG3	2.11	0.50
1:G:35:GLU:HG3	1:G:37:ARG:HG3	1.93	0.50
1:D:55:MET:HG3	1:D:120:LEU:O	2.12	0.50
1:J:68:ASN:ND2	1:J:188:ASN:HB2	2.26	0.50
1:E:344:GLN:NE2	1:E:352:TYR:HA	2.27	0.50
1:E:380:SER:OG	1:B:353:ARG:NE	2.44	0.50
1:G:341:ASP:HB2	1:G:370:ARG:NH1	2.26	0.50
1:J:134:LEU:HD11	1:J:160:LYS:HE3	1.93	0.50
1:L:273:MET:O	1:L:276:LEU:HD22	2.11	0.50
1:A:74:VAL:HG13	1:A:75:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:ASP:HB2	1:F:282:SER:HB2	1.94	0.49
1:C:158:LEU:HD23	1:C:161:GLN:NE2	2.26	0.49
1:G:198:MET:HB2	1:G:275:TYR:CE2	2.47	0.49
1:I:404:PRO:HB2	1:I:411:LYS:HG2	1.94	0.49
1:H:248:LEU:HD12	1:H:328:ALA:HB1	1.94	0.49
1:J:100:ILE:HG13	1:J:104:ASN:HD21	1.77	0.49
1:A:232:VAL:HA	1:A:235:ILE:HG22	1.94	0.49
1:L:390:MET:O	1:L:393:MET:HG3	2.12	0.49
1:E:26:PRO:HB2	1:E:89:PHE:CZ	2.47	0.49
1:E:314:ALA:O	1:E:409:VAL:HG23	2.12	0.49
1:F:135:PHE:HZ	1:F:173:VAL:HB	1.77	0.49
1:I:342:ILE:HG23	1:I:342:ILE:O	2.13	0.49
1:B:242:GLU:O	1:B:245:THR:HG22	2.12	0.49
1:L:61:ASN:O	1:L:119:LYS:NZ	2.43	0.49
1:E:39:TYR:O	1:E:188:ASN:ND2	2.44	0.49
1:E:132:LEU:HB3	1:E:133:PRO:HD3	1.93	0.49
1:F:166:LYS:HG2	1:K:63:ARG:HH11	1.77	0.49
1:K:412:TRP:O	1:K:416:THR:HG22	2.13	0.49
1:H:305:LEU:HA	1:H:397:VAL:HG11	1.93	0.49
1:F:261:LYS:O	1:F:264:GLN:HG2	2.12	0.49
1:F:29:PHE:HE2	1:F:36:ILE:HG22	1.78	0.49
1:G:81:LEU:HD21	1:G:97:GLY:HA2	1.95	0.49
1:H:388:ASP:O	1:H:389:ASP:HB2	2.12	0.49
1:J:135:PHE:HD1	1:J:161:GLN:HE22	1.60	0.49
1:I:41:ASN:OD1	1:I:111:ILE:HG21	2.12	0.49
1:K:41:ASN:ND2	1:K:69:ALA:HB2	2.28	0.49
1:C:137:LEU:HD22	1:C:193:VAL:HG22	1.94	0.49
1:A:93:ILE:HG22	1:A:100:ILE:HD11	1.94	0.49
1:A:367:PRO:HG2	1:A:375:TRP:CE2	2.48	0.49
1:E:36:ILE:HG13	1:E:106:VAL:HG23	1.95	0.49
1:I:87:ASP:HB3	1:I:92:LYS:HG3	1.95	0.49
1:G:41:ASN:ND2	1:G:116:PRO:HD3	2.28	0.49
1:G:411:LYS:HE2	1:G:415:GLN:NE2	2.28	0.49
1:H:261:LYS:O	1:H:264:GLN:HG2	2.13	0.49
1:A:100:ILE:HG13	1:A:104:ASN:HD21	1.78	0.48
1:A:137:LEU:HD13	1:A:196:VAL:HG11	1.95	0.48
1:E:66:HIS:NE2	1:E:116:PRO:HB2	2.28	0.48
1:E:182:VAL:HG13	1:B:163:LYS:HG3	1.95	0.48
1:J:57:LEU:HG	1:J:172:PRO:HB2	1.94	0.48
1:J:226:LEU:HD13	1:J:287:TYR:HB3	1.94	0.48
1:E:50:ARG:NH1	1:E:126:ALA:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:ILE:HD12	1:F:240:ILE:H	1.78	0.48
1:K:56:GLY:HA3	1:K:62:CYS:HA	1.94	0.48
1:L:39:TYR:HB3	1:L:111:ILE:HG22	1.94	0.48
1:A:23:ALA:HB2	1:A:284:LYS:HE3	1.95	0.48
1:A:321:ASP:HA	1:I:235:ILE:O	2.13	0.48
1:E:47:ASP:O	1:E:51:GLN:HG3	2.14	0.48
1:E:139:LEU:HD12	1:E:183:TRP:CZ3	2.48	0.48
1:F:252:VAL:HG13	1:F:295:PHE:HA	1.95	0.48
1:G:26:PRO:HB2	1:G:89:PHE:CZ	2.48	0.48
1:H:128:ASP:HB2	1:H:131:TRP:NE1	2.28	0.48
1:E:182:VAL:HG22	1:B:163:LYS:HG3	1.94	0.48
1:D:70:TYR:CZ	1:D:132:LEU:HD23	2.49	0.48
1:L:261:LYS:O	1:L:264:GLN:HG2	2.13	0.48
1:C:178:LYS:HB2	1:C:181:ASP:OD2	2.14	0.48
1:A:246:TRP:CE2	1:A:372:VAL:HG22	2.48	0.48
1:G:182:VAL:HG13	1:J:163:LYS:HG3	1.95	0.48
1:H:218:SER:OG	1:H:278:ASP:OD2	2.26	0.48
1:H:353:ARG:O	1:H:353:ARG:HG2	2.14	0.48
1:L:46:LEU:HD13	1:L:73:ALA:HB1	1.95	0.48
1:L:218:SER:OG	1:L:278:ASP:OD2	2.16	0.48
1:A:226:LEU:HD21	1:A:266:ILE:HG23	1.96	0.48
1:I:207:ILE:HD12	1:I:207:ILE:H	1.79	0.48
1:K:41:ASN:HB2	1:K:115:LEU:HD13	1.96	0.48
1:C:246:TRP:CE2	1:C:372:VAL:HG22	2.49	0.48
1:K:242:GLU:O	1:K:245:THR:HG22	2.14	0.48
1:G:70:TYR:OH	1:G:129:ASP:OD1	2.22	0.48
1:G:369:ASN:ND2	1:G:374:GLU:OE1	2.45	0.48
1:H:197:ASP:O	1:H:201:ASN:N	2.47	0.48
1:J:197:ASP:OD2	1:J:275:TYR:OH	2.17	0.48
1:J:314:ALA:O	1:J:409:VAL:HG23	2.14	0.48
1:A:128:ASP:HB2	1:A:131:TRP:NE1	2.29	0.47
1:E:247:VAL:HG11	1:E:253:ALA:HB2	1.95	0.47
1:C:66:HIS:NE2	1:C:116:PRO:HB2	2.30	0.47
1:I:7:LYS:HA	1:I:12:VAL:HA	1.96	0.47
1:L:238:LEU:HD21	1:L:370:ARG:HD3	1.96	0.47
1:K:261:LYS:O	1:K:264:GLN:HG2	2.13	0.47
1:D:197:ASP:OD1	1:D:275:TYR:OH	2.28	0.47
1:E:342:ILE:HG23	1:E:342:ILE:O	2.14	0.47
1:B:235:ILE:HG12	1:B:308:SER:HB3	1.96	0.47
1:J:224:ALA:O	1:J:228:THR:HG23	2.14	0.47
1:A:409:VAL:O	1:A:413:ILE:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:GLU:O	1:E:127:GLU:HG2	2.13	0.47
1:F:358:GLU:OE1	1:F:358:GLU:N	2.46	0.47
1:B:198:MET:HE1	1:B:272:TYR:HA	1.97	0.47
1:D:52:TYR:HB3	1:D:66:HIS:CD2	2.49	0.47
1:J:166:LYS:CG	1:J:167:SER:H	2.25	0.47
1:A:315:ARG:H	1:A:315:ARG:HD3	1.79	0.47
1:I:193:VAL:HG13	1:I:215:THR:HG22	1.96	0.47
1:I:367:PRO:HG2	1:I:375:TRP:CE2	2.49	0.47
1:I:386:PRO:HB2	1:I:391:LEU:HD22	1.96	0.47
1:D:66:HIS:CE1	1:D:119:LYS:HD2	2.49	0.47
1:D:86:TRP:HH2	1:D:198:MET:HG2	1.80	0.47
1:J:144:ARG:HD2	1:J:217:VAL:HG21	1.95	0.47
1:A:286:PRO:HA	1:A:291:LYS:HG2	1.95	0.47
1:E:353:ARG:NH2	1:I:380:SER:OG	2.48	0.47
1:F:246:TRP:CD2	1:F:332:MET:HG3	2.49	0.47
1:F:314:ALA:HB3	1:F:409:VAL:HG23	1.97	0.47
1:I:21:ASP:OD1	1:I:22:GLN:N	2.48	0.47
1:I:74:VAL:HG13	1:I:75:LEU:HG	1.96	0.47
1:K:74:VAL:HG13	1:K:75:LEU:HG	1.95	0.47
1:K:112:PRO:O	1:K:114:GLY:N	2.48	0.47
1:K:267:ASP:OD1	1:K:267:ASP:N	2.47	0.47
1:B:135:PHE:CZ	1:B:173:VAL:HB	2.50	0.47
1:G:39:TYR:HB3	1:G:111:ILE:HA	1.97	0.47
1:D:135:PHE:HE1	1:D:139:LEU:HD11	1.80	0.47
1:K:128:ASP:HB3	1:K:131:TRP:CH2	2.50	0.47
1:C:342:ILE:HG23	1:C:342:ILE:O	2.15	0.47
1:G:140:TYR:CD2	1:G:193:VAL:HG11	2.50	0.47
1:D:66:HIS:NE2	1:D:116:PRO:HB2	2.30	0.47
1:D:86:TRP:HZ3	1:D:93:ILE:HD13	1.80	0.47
1:D:317:PRO:HG2	1:D:320:ILE:HD13	1.96	0.47
1:D:404:PRO:HG2	1:D:411:LYS:HE3	1.96	0.47
1:J:108:VAL:HG12	1:J:108:VAL:O	2.14	0.47
1:F:24:ASP:O	1:F:25:TYR:HB2	2.14	0.47
1:I:56:GLY:HA2	1:I:119:LYS:HZ2	1.79	0.47
1:K:135:PHE:CZ	1:K:173:VAL:HB	2.50	0.47
1:B:111:ILE:HG13	1:B:112:PRO:HD2	1.97	0.47
1:C:63:ARG:HH11	1:G:166:LYS:HB3	1.79	0.47
1:G:182:VAL:HG13	1:J:163:LYS:HA	1.96	0.47
1:J:36:ILE:HG13	1:J:106:VAL:HG23	1.97	0.47
1:A:135:PHE:HZ	1:A:173:VAL:HB	1.80	0.47
1:A:382:VAL:HG12	1:A:382:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TRP:CE2	1:D:270:THR:HG23	2.50	0.47
1:D:242:GLU:O	1:D:245:THR:OG1	2.30	0.47
1:L:320:ILE:HG13	1:L:321:ASP:H	1.80	0.47
1:L:387:THR:HG23	1:L:390:MET:H	1.80	0.47
1:E:41:ASN:HD21	1:E:115:LEU:HA	1.80	0.46
1:B:367:PRO:HG2	1:B:375:TRP:CE2	2.50	0.46
1:G:16:LEU:HD13	1:J:267:ASP:HB3	1.97	0.46
1:H:212:ARG:O	1:H:216:ILE:HG13	2.15	0.46
1:D:342:ILE:HG23	1:D:342:ILE:O	2.14	0.46
1:E:235:ILE:HD12	1:I:320:ILE:O	2.15	0.46
1:A:100:ILE:CG1	1:A:104:ASN:HD21	2.28	0.46
1:A:135:PHE:CZ	1:A:173:VAL:HB	2.50	0.46
1:I:24:ASP:O	1:I:286:PRO:HD3	2.15	0.46
1:K:72:TYR:HA	1:K:103:PHE:HE2	1.80	0.46
1:L:212:ARG:HH21	1:L:216:ILE:HD13	1.79	0.46
1:F:404:PRO:HB2	1:F:411:LYS:HG2	1.96	0.46
1:I:139:LEU:O	1:I:143:GLY:N	2.40	0.46
1:J:207:ILE:H	1:J:207:ILE:HD12	1.79	0.46
1:L:248:LEU:HD21	1:L:376:ILE:HD11	1.98	0.46
1:E:64:ILE:HD13	1:E:183:TRP:CG	2.50	0.46
1:E:219:ARG:NH1	1:E:274:PRO:HG2	2.30	0.46
1:F:51:GLN:CB	1:F:121:ASN:HB3	2.44	0.46
1:F:87:ASP:OD1	1:F:92:LYS:HD3	2.16	0.46
1:F:177:HIS:NE2	1:F:179:TYR:HB3	2.31	0.46
1:F:233:VAL:HG21	1:F:240:ILE:HG13	1.97	0.46
1:I:74:VAL:HG11	1:I:133:PRO:HG3	1.98	0.46
1:I:314:ALA:O	1:I:409:VAL:HG23	2.15	0.46
1:B:100:ILE:HG13	1:B:104:ASN:HD21	1.80	0.46
1:G:79:ARG:HG3	1:G:99:LYS:HB3	1.96	0.46
1:D:135:PHE:HZ	1:D:173:VAL:HB	1.79	0.46
1:D:207:ILE:HD12	1:D:207:ILE:H	1.80	0.46
1:J:364:SER:O	1:J:378:TRP:NE1	2.39	0.46
1:A:241:GLU:HA	1:F:6:ILE:HD11	1.97	0.46
1:F:47:ASP:O	1:F:51:GLN:HG3	2.15	0.46
1:G:53:VAL:HG13	1:G:67:VAL:HG12	1.97	0.46
1:G:305:LEU:HD23	1:G:413:ILE:HD13	1.97	0.46
1:D:55:MET:HG2	1:D:122:ALA:HB2	1.97	0.46
1:D:131:TRP:CD1	1:D:165:ILE:HG21	2.49	0.46
1:I:79:ARG:HA	1:I:101:GLY:HA2	1.98	0.46
1:C:158:LEU:HA	1:C:161:GLN:HE21	1.80	0.46
1:C:367:PRO:HG2	1:C:375:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:TYR:CD2	1:G:390:MET:HG2	2.50	0.46
1:D:256:LEU:O	1:D:260:MET:HG2	2.15	0.46
1:J:128:ASP:O	1:J:132:LEU:HD23	2.15	0.46
1:A:235:ILE:HD12	1:F:320:ILE:O	2.16	0.46
1:A:316:GLN:H	1:A:408:SER:HA	1.81	0.46
1:E:6:ILE:HG13	1:E:15:VAL:HG11	1.98	0.46
1:E:247:VAL:HG13	1:E:252:VAL:HG23	1.98	0.46
1:F:223:CYS:CB	1:F:287:TYR:HB2	2.46	0.46
1:I:59:GLU:C	1:I:61:ASN:H	2.18	0.46
1:C:93:ILE:HD11	1:C:272:TYR:HE1	1.81	0.46
1:G:183:TRP:N	1:G:183:TRP:CD1	2.84	0.46
1:D:41:ASN:ND2	1:D:115:LEU:HD13	2.24	0.46
1:L:367:PRO:HG2	1:L:375:TRP:CE2	2.51	0.46
1:K:35:GLU:OE2	1:K:91:HIS:NE2	2.46	0.46
1:B:38:LEU:HA	1:B:191:LYS:HD3	1.97	0.46
1:H:156:GLU:O	1:H:160:LYS:HG3	2.16	0.46
1:E:382:VAL:HG11	1:E:387:THR:HG22	1.98	0.46
1:E:392:MET:O	1:E:396:ARG:HG2	2.15	0.46
1:F:150:TYR:HE2	1:F:176:THR:HA	1.81	0.46
1:K:100:ILE:HG13	1:K:104:ASN:HD21	1.80	0.46
1:B:314:ALA:O	1:B:409:VAL:HG23	2.16	0.46
1:C:55:MET:HG3	1:C:120:LEU:O	2.16	0.46
1:C:342:ILE:HD11	1:H:248:LEU:HD13	1.98	0.46
1:J:358:GLU:O	1:J:360:SER:N	2.48	0.46
1:E:22:GLN:HA	1:E:291:LYS:HE2	1.98	0.45
1:F:342:ILE:O	1:F:342:ILE:HG13	2.16	0.45
1:G:6:ILE:HD12	1:G:15:VAL:HG12	1.97	0.45
1:G:70:TYR:CZ	1:G:132:LEU:HD23	2.51	0.45
1:H:108:VAL:HG13	1:H:109:GLU:H	1.81	0.45
1:H:131:TRP:CD1	1:H:165:ILE:HD11	2.50	0.45
1:D:261:LYS:HG3	1:D:264:GLN:HE21	1.80	0.45
1:A:380:SER:OG	1:I:353:ARG:NH1	2.49	0.45
1:F:29:PHE:CE2	1:F:36:ILE:HG22	2.51	0.45
1:F:267:ASP:HB3	1:K:16:LEU:HB3	1.97	0.45
1:K:131:TRP:CE2	1:K:169:TRP:HZ3	2.33	0.45
1:K:321:ASP:HB3	1:K:325:ILE:HG13	1.96	0.45
1:G:26:PRO:HA	1:G:281:ILE:HG22	1.99	0.45
1:E:198:MET:HE1	1:E:272:TYR:CD1	2.52	0.45
1:C:246:TRP:CD2	1:C:332:MET:HG3	2.51	0.45
1:H:267:ASP:OD1	1:H:267:ASP:N	2.48	0.45
1:D:120:LEU:HG	1:D:121:ASN:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:307:ARG:HE	1:L:397:VAL:HG22	1.81	0.45
1:I:221:LYS:HD2	1:I:277:ILE:HG21	1.97	0.45
1:I:340:PRO:O	1:I:342:ILE:N	2.49	0.45
1:B:226:LEU:HD11	1:B:266:ILE:HD11	1.99	0.45
1:E:38:LEU:HD11	1:E:192:ILE:HG22	1.98	0.45
1:E:285:SER:OG	1:E:288:SER:OG	2.29	0.45
1:I:304:ALA:O	1:I:307:ARG:N	2.42	0.45
1:D:36:ILE:HB	1:D:106:VAL:HG23	1.99	0.45
1:L:228:THR:O	1:L:232:VAL:HG23	2.15	0.45
1:A:261:LYS:HD3	1:A:262:PRO:HD2	1.97	0.45
1:F:149:ALA:HA	1:F:152:THR:HG22	1.97	0.45
1:F:158:LEU:HD21	1:F:173:VAL:HG11	1.98	0.45
1:F:269:SER:OG	1:F:270:THR:N	2.50	0.45
1:B:228:THR:O	1:B:232:VAL:HG23	2.17	0.45
1:C:307:ARG:HE	1:H:416:THR:HG22	1.80	0.45
1:D:38:LEU:HD11	1:D:192:ILE:HG23	1.99	0.45
1:J:293:PRO:O	1:J:296:HIS:N	2.49	0.45
1:L:137:LEU:HD13	1:L:196:VAL:HG11	1.99	0.45
1:A:132:LEU:HB3	1:A:133:PRO:HD3	1.99	0.45
1:A:221:LYS:HG2	1:A:222:ASP:N	2.31	0.45
1:I:238:LEU:HD13	1:I:242:GLU:HB3	1.99	0.45
1:K:404:PRO:HG2	1:K:411:LYS:HE2	1.98	0.45
1:G:26:PRO:HB3	1:G:276:LEU:CD2	2.46	0.45
1:J:100:ILE:CG1	1:J:104:ASN:HD21	2.29	0.45
1:G:82:LEU:HA	1:G:203:PHE:HE1	1.81	0.45
1:J:261:LYS:O	1:J:264:GLN:NE2	2.39	0.45
1:E:80:GLU:O	1:E:100:ILE:HG22	2.17	0.45
1:F:233:VAL:HG11	1:F:240:ILE:HG13	1.99	0.45
1:K:86:TRP:CD2	1:K:93:ILE:HD11	2.52	0.45
1:B:273:MET:O	1:B:276:LEU:HG	2.16	0.45
1:C:309:LYS:NZ	1:C:400:THR:HB	2.32	0.45
1:G:142:VAL:HG22	1:G:153:LEU:HB3	1.98	0.45
1:G:160:LYS:HE2	1:G:213:TRP:HB2	1.98	0.45
1:G:226:LEU:HD13	1:G:287:TYR:HB3	1.99	0.45
1:D:228:THR:O	1:D:232:VAL:HG23	2.17	0.45
1:A:221:LYS:HD2	1:A:277:ILE:HB	1.99	0.45
1:E:140:TYR:CD2	1:E:193:VAL:HG11	2.51	0.45
1:F:105:LEU:HD12	1:F:105:LEU:H	1.82	0.45
1:K:167:SER:OG	1:L:61:ASN:OD1	2.29	0.45
1:H:220:PHE:CE1	1:H:274:PRO:HB3	2.52	0.45
1:D:6:ILE:HD11	1:L:241:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLU:HB2	1:D:107:ARG:HH21	1.82	0.45
1:D:63:ARG:HE	1:L:166:LYS:HD3	1.82	0.45
1:D:231:HIS:HD1	1:J:319:GLU:HG2	1.81	0.45
1:L:304:ALA:O	1:L:307:ARG:N	2.47	0.45
1:A:334:TYR:CD2	1:A:390:MET:HG3	2.52	0.44
1:E:89:PHE:HE1	1:E:265:GLU:HB2	1.81	0.44
1:E:261:LYS:O	1:E:264:GLN:HG2	2.16	0.44
1:K:93:ILE:HG13	1:K:94:GLY:N	2.32	0.44
1:B:37:ARG:HE	1:B:109:GLU:HG3	1.82	0.44
1:G:128:ASP:HB3	1:G:131:TRP:NE1	2.32	0.44
1:D:350:ASN:HB3	1:J:373:VAL:HG21	1.99	0.44
1:J:304:ALA:C	1:J:306:CYS:H	2.21	0.44
1:F:100:ILE:CG1	1:F:104:ASN:HD21	2.30	0.44
1:C:221:LYS:HD3	1:C:277:ILE:HD11	1.99	0.44
1:G:304:ALA:O	1:G:307:ARG:N	2.42	0.44
1:G:363:VAL:HG13	1:G:364:SER:N	2.32	0.44
1:E:342:ILE:HD11	1:I:248:LEU:HD13	2.00	0.44
1:I:236:THR:HG23	1:I:336:LEU:CD1	2.47	0.44
1:K:193:VAL:O	1:K:215:THR:OG1	2.32	0.44
1:C:138:GLY:HA2	1:C:214:GLY:HA3	1.98	0.44
1:J:159:ILE:HG23	1:J:163:LYS:NZ	2.33	0.44
1:J:212:ARG:HH21	1:J:216:ILE:HD13	1.83	0.44
1:K:55:MET:HG3	1:K:120:LEU:O	2.17	0.44
1:C:70:TYR:HE2	1:C:132:LEU:HB3	1.83	0.44
1:L:26:PRO:HA	1:L:281:ILE:HG22	1.99	0.44
1:A:6:ILE:HD11	1:I:241:GLU:HA	1.99	0.44
1:F:45:LYS:HA	1:F:45:LYS:HD3	1.59	0.44
1:F:304:ALA:O	1:F:307:ARG:N	2.47	0.44
1:I:246:TRP:O	1:I:248:LEU:HG	2.17	0.44
1:D:235:ILE:HD12	1:J:320:ILE:O	2.17	0.44
1:D:318:ASP:OD1	1:D:318:ASP:N	2.48	0.44
1:J:113:ASP:OD1	1:J:115:LEU:HD23	2.16	0.44
1:L:38:LEU:O	1:L:109:GLU:HB2	2.17	0.44
1:L:42:ARG:HG2	1:L:110:ASP:OD2	2.17	0.44
1:E:197:ASP:OD2	1:E:275:TYR:OH	2.22	0.44
1:I:276:LEU:HD11	1:I:285:SER:HB2	2.00	0.44
1:C:317:PRO:O	1:C:318:ASP:HB3	2.18	0.44
1:H:67:VAL:HG13	1:H:136:LEU:HD13	2.00	0.44
1:J:37:ARG:O	1:J:37:ARG:HG2	2.18	0.44
1:E:133:PRO:HB2	1:E:211:PHE:CZ	2.52	0.44
1:K:368:LYS:HE3	1:L:383:ASP:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:ILE:HG22	1:J:100:ILE:HD11	2.00	0.44
1:J:186:ASP:OD2	1:J:189:TYR:N	2.42	0.44
1:E:372:VAL:O	1:E:376:ILE:HG13	2.18	0.44
1:K:160:LYS:HE2	1:K:213:TRP:HB3	1.98	0.44
1:B:25:TYR:CE2	1:B:261:LYS:HD2	2.52	0.44
1:H:132:LEU:HB3	1:H:133:PRO:HD3	2.00	0.44
1:H:382:VAL:HG12	1:H:382:VAL:O	2.18	0.44
1:D:46:LEU:HG	1:D:73:ALA:HB1	2.00	0.44
1:D:290:ILE:HD12	1:D:290:ILE:H	1.82	0.44
1:D:412:TRP:CE2	1:D:416:THR:HG21	2.53	0.44
1:L:254:ASP:HA	1:L:257:VAL:HG22	1.99	0.44
1:I:89:PHE:HE1	1:I:265:GLU:HG3	1.83	0.44
1:I:358:GLU:O	1:I:360:SER:N	2.51	0.44
1:B:256:LEU:O	1:B:260:MET:HG2	2.18	0.44
1:D:35:GLU:CD	1:D:107:ARG:HE	2.21	0.44
1:J:28:THR:O	1:J:31:GLU:HG2	2.17	0.44
1:L:269:SER:O	1:L:271:SER:N	2.51	0.44
1:E:255:GLU:HB3	1:E:292:ASN:HB3	1.98	0.43
1:E:357:LYS:HD2	1:E:357:LYS:HA	1.80	0.43
1:G:221:LYS:HE2	1:G:277:ILE:HB	1.99	0.43
1:H:47:ASP:O	1:H:51:GLN:HG3	2.18	0.43
1:H:301:LEU:HD23	1:H:305:LEU:HD13	2.00	0.43
1:H:363:VAL:HG13	1:H:364:SER:N	2.32	0.43
1:D:26:PRO:HA	1:D:281:ILE:HG22	1.99	0.43
1:J:60:LYS:O	1:J:60:LYS:HG2	2.17	0.43
1:B:219:ARG:HD3	1:B:275:TYR:OH	2.19	0.43
1:C:277:ILE:HG13	1:C:278:ASP:N	2.32	0.43
1:G:67:VAL:HB	1:G:136:LEU:HD13	2.00	0.43
1:G:125:SER:HB2	1:G:128:ASP:HB2	2.00	0.43
1:G:178:LYS:HB2	1:G:181:ASP:OD2	2.18	0.43
1:H:19:ASN:CG	1:H:20:GLU:H	2.22	0.43
1:H:405:ARG:HB2	1:H:408:SER:HB2	2.00	0.43
1:J:262:PRO:O	1:J:264:GLN:N	2.45	0.43
1:E:76:LYS:O	1:E:79:ARG:NE	2.47	0.43
1:H:74:VAL:HG13	1:H:75:LEU:HG	1.99	0.43
1:H:235:ILE:HD13	1:H:308:SER:HB3	2.00	0.43
1:D:100:ILE:O	1:D:104:ASN:ND2	2.51	0.43
1:J:222:ASP:HB2	1:J:277:ILE:HD11	2.00	0.43
1:L:387:THR:HG22	1:L:390:MET:HG3	2.00	0.43
1:A:269:SER:O	1:A:271:SER:N	2.51	0.43
1:F:297:PHE:HE1	1:F:409:VAL:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ALA:O	1:C:409:VAL:HG23	2.19	0.43
1:E:26:PRO:HB3	1:E:276:LEU:HD21	2.00	0.43
1:I:356:PRO:HG2	1:I:358:GLU:OE2	2.19	0.43
1:C:382:VAL:HG12	1:C:382:VAL:O	2.18	0.43
1:H:3:VAL:HG13	1:H:4:ILE:N	2.33	0.43
1:H:393:MET:HA	1:H:396:ARG:HD2	2.01	0.43
1:D:165:ILE:HG13	1:D:166:LYS:N	2.26	0.43
1:K:55:MET:CG	1:K:122:ALA:HB2	2.42	0.43
1:K:157:SER:O	1:K:161:GLN:HG2	2.18	0.43
1:K:363:VAL:HG13	1:K:364:SER:N	2.34	0.43
1:G:135:PHE:CZ	1:G:173:VAL:HB	2.51	0.43
1:L:330:LEU:HD22	1:L:417:TYR:CE1	2.53	0.43
1:A:228:THR:O	1:A:232:VAL:HG13	2.19	0.43
1:E:83:GLU:O	1:E:96:GLN:NE2	2.51	0.43
1:E:270:THR:O	1:E:270:THR:OG1	2.31	0.43
1:F:29:PHE:CD2	1:F:281:ILE:HA	2.53	0.43
1:I:101:GLY:N	1:I:104:ASN:OD1	2.44	0.43
1:I:273:MET:HG3	1:I:274:PRO:HD3	2.01	0.43
1:C:27:SER:O	1:C:31:GLU:HG3	2.19	0.43
1:G:24:ASP:HB2	1:G:282:SER:HB2	2.00	0.43
1:D:144:ARG:HH22	1:D:221:LYS:CD	2.31	0.43
1:J:60:LYS:HB3	1:J:60:LYS:HE2	1.76	0.43
1:L:37:ARG:HD3	1:L:109:GLU:HG3	2.01	0.43
1:L:64:ILE:HA	1:L:67:VAL:HG22	2.01	0.43
1:L:363:VAL:HG13	1:L:364:SER:N	2.33	0.43
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.78	0.43
1:F:25:TYR:CD1	1:F:286:PRO:HG3	2.53	0.43
1:B:198:MET:HB2	1:B:275:TYR:CE2	2.54	0.43
1:H:158:LEU:HD22	1:H:169:TRP:HE1	1.84	0.43
1:A:330:LEU:HD12	1:A:417:TYR:CE2	2.54	0.43
1:E:53:VAL:HG11	1:E:136:LEU:HD11	2.00	0.43
1:E:165:ILE:HG13	1:E:166:LYS:N	2.30	0.43
1:E:249:GLN:HE21	1:E:325:ILE:HA	1.83	0.43
1:F:387:THR:HG23	1:F:390:MET:H	1.84	0.43
1:I:47:ASP:HA	1:I:50:ARG:HD2	2.00	0.43
1:I:186:ASP:O	1:I:190:LEU:HG	2.18	0.43
1:D:363:VAL:HG22	1:D:364:SER:N	2.31	0.43
1:D:364:SER:O	1:D:366:GLU:N	2.51	0.43
1:L:25:TYR:OH	1:L:258:LYS:O	2.33	0.43
1:A:255:GLU:O	1:A:259:MET:HB2	2.19	0.43
1:A:264:GLN:HB2	1:A:266:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:LEU:HD23	1:F:401:ILE:HG23	2.01	0.43
1:B:70:TYR:CZ	1:B:132:LEU:HD23	2.54	0.43
1:B:131:TRP:CD1	1:B:165:ILE:HD11	2.54	0.43
1:C:70:TYR:OH	1:C:129:ASP:OD1	2.32	0.43
1:C:75:LEU:O	1:C:102:PRO:HG2	2.19	0.43
1:C:100:ILE:HG23	1:C:101:GLY:N	2.32	0.43
1:H:60:LYS:HE3	1:H:60:LYS:HB2	1.89	0.43
1:H:204:LYS:HE3	1:H:204:LYS:HB2	1.89	0.43
1:H:382:VAL:HG11	1:H:387:THR:CG2	2.48	0.43
1:A:249:GLN:HB2	1:A:252:VAL:HG23	2.01	0.42
1:A:261:LYS:O	1:A:264:GLN:HG2	2.19	0.42
1:E:59:GLU:C	1:E:61:ASN:H	2.23	0.42
1:E:128:ASP:OD1	1:E:128:ASP:N	2.47	0.42
1:B:41:ASN:OD1	1:B:111:ILE:HD13	2.19	0.42
1:B:111:ILE:HG12	1:B:112:PRO:O	2.19	0.42
1:J:256:LEU:HD21	1:J:295:PHE:CE1	2.54	0.42
1:A:218:SER:OG	1:A:278:ASP:OD2	2.27	0.42
1:B:38:LEU:HD23	1:B:106:VAL:HG11	2.00	0.42
1:G:286:PRO:HA	1:G:291:LYS:HG2	1.99	0.42
1:H:269:SER:O	1:H:271:SER:N	2.50	0.42
1:D:230:GLY:O	1:D:234:LYS:HD2	2.19	0.42
1:A:50:ARG:CZ	1:A:126:ALA:HA	2.49	0.42
1:E:320:ILE:O	1:B:235:ILE:HD12	2.18	0.42
1:K:63:ARG:HG2	1:K:119:LYS:HE3	2.01	0.42
1:B:152:THR:O	1:B:156:GLU:HG3	2.20	0.42
1:C:256:LEU:HD21	1:C:295:PHE:CE1	2.54	0.42
1:C:261:LYS:O	1:C:264:GLN:HG2	2.18	0.42
1:G:166:LYS:CG	1:G:167:SER:H	2.28	0.42
1:D:59:GLU:C	1:D:61:ASN:H	2.22	0.42
1:L:255:GLU:OE1	1:L:295:PHE:N	2.42	0.42
1:A:248:LEU:HD13	1:I:342:ILE:HD11	2.00	0.42
1:A:376:ILE:HG22	1:I:353:ARG:HB2	2.01	0.42
1:E:66:HIS:CE1	1:E:116:PRO:HB2	2.54	0.42
1:C:140:TYR:CD2	1:C:193:VAL:HG11	2.55	0.42
1:H:45:LYS:O	1:H:48:VAL:HG22	2.20	0.42
1:D:232:VAL:O	1:D:236:THR:OG1	2.27	0.42
1:J:151:ARG:NH2	1:J:175:ALA:O	2.52	0.42
1:J:228:THR:HG22	1:J:300:GLN:NE2	2.34	0.42
1:L:305:LEU:HA	1:L:397:VAL:HG11	2.02	0.42
1:E:27:SER:HB2	1:E:263:GLY:O	2.18	0.42
1:F:93:ILE:HD13	1:F:105:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:ASP:HB3	1:I:282:SER:OG	2.20	0.42
1:I:159:ILE:O	1:I:163:LYS:HD3	2.20	0.42
1:K:290:ILE:HD12	1:K:290:ILE:H	1.83	0.42
1:G:41:ASN:OD1	1:G:41:ASN:N	2.53	0.42
1:G:197:ASP:CG	1:G:212:ARG:HE	2.23	0.42
1:H:72:TYR:O	1:H:76:LYS:HB2	2.20	0.42
1:H:134:LEU:HB2	1:H:211:PHE:CD1	2.55	0.42
1:A:247:VAL:HG13	1:A:252:VAL:HB	2.01	0.42
1:F:253:ALA:O	1:F:257:VAL:HG22	2.19	0.42
1:C:51:GLN:OE1	1:C:121:ASN:HB3	2.20	0.42
1:C:62:CYS:SG	1:C:183:TRP:HZ2	2.43	0.42
1:G:16:LEU:HD12	1:G:16:LEU:O	2.18	0.42
1:J:131:TRP:CZ2	1:J:169:TRP:HZ3	2.38	0.42
1:E:197:ASP:HA	1:E:212:ARG:HD2	2.02	0.42
1:E:367:PRO:HG2	1:E:375:TRP:CE2	2.54	0.42
1:F:54:TYR:O	1:F:58:VAL:HG23	2.19	0.42
1:F:201:ASN:HB2	1:F:212:ARG:NH1	2.35	0.42
1:I:89:PHE:CE1	1:I:265:GLU:HG3	2.55	0.42
1:K:219:ARG:HE	1:K:274:PRO:HG2	1.85	0.42
1:K:367:PRO:HG2	1:K:375:TRP:CE2	2.55	0.42
1:C:395:LYS:HG3	1:C:418:GLY:HA2	2.01	0.42
1:H:137:LEU:HD22	1:H:193:VAL:HG23	2.02	0.42
1:A:166:LYS:NZ	1:F:63:ARG:HH12	2.17	0.42
1:F:308:SER:O	1:F:309:LYS:HB2	2.20	0.42
1:G:314:ALA:O	1:G:409:VAL:HG23	2.19	0.42
1:H:266:ILE:HA	1:H:273:MET:HE2	2.02	0.42
1:D:39:TYR:HA	1:D:109:GLU:O	2.19	0.42
1:J:136:LEU:O	1:J:189:TYR:OH	2.30	0.42
1:A:74:VAL:HG11	1:A:133:PRO:HG3	2.01	0.42
1:A:345:GLN:HG3	1:F:250:THR:HA	2.02	0.42
1:E:266:ILE:HA	1:E:273:MET:HE2	2.02	0.42
1:K:238:LEU:HD23	1:K:336:LEU:HD21	2.02	0.42
1:B:336:LEU:HD22	1:B:370:ARG:NH1	2.35	0.42
1:C:63:ARG:HB2	1:C:66:HIS:ND1	2.34	0.42
1:C:124:VAL:HG12	1:C:124:VAL:O	2.19	0.42
1:H:150:TYR:HE2	1:H:176:THR:HA	1.85	0.42
1:D:197:ASP:OD2	1:D:215:THR:HG23	2.19	0.42
1:J:88:SER:HB2	1:J:271:SER:HA	2.00	0.42
1:J:120:LEU:HD12	1:J:120:LEU:HA	1.82	0.42
1:J:231:HIS:CD2	1:J:235:ILE:HG13	2.55	0.42
1:J:266:ILE:HA	1:J:273:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:346:PHE:C	1:J:347:SER:HG	2.23	0.42
1:J:363:VAL:HG13	1:J:364:SER:N	2.34	0.42
1:L:100:ILE:HG23	1:L:101:GLY:N	2.30	0.42
1:E:246:TRP:CE2	1:E:372:VAL:HG22	2.55	0.42
1:E:331:LEU:HD22	1:E:379:TYR:CD2	2.55	0.42
1:I:222:ASP:O	1:I:285:SER:OG	2.37	0.42
1:G:51:GLN:NE2	1:G:124:VAL:HA	2.35	0.42
1:H:57:LEU:HD11	1:H:135:PHE:HE2	1.84	0.42
1:J:382:VAL:HG12	1:J:382:VAL:O	2.19	0.42
1:L:40:VAL:HG11	1:L:192:ILE:HD11	2.01	0.42
1:L:158:LEU:HD23	1:L:161:GLN:NE2	2.27	0.42
1:L:212:ARG:HA	1:L:215:THR:HG22	2.01	0.42
1:E:231:HIS:ND1	1:I:319:GLU:HG2	2.35	0.41
1:K:340:PRO:HA	1:K:370:ARG:HH21	1.85	0.41
1:G:328:ALA:HB2	1:J:342:ILE:HD12	2.02	0.41
1:H:142:VAL:HG22	1:H:153:LEU:HB3	2.02	0.41
1:J:246:TRP:CE2	1:J:372:VAL:HG22	2.55	0.41
1:L:248:LEU:HA	1:L:248:LEU:HD23	1.77	0.41
1:B:151:ARG:HD2	1:B:151:ARG:HA	1.92	0.41
1:B:190:LEU:HA	1:B:193:VAL:HG12	2.02	0.41
1:C:55:MET:SD	1:C:122:ALA:HB2	2.60	0.41
1:G:219:ARG:HG3	1:G:220:PHE:CD2	2.54	0.41
1:G:246:TRP:CE2	1:G:372:VAL:HG22	2.56	0.41
1:A:51:GLN:HE22	1:A:124:VAL:HG12	1.85	0.41
1:A:284:LYS:HE3	1:A:291:LYS:HD3	2.01	0.41
1:A:416:THR:HG23	1:A:417:TYR:N	2.36	0.41
1:I:346:PHE:C	1:I:347:SER:HG	2.24	0.41
1:I:355:PRO:HA	1:I:356:PRO:HD3	1.93	0.41
1:K:276:LEU:HD12	1:K:281:ILE:HB	2.02	0.41
1:B:226:LEU:HD12	1:B:226:LEU:HA	1.89	0.41
1:C:327:ASN:OD1	1:G:340:PRO:HG3	2.20	0.41
1:C:382:VAL:HG11	1:C:387:THR:HG22	2.00	0.41
1:D:318:ASP:O	1:D:320:ILE:HG23	2.20	0.41
1:E:353:ARG:NH1	1:E:355:PRO:HB3	2.35	0.41
1:K:340:PRO:HB2	1:K:342:ILE:HD11	2.02	0.41
1:C:26:PRO:HB2	1:C:89:PHE:HE2	1.85	0.41
1:D:249:GLN:NE2	1:D:325:ILE:HA	2.35	0.41
1:J:100:ILE:HG23	1:J:101:GLY:N	2.30	0.41
1:J:367:PRO:HG2	1:J:375:TRP:CE2	2.56	0.41
1:L:178:LYS:HE2	1:L:178:LYS:HB3	1.91	0.41
1:L:290:ILE:HD12	1:L:290:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:PHE:CE1	1:L:316:GLN:HG2	2.55	0.41
1:E:42:ARG:HH21	1:E:110:ASP:HB2	1.86	0.41
1:F:160:LYS:HA	1:F:163:LYS:HE3	2.02	0.41
1:B:55:MET:HG3	1:B:120:LEU:O	2.19	0.41
1:B:78:GLU:O	1:B:78:GLU:HG3	2.20	0.41
1:C:17:PRO:HD3	1:G:240:ILE:HD13	2.03	0.41
1:C:233:VAL:HG22	1:C:243:VAL:HG21	2.03	0.41
1:F:26:PRO:HB3	1:F:276:LEU:HD13	2.02	0.41
1:F:166:LYS:HG2	1:K:63:ARG:HD3	2.03	0.41
1:B:113:ASP:OD1	1:B:114:GLY:N	2.49	0.41
1:B:364:SER:C	1:B:366:GLU:H	2.23	0.41
1:C:310:ARG:NH1	1:H:318:ASP:OD2	2.48	0.41
1:D:299:GLY:HA2	1:D:302:VAL:HB	2.03	0.41
1:A:166:LYS:CG	1:A:167:SER:H	2.30	0.41
1:I:135:PHE:HZ	1:I:173:VAL:HB	1.85	0.41
1:I:198:MET:HE2	1:I:275:TYR:CD1	2.56	0.41
1:B:39:TYR:HA	1:B:109:GLU:O	2.21	0.41
1:C:253:ALA:CB	1:G:345:GLN:HG2	2.51	0.41
1:G:19:ASN:CG	1:G:20:GLU:H	2.23	0.41
1:H:340:PRO:HA	1:H:370:ARG:HH21	1.85	0.41
1:D:183:TRP:CD1	1:D:183:TRP:N	2.88	0.41
1:J:372:VAL:O	1:J:376:ILE:HG23	2.21	0.41
1:L:82:LEU:O	1:L:83:GLU:HG2	2.21	0.41
1:A:64:ILE:HD13	1:A:183:TRP:CG	2.56	0.41
1:E:23:ALA:HB1	1:E:284:LYS:O	2.21	0.41
1:F:157:SER:O	1:F:161:GLN:HG2	2.21	0.41
1:I:139:LEU:HD12	1:I:180:PHE:CG	2.56	0.41
1:B:8:THR:HG22	1:B:9:ASN:H	1.86	0.41
1:C:6:ILE:HA	1:J:347:SER:O	2.21	0.41
1:D:355:PRO:HA	1:D:356:PRO:HD3	1.90	0.41
1:L:207:ILE:H	1:L:207:ILE:HD12	1.86	0.41
1:L:404:PRO:HB2	1:L:411:LYS:HB2	2.02	0.41
1:A:100:ILE:HG23	1:A:101:GLY:N	2.30	0.41
1:A:373:VAL:HG11	1:I:350:ASN:HB3	2.02	0.41
1:E:225:ALA:O	1:E:228:THR:HG22	2.21	0.41
1:F:120:LEU:HD12	1:F:120:LEU:HA	1.86	0.41
1:I:62:CYS:HB3	1:I:179:TYR:HE2	1.86	0.41
1:I:64:ILE:HG22	1:I:68:ASN:ND2	2.35	0.41
1:C:36:ILE:HG21	1:C:279:MET:HG3	2.03	0.41
1:C:363:VAL:HG13	1:C:364:SER:N	2.34	0.41
1:G:56:GLY:C	1:G:62:CYS:HB3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:LEU:HD21	1:G:295:PHE:CE1	2.56	0.41
1:H:190:LEU:O	1:H:278:ASP:HB3	2.21	0.41
1:H:321:ASP:O	1:H:324:SER:N	2.52	0.41
1:H:386:PRO:HB2	1:H:391:LEU:HD21	2.02	0.41
1:D:363:VAL:HG11	1:D:366:GLU:HB2	2.03	0.41
1:J:137:LEU:HD11	1:J:196:VAL:HG21	2.03	0.41
1:J:139:LEU:HD12	1:J:183:TRP:CZ3	2.56	0.41
1:J:225:ALA:O	1:J:228:THR:OG1	2.35	0.41
1:J:246:TRP:CD2	1:J:372:VAL:HG22	2.56	0.41
1:I:63:ARG:NH1	1:I:117:ASP:HB2	2.36	0.41
1:B:72:TYR:O	1:B:76:LYS:HB2	2.21	0.41
1:D:231:HIS:ND1	1:J:319:GLU:HG2	2.36	0.41
1:D:301:LEU:HD23	1:D:305:LEU:HG	2.02	0.41
1:J:275:TYR:O	1:J:279:MET:HB2	2.21	0.41
1:A:248:LEU:HB3	1:I:342:ILE:HD12	2.02	0.40
1:E:317:PRO:O	1:E:320:ILE:HG12	2.21	0.40
1:F:272:TYR:HD2	1:F:281:ILE:HD11	1.86	0.40
1:I:249:GLN:HE22	1:I:328:ALA:CB	2.34	0.40
1:K:198:MET:HB2	1:K:275:TYR:CE2	2.56	0.40
1:K:334:TYR:CD1	1:K:334:TYR:O	2.74	0.40
1:K:401:ILE:HD13	1:K:410:GLY:HA2	2.02	0.40
1:B:135:PHE:HZ	1:B:173:VAL:HB	1.86	0.40
1:C:276:LEU:HA	1:C:281:ILE:HG22	2.02	0.40
1:G:103:PHE:CZ	1:G:192:ILE:HG23	2.56	0.40
1:H:59:GLU:C	1:H:61:ASN:H	2.24	0.40
1:J:77:GLY:HA2	1:J:79:ARG:NH1	2.37	0.40
1:A:67:VAL:HG13	1:A:136:LEU:HD13	2.02	0.40
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.84	0.40
1:A:137:LEU:HD22	1:A:193:VAL:HG23	2.03	0.40
1:E:37:ARG:HD2	1:E:109:GLU:HG3	2.02	0.40
1:F:70:TYR:HE2	1:F:132:LEU:HB3	1.86	0.40
1:I:208:LYS:HD2	1:I:211:PHE:CE2	2.55	0.40
1:K:78:GLU:OE1	1:K:200:TYR:OH	2.38	0.40
1:B:132:LEU:HB3	1:B:133:PRO:HD3	2.03	0.40
1:B:183:TRP:CD1	1:B:183:TRP:N	2.89	0.40
1:C:226:LEU:HD13	1:C:287:TYR:HB3	2.02	0.40
1:G:139:LEU:HD12	1:G:180:PHE:CD1	2.57	0.40
1:G:139:LEU:O	1:G:143:GLY:N	2.50	0.40
1:G:238:LEU:HD21	1:G:370:ARG:HD3	2.03	0.40
1:J:7:LYS:HG2	1:J:8:THR:N	2.35	0.40
1:J:139:LEU:HB3	1:J:180:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:LEU:O	1:L:158:LEU:N	2.40	0.40
1:L:257:VAL:C	1:L:259:MET:H	2.25	0.40
1:E:363:VAL:HG13	1:E:364:SER:N	2.35	0.40
1:F:235:ILE:HA	1:K:320:ILE:O	2.22	0.40
1:I:61:ASN:O	1:I:119:LYS:NZ	2.27	0.40
1:K:334:TYR:O	1:K:334:TYR:HD1	2.05	0.40
1:G:305:LEU:HD23	1:G:305:LEU:HA	1.93	0.40
1:H:353:ARG:H	1:H:353:ARG:HD3	1.86	0.40
1:D:79:ARG:HB3	1:D:99:LYS:HB3	2.02	0.40
1:J:19:ASN:CG	1:J:20:GLU:H	2.25	0.40
1:J:224:ALA:HB3	1:J:289:THR:HG23	2.03	0.40
1:A:363:VAL:HG13	1:A:364:SER:N	2.32	0.40
1:E:120:LEU:O	1:E:120:LEU:HD23	2.21	0.40
1:E:129:ASP:O	1:E:133:PRO:HD2	2.21	0.40
1:I:132:LEU:HB3	1:I:133:PRO:HD3	2.03	0.40
1:K:224:ALA:O	1:K:228:THR:HG23	2.21	0.40
1:D:86:TRP:HE1	1:D:202:HIS:CD2	2.39	0.40
1:D:247:VAL:O	1:D:247:VAL:HG12	2.21	0.40
1:F:257:VAL:C	1:F:259:MET:H	2.24	0.40
1:F:267:ASP:OD1	1:F:267:ASP:N	2.54	0.40
1:K:159:ILE:O	1:K:163:LYS:HD3	2.22	0.40
1:C:64:ILE:HD13	1:C:183:TRP:CD1	2.56	0.40
1:G:219:ARG:HD2	1:G:274:PRO:HB2	2.02	0.40
1:G:248:LEU:HD13	1:J:342:ILE:HG23	2.02	0.40
1:G:261:LYS:O	1:G:264:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	415/418 (99%)	346 (83%)	64 (15%)	5 (1%)	13 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	415/418 (99%)	345 (83%)	67 (16%)	3 (1%)	22 60
1	C	415/418 (99%)	352 (85%)	59 (14%)	4 (1%)	15 52
1	D	415/418 (99%)	342 (82%)	65 (16%)	8 (2%)	8 40
1	E	415/418 (99%)	349 (84%)	63 (15%)	3 (1%)	22 60
1	F	415/418 (99%)	350 (84%)	59 (14%)	6 (1%)	11 45
1	G	415/418 (99%)	350 (84%)	64 (15%)	1 (0%)	47 79
1	H	415/418 (99%)	345 (83%)	66 (16%)	4 (1%)	15 52
1	I	415/418 (99%)	355 (86%)	56 (14%)	4 (1%)	15 52
1	J	415/418 (99%)	357 (86%)	56 (14%)	2 (0%)	29 66
1	K	415/418 (99%)	347 (84%)	61 (15%)	7 (2%)	9 42
1	L	415/418 (99%)	346 (83%)	61 (15%)	8 (2%)	8 40
All	All	4980/5016 (99%)	4184 (84%)	741 (15%)	55 (1%)	14 50

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	268	LYS
1	I	365	GLU
1	B	79	ARG
1	D	79	ARG
1	D	126	ALA
1	D	363	VAL
1	D	365	GLU
1	L	79	ARG
1	L	83	GLU
1	A	79	ARG
1	A	408	SER
1	F	60	LYS
1	F	219	ARG
1	F	220	PHE
1	F	322	SER
1	I	79	ARG
1	K	20	GLU
1	K	79	ARG
1	K	322	SER
1	C	79	ARG
1	C	89	PHE
1	H	79	ARG

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Mol	Chain	Res	Type
1	D	60	LYS
1	J	79	ARG
1	J	359	ALA
1	E	4	ILE
1	E	60	LYS
1	E	79	ARG
1	F	79	ARG
1	K	222	ASP
1	B	359	ALA
1	H	60	LYS
1	D	357	LYS
1	L	60	LYS
1	L	82	LEU
1	L	222	ASP
1	I	60	LYS
1	B	39	TYR
1	G	293	PRO
1	H	345	GLN
1	L	270	THR
1	A	284	LYS
1	A	365	GLU
1	K	347	SER
1	K	365	GLU
1	D	145	ALA
1	L	85	ASP
1	F	25	TYR
1	K	113	ASP
1	C	305	LEU
1	C	365	GLU
1	D	315	ARG
1	L	359	ALA
1	A	262	PRO
1	H	262	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	356/357 (100%)	355 (100%)	1 (0%)	92 95
1	B	356/357 (100%)	356 (100%)	0	100 100
1	C	356/357 (100%)	356 (100%)	0	100 100
1	D	356/357 (100%)	353 (99%)	3 (1%)	81 88
1	E	356/357 (100%)	355 (100%)	1 (0%)	92 95
1	F	356/357 (100%)	355 (100%)	1 (0%)	92 95
1	G	356/357 (100%)	356 (100%)	0	100 100
1	H	356/357 (100%)	355 (100%)	1 (0%)	92 95
1	I	356/357 (100%)	355 (100%)	1 (0%)	92 95
1	J	356/357 (100%)	355 (100%)	1 (0%)	92 95
1	K	356/357 (100%)	355 (100%)	1 (0%)	92 95
1	L	356/357 (100%)	354 (99%)	2 (1%)	86 91
All	All	4272/4284 (100%)	4260 (100%)	12 (0%)	92 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ARG
1	E	354	LYS
1	F	327	ASN
1	I	327	ASN
1	K	327	ASN
1	H	353	ARG
1	D	5	ARG
1	D	42	ARG
1	D	86	TRP
1	J	37	ARG
1	L	86	TRP
1	L	201	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	249	GLN
1	A	345	GLN
1	E	61	ASN
1	F	104	ASN

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Mol	Chain	Res	Type
1	F	188	ASN
1	F	249	GLN
1	I	161	GLN
1	C	161	GLN
1	G	51	GLN
1	G	249	GLN
1	D	41	ASN
1	D	104	ASN
1	D	249	GLN
1	J	104	ASN
1	J	344	GLN
1	L	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	417/418 (99%)	0.26	11 (2%)	56	46	102, 138, 187, 246	0
1	B	417/418 (99%)	0.39	30 (7%)	15	12	109, 162, 217, 242	0
1	C	417/418 (99%)	0.37	18 (4%)	35	29	111, 146, 199, 249	0
1	D	417/418 (99%)	0.27	21 (5%)	28	25	114, 148, 198, 244	0
1	E	417/418 (99%)	0.28	12 (2%)	51	41	108, 144, 199, 236	0
1	F	417/418 (99%)	0.21	9 (2%)	62	52	102, 145, 204, 231	0
1	G	417/418 (99%)	0.37	18 (4%)	35	29	107, 161, 212, 246	0
1	H	417/418 (99%)	0.43	24 (5%)	23	19	110, 171, 220, 235	0
1	I	417/418 (99%)	0.19	8 (1%)	66	58	106, 139, 191, 236	0
1	J	417/418 (99%)	0.35	25 (5%)	21	17	116, 150, 208, 259	0
1	K	417/418 (99%)	0.28	12 (2%)	51	41	109, 166, 214, 240	0
1	L	417/418 (99%)	0.51	35 (8%)	11	10	112, 177, 228, 245	0
All	All	5004/5016 (99%)	0.33	223 (4%)	33	28	102, 151, 214, 259	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	SER	7.7
1	I	362	LEU	7.7
1	L	353	ARG	7.4
1	L	361	TYR	6.6
1	I	363	VAL	6.2
1	C	363	VAL	6.1
1	D	362	LEU	5.6
1	J	364	SER	5.6
1	C	362	LEU	5.6
1	J	358	GLU	5.5
1	F	150	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	360	SER	5.0
1	H	359	ALA	4.8
1	H	2	SER	4.7
1	I	361	TYR	4.5
1	B	2	SER	4.3
1	G	362	LEU	4.3
1	C	364	SER	4.3
1	F	167	SER	4.3
1	K	38	LEU	4.2
1	E	363	VAL	4.1
1	B	167	SER	4.0
1	B	100	ILE	4.0
1	A	150	TYR	4.0
1	G	357	LYS	4.0
1	H	179	TYR	3.9
1	K	100	ILE	3.9
1	H	360	SER	3.9
1	G	361	TYR	3.8
1	H	100	ILE	3.8
1	L	105	LEU	3.7
1	G	167	SER	3.7
1	L	363	VAL	3.7
1	G	363	VAL	3.7
1	L	82	LEU	3.6
1	H	150	TYR	3.6
1	D	353	ARG	3.6
1	E	358	GLU	3.6
1	L	166	LYS	3.5
1	D	363	VAL	3.5
1	C	361	TYR	3.4
1	B	99	LYS	3.4
1	J	100	ILE	3.4
1	C	167	SER	3.4
1	L	360	SER	3.4
1	B	355	PRO	3.4
1	F	177	HIS	3.4
1	L	15	VAL	3.4
1	G	352	TYR	3.3
1	J	362	LEU	3.3
1	L	91	HIS	3.3
1	L	356	PRO	3.3
1	B	353	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	360	SER	3.3
1	L	401	ILE	3.2
1	C	2	SER	3.2
1	L	88	SER	3.2
1	H	3	VAL	3.2
1	J	361	TYR	3.2
1	K	2	SER	3.2
1	J	2	SER	3.2
1	E	361	TYR	3.1
1	L	5	ARG	3.1
1	J	359	ALA	3.1
1	F	166	LYS	3.1
1	G	38	LEU	3.1
1	I	364	SER	3.1
1	E	362	LEU	3.1
1	D	361	TYR	3.0
1	B	359	ALA	3.0
1	J	363	VAL	3.0
1	L	362	LEU	3.0
1	G	37	ARG	2.9
1	B	78	GLU	2.9
1	E	3	VAL	2.9
1	H	276	LEU	2.9
1	H	361	TYR	2.9
1	A	100	ILE	2.8
1	G	119	LYS	2.8
1	C	3	VAL	2.8
1	B	3	VAL	2.8
1	H	30	PHE	2.8
1	H	177	HIS	2.8
1	J	44	GLU	2.7
1	E	294	SER	2.7
1	I	272	TYR	2.7
1	G	2	SER	2.7
1	D	63	ARG	2.7
1	G	166	LYS	2.7
1	H	167	SER	2.7
1	A	272	TYR	2.7
1	L	351	THR	2.7
1	A	363	VAL	2.7
1	L	287	TYR	2.7
1	B	279	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	363	VAL	2.7
1	H	344	GLN	2.7
1	D	119	LYS	2.7
1	A	119	LYS	2.6
1	L	2	SER	2.6
1	D	360	SER	2.6
1	D	66	HIS	2.6
1	K	150	TYR	2.6
1	J	165	ILE	2.6
1	L	89	PHE	2.6
1	G	356	PRO	2.6
1	A	40	VAL	2.6
1	A	362	LEU	2.6
1	K	364	SER	2.6
1	D	61	ASN	2.5
1	H	346	PHE	2.5
1	J	161	GLN	2.5
1	B	363	VAL	2.5
1	H	93	ILE	2.5
1	C	119	LYS	2.5
1	H	119	LYS	2.5
1	L	272	TYR	2.5
1	C	105	LEU	2.5
1	D	183	TRP	2.5
1	I	2	SER	2.5
1	L	279	MET	2.4
1	I	34	ASN	2.4
1	L	286	PRO	2.4
1	C	413	ILE	2.4
1	G	91	HIS	2.4
1	A	2	SER	2.4
1	D	41	ASN	2.4
1	D	15	VAL	2.4
1	L	167	SER	2.4
1	C	42	ARG	2.4
1	B	94	GLY	2.4
1	B	93	ILE	2.4
1	D	167	SER	2.4
1	E	93	ILE	2.4
1	C	346	PHE	2.4
1	B	161	GLN	2.4
1	F	38	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	357	LYS	2.4
1	B	5	ARG	2.3
1	A	103	PHE	2.3
1	F	100	ILE	2.3
1	H	362	LEU	2.3
1	L	276	LEU	2.3
1	B	130	ALA	2.3
1	L	87	ASP	2.3
1	H	244	PHE	2.3
1	G	93	ILE	2.3
1	G	100	ILE	2.3
1	D	281	ILE	2.3
1	H	272	TYR	2.3
1	B	360	SER	2.3
1	D	179	TYR	2.3
1	B	231	HIS	2.3
1	C	305	LEU	2.3
1	G	353	ARG	2.3
1	L	165	ILE	2.3
1	D	297	PHE	2.3
1	K	181	ASP	2.3
1	H	6	ILE	2.3
1	D	139	LEU	2.3
1	B	200	TYR	2.3
1	K	285	SER	2.3
1	H	281	ILE	2.3
1	B	272	TYR	2.3
1	J	145	ALA	2.2
1	J	357	LYS	2.2
1	E	272	TYR	2.2
1	E	353	ARG	2.2
1	F	179	TYR	2.2
1	F	71	LEU	2.2
1	B	102	PRO	2.2
1	B	244	PHE	2.2
1	G	121	ASN	2.2
1	D	178	LYS	2.2
1	B	87	ASP	2.2
1	C	81	LEU	2.2
1	D	112	PRO	2.2
1	C	360	SER	2.2
1	D	364	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	40	VAL	2.2
1	J	105	LEU	2.2
1	L	346	PHE	2.2
1	K	358	GLU	2.2
1	L	6	ILE	2.2
1	L	364	SER	2.2
1	B	356	PRO	2.2
1	C	236	THR	2.2
1	J	305	LEU	2.2
1	L	119	LYS	2.2
1	F	161	GLN	2.2
1	K	173	VAL	2.2
1	L	141	ARG	2.2
1	L	344	GLN	2.2
1	L	273	MET	2.1
1	B	121	ASN	2.1
1	G	106	VAL	2.1
1	A	38	LEU	2.1
1	J	75	LEU	2.1
1	B	199	PHE	2.1
1	J	103	PHE	2.1
1	B	364	SER	2.1
1	J	356	PRO	2.1
1	H	60	LYS	2.1
1	J	40	VAL	2.1
1	C	145	ALA	2.1
1	J	163	LYS	2.1
1	C	102	PRO	2.1
1	J	307	ARG	2.1
1	K	218	SER	2.1
1	K	286	PRO	2.1
1	E	140	TYR	2.0
1	H	401	ILE	2.0
1	B	178	LYS	2.0
1	J	6	ILE	2.0
1	J	334	TYR	2.0
1	L	347	SER	2.0
1	B	166	LYS	2.0
1	E	179	TYR	2.0
1	K	203	PHE	2.0
1	L	75	LEU	2.0
1	J	146	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	287	TYR	2.0
1	B	82	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.