



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:24 PM UTC

PDB ID : 7XPN / pdb_00007xpn
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

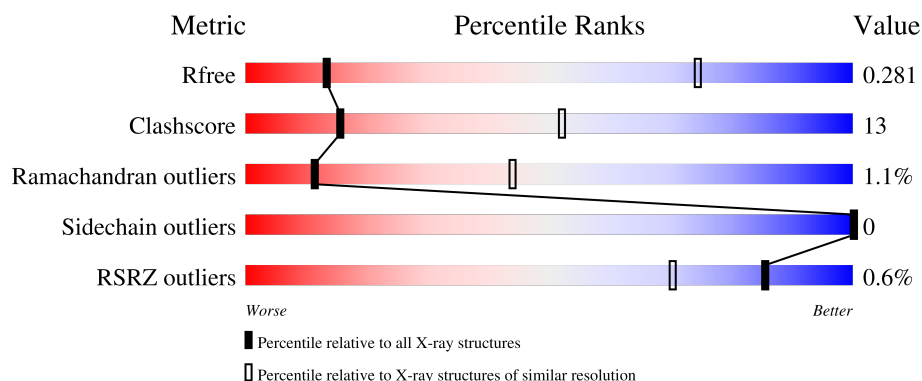
1 Overall quality at a glance

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}	180053	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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

Mol	Chain	Length	Quality of chain
1	A	418	68% 31% .
1	B	418	69% 30%
1	C	418	73% 26% .
1	D	418	67% 32% .
1	E	418	63% 36%

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Mol	Chain	Length	Quality of chain
1	F	418	68%31%
1	G	418	67%33%
1	H	418	70%29%
1	I	418	% 67%32%
1	J	418	68%32%
1	K	418	% 71%28%
1	L	418	% 70%29%

2 Entry composition

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.

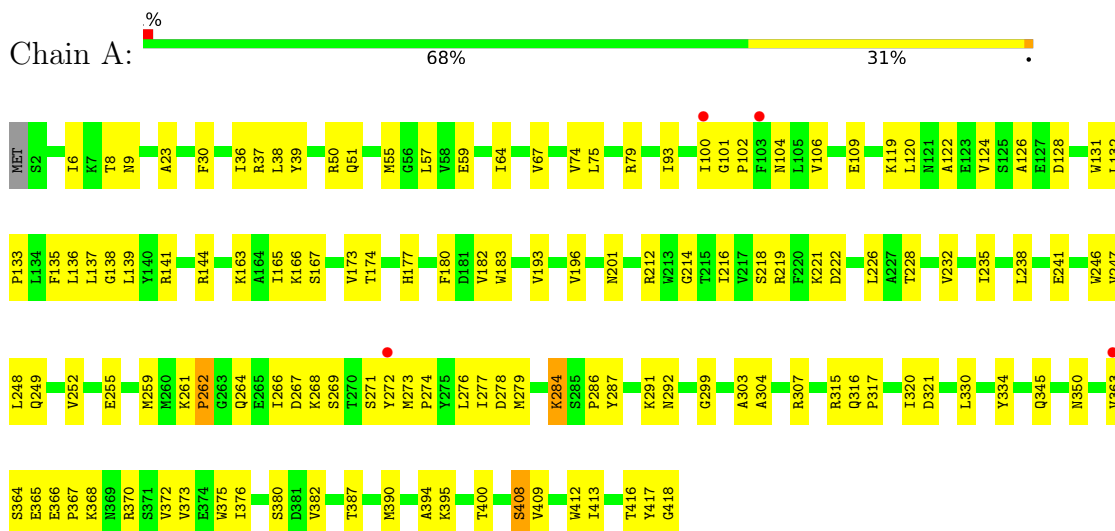
- Molecule 1 is a protein called Nucleoprotein.

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			

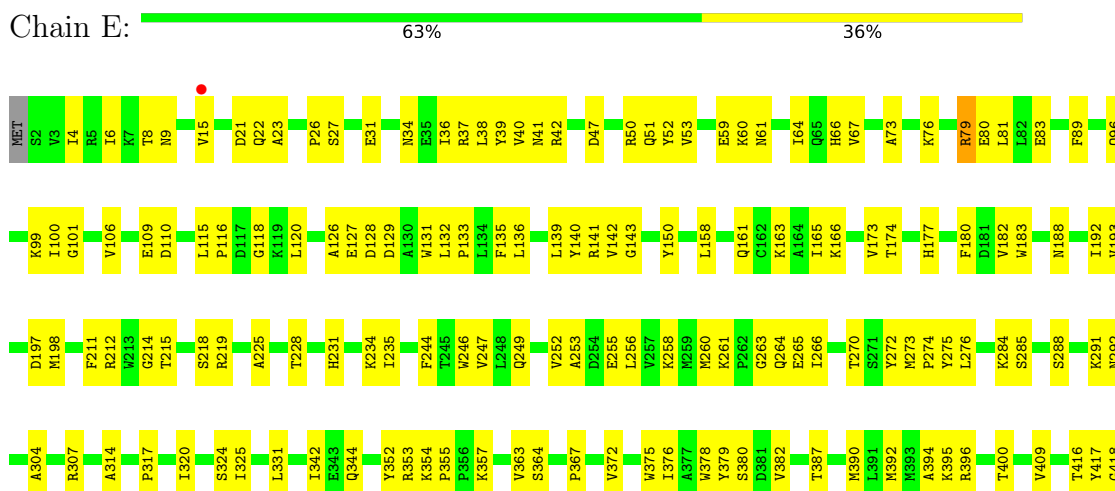
3 Residue-property plots

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

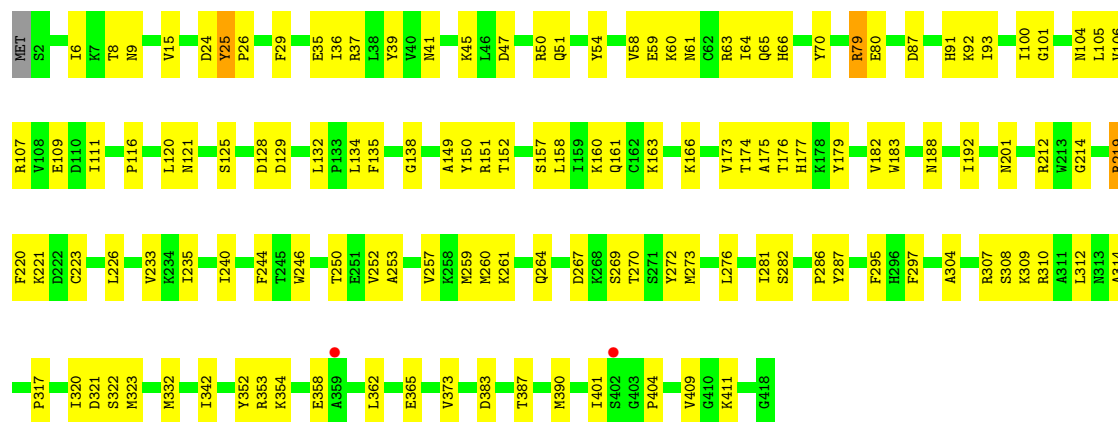


• Molecule 1: Nucleoprotein

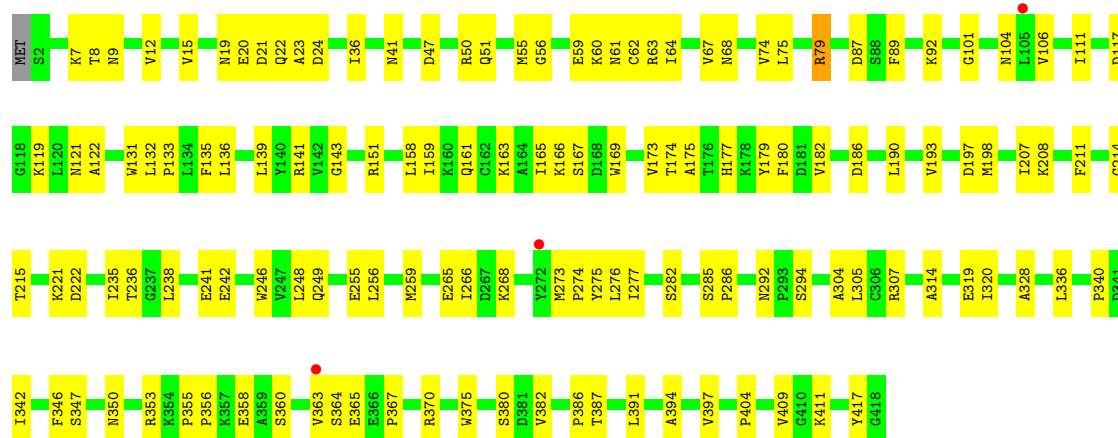


• Molecule 1: Nucleoprotein

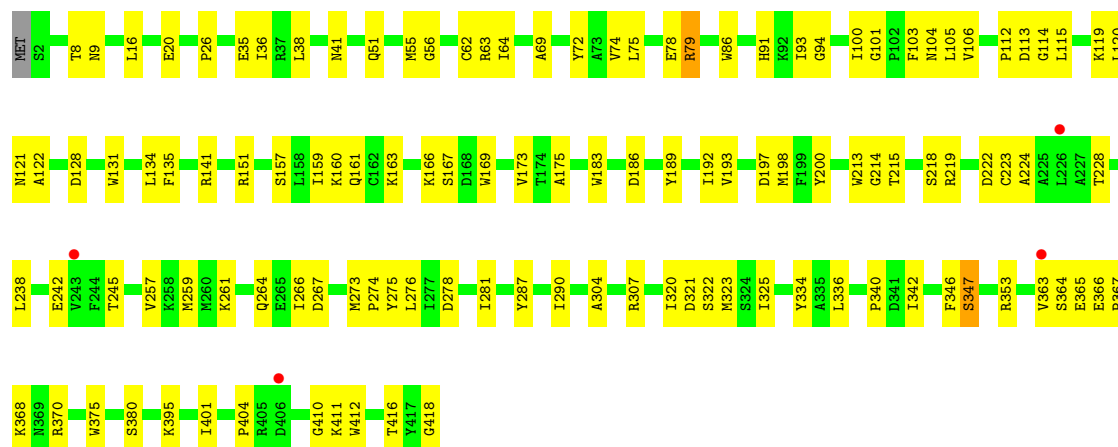
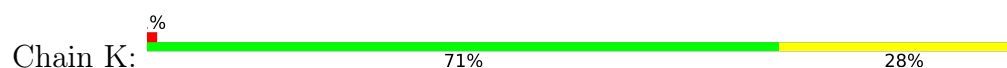




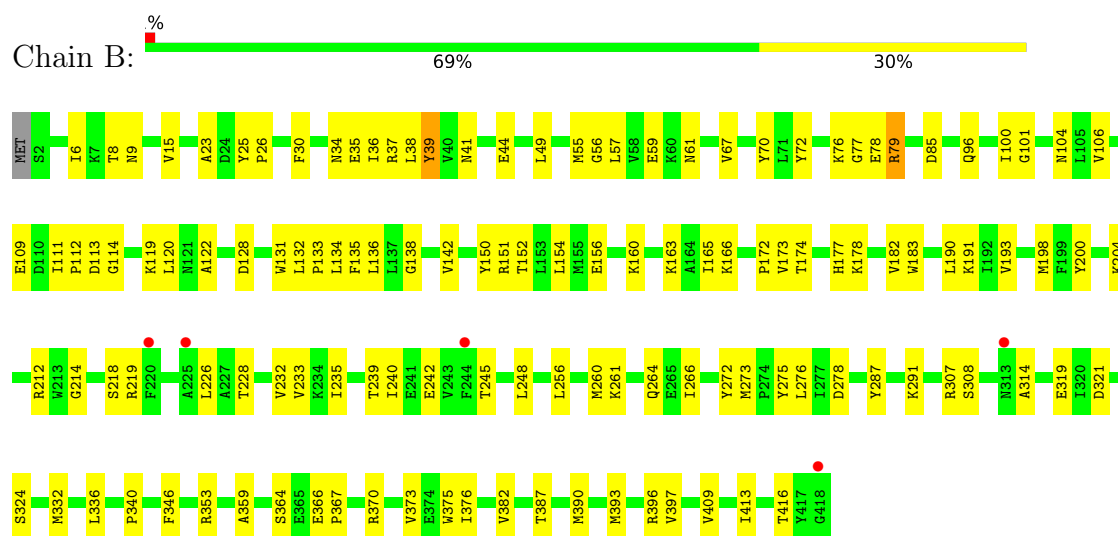
• Molecule 1: Nucleoprotein



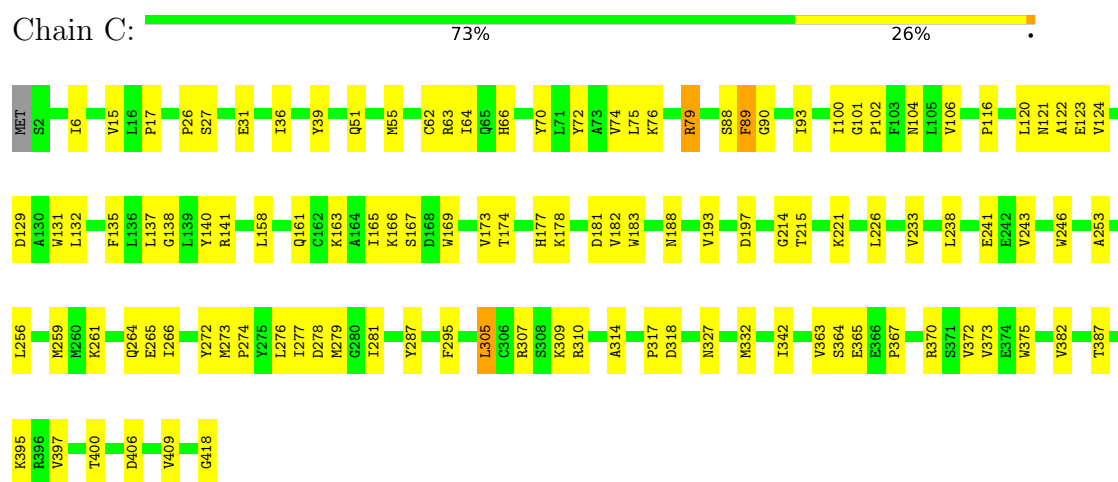
• Molecule 1: Nucleoprotein



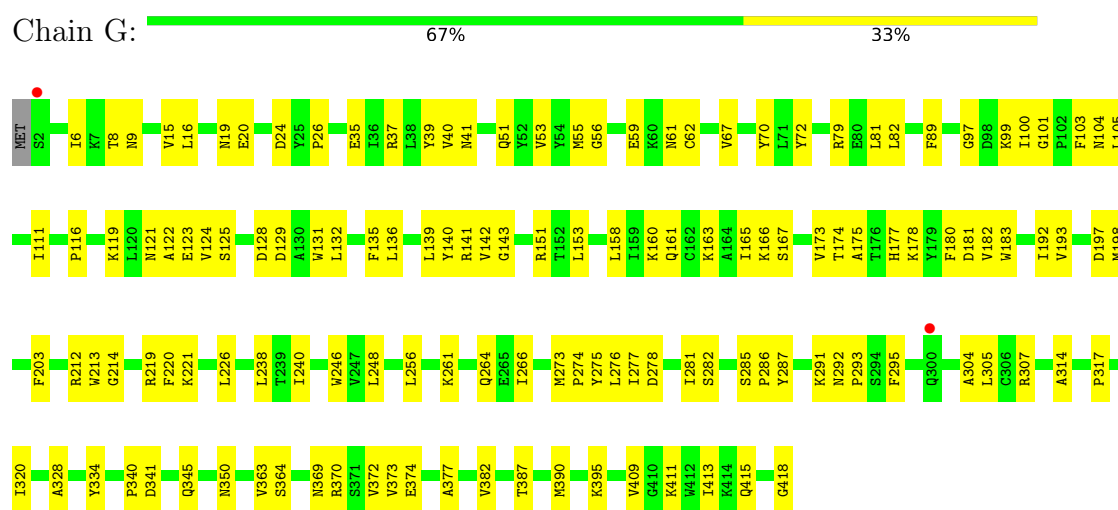
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

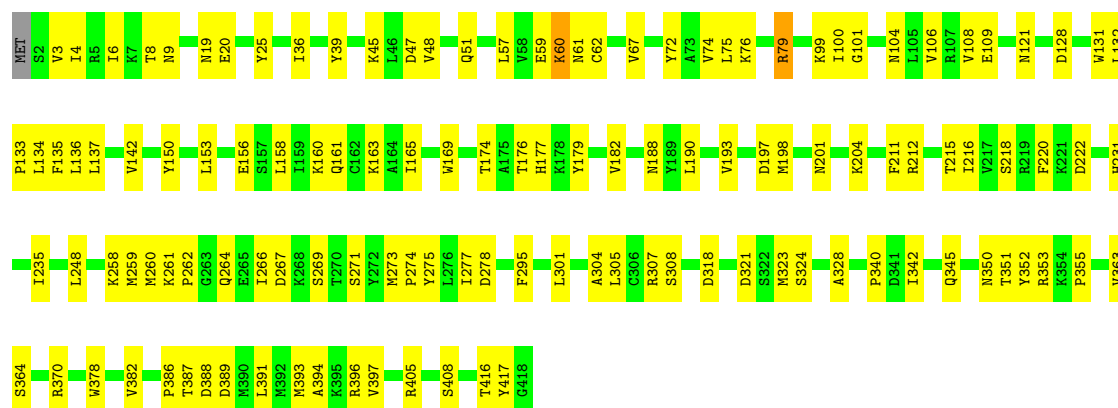


• Molecule 1: Nucleoprotein



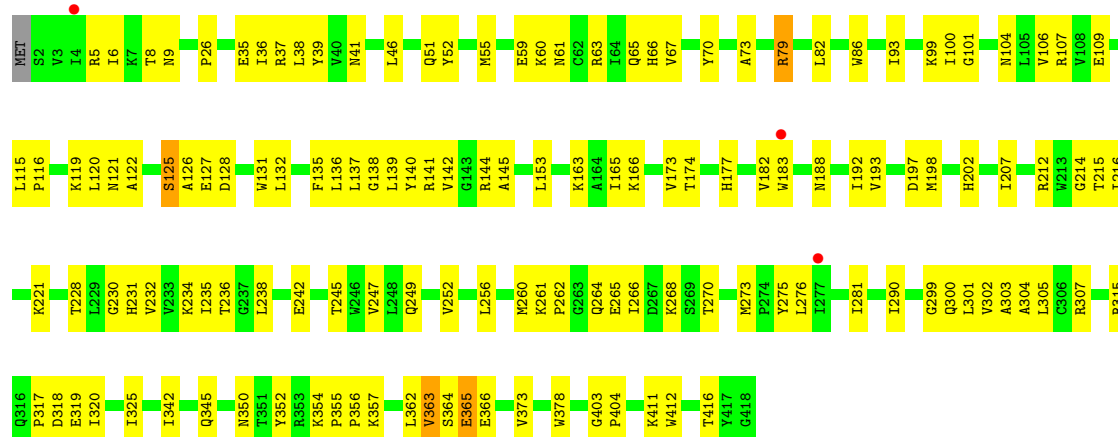
• Molecule 1: Nucleoprotein

Chain H:  70% 29%



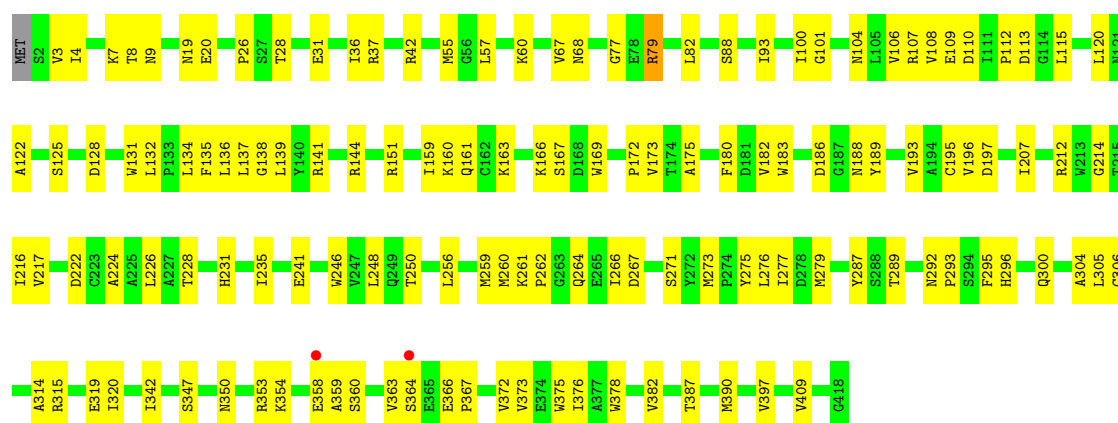
• Molecule 1: Nucleoprotein

Chain D:  67% 32%

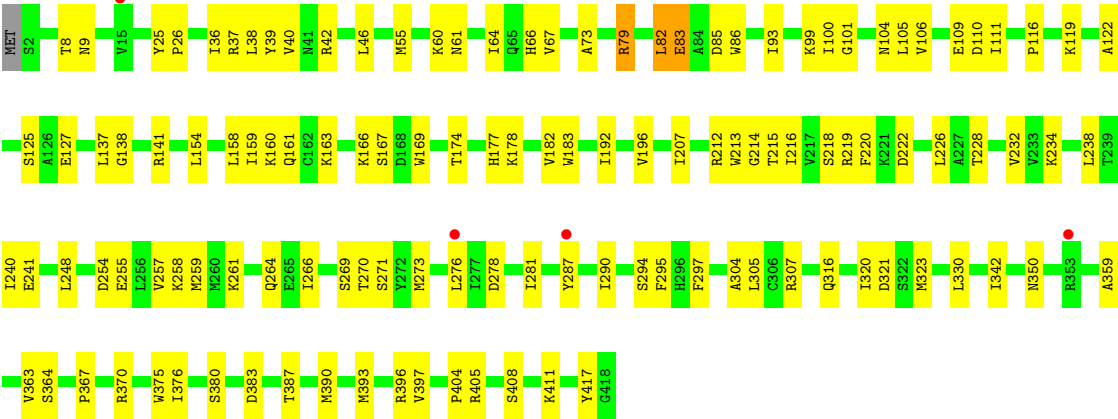


• Molecule 1: Nucleoprotein

Chain J:  68% 32%



• Molecule 1: Nucleoprotein



4 Data and refinement statistics

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 72.86 – 3.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.86-3.98) 91.4 (72.86-3.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.255 , 0.284 0.256 , 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)	0.31 , 108.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.16	0/3375	0.51	1/4575 (0.0%)
1	B	0.14	0/3375	0.46	0/4575
1	C	0.14	0/3375	0.46	0/4575
1	D	0.16	0/3375	0.50	0/4575
1	E	0.15	0/3375	0.48	0/4575
1	F	0.15	0/3375	0.48	0/4575
1	G	0.14	0/3375	0.47	0/4575
1	H	0.14	0/3375	0.48	2/4575 (0.0%)
1	I	0.14	0/3375	0.45	0/4575
1	J	0.14	0/3375	0.46	0/4575
1	K	0.14	0/3375	0.47	0/4575
1	L	0.14	0/3375	0.49	0/4575
All	All	0.15	0/40500	0.48	3/54900 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	TYR	N-CA-C	6.38	119.00	111.02
1	H	351	THR	CA-C-N	5.00	131.10	121.54
1	H	351	THR	C-N-CA	5.00	131.10	121.54

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

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	100	0
1	B	3299	0	3279	94	0
1	C	3299	0	3279	88	0
1	D	3299	0	3279	102	0
1	E	3299	0	3279	114	0
1	F	3299	0	3279	98	0
1	G	3299	0	3279	100	0
1	H	3299	0	3279	89	0
1	I	3299	0	3279	91	0
1	J	3299	0	3279	105	0
1	K	3299	0	3279	79	0
1	L	3299	0	3279	86	0
All	All	39588	0	39348	1060	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 (1060) 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:B:239:THR:OG1	1:B:242:GLU:OE1	2.06	0.73
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: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:A:387:THR:H	1:A:390:MET:HE3	1.55	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: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:266:ILE:HG22	1:I:273:MET:HE3	1.78	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:G:55:MET:HE3	1:G:122:ALA:HB2	1.80	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:A:266:ILE:HA	1:A:273:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:307:ARG:HH11	1:H:323:MET:HE1	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:I:256:LEU:HA	1:I:259:MET:HE2	1.81	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:L:218:SER:OG	1:L:278:ASP:OD2	2.16	0.61
1:I:197:ASP:OD2	1:I:275:TYR:OH	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:51:GLN:HE22	1:G:123:GLU:C	2.10	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:G:59:GLU:OE1	1:G:119:LYS:NZ	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:266:ILE:HA	1:E:273:MET:HE2	1.87	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
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:F:226:LEU:HD12	1:F:259:MET:HE3	1.87	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:K:197:ASP:OD2	1:K:275:TYR:OH	2.20	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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:387:THR:H	1:B:390:MET:HE3	1.75	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:B:319:GLU:HG2	1:H:231:HIS:CE1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:GLN:CG	1:H:121:ASN:HB3	2.39	0.51
1:D:232:VAL:O	1:D:236:THR:OG1	2.27	0.51
1:A:36:ILE:HG21	1:A:279:MET:HE3	1.92	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:C:226:LEU:HD12	1:C:259:MET:HE3	1.91	0.51
1:H:222:ASP:HB2	1:H:277:ILE:HD11	1.92	0.51
1:I:249:GLN:N	1:I:249:GLN:OE1	2.44	0.51
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:F:244:PHE:HZ	1:F:260:MET:HE3	1.76	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:I:59:GLU:C	1:I:61:ASN:H	2.18	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:B:198:MET:HE3	1:B:275:TYR:CD2	2.47	0.50
1:G:105:LEU:HD22	1:G:198:MET:HE3	1.93	0.50
1:J:387:THR:H	1:J:390:MET:HE3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:342:ILE:HG13	1:L:342:ILE:O	2.11	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
1:F:24:ASP:HB2	1:F:282:SER:HB2	1.94	0.49
1:K:218:SER:OG	1:K:278:ASP:OD2	2.23	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:H:266:ILE:HA	1:H:273:MET:HE2	1.94	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:B:198:MET:HE1	1:B:272:TYR:HA	1.94	0.49
1:H:305:LEU:HA	1:H:397:VAL:HG11	1.93	0.49
1:J:197:ASP:OD2	1:J:275:TYR:OH	2.17	0.49
1:J:304:ALA:C	1:J:306:CYS:H	2.21	0.49
1:F:261:LYS:O	1:F:264:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:387:THR:H	1:E:390:MET:HE3	1.77	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
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:D:35:GLU:CD	1:D:107:ARG:HE	2.21	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:H:19:ASN:CG	1:H:20:GLU:H	2.22	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:B:198:MET:HE1	1:B:272:TYR:HD1	1.77	0.48
1:C:178:LYS:HB2	1:C:181:ASP:OD2	2.14	0.48
1:D:366:GLU:H	1:D:378:TRP:CD1	2.32	0.48
1:A:246:TRP:CE2	1:A:372:VAL:HG22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:VAL:HG13	1:J:163:LYS:HG3	1.95	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: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: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:B:15:VAL:HA	1:H:260:MET:HE3	1.96	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:59:GLU:C	1:E:61:ASN:H	2.23	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:C:307:ARG:NH1	1:H:323:MET:HE1	2.30	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
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:D:52:TYR:HB3	1:D:66:HIS:CD2	2.49	0.47
1:D:59:GLU:C	1:D:61:ASN:H	2.22	0.47
1:J:166:LYS:CG	1:J:167:SER:H	2.25	0.47
1:J:256:LEU:HD23	1:J:259:MET:HE2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:266:ILE:HG12	1:C:273:MET:HE3	1.97	0.47
1:G:39:TYR:HB3	1:G:111:ILE:HA	1.97	0.47
1:G:197:ASP:CG	1:G:212:ARG:HE	2.23	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
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:B:364:SER:C	1:B:366:GLU:H	2.23	0.46
1:A:100:ILE:CG1	1:A:104:ASN:HD21	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:273:MET:HE1	1:F:287:TYR:CD2	2.50	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:19:ASN:CG	1:G:20:GLU:H	2.23	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
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:C:93:ILE:HD11	1:C:272:TYR:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:198:MET:HE1	1:E:272:TYR:CD1	2.51	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:G:56:GLY:C	1:G:62:CYS:HB3	2.40	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
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:H:59:GLU:C	1:H:61:ASN:H	2.24	0.45
1:J:195:CYS:SG	1:J:279:MET:HE1	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:257:VAL:C	1:L:259:MET:H	2.25	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:19:ASN:CG	1:J:20:GLU:H	2.25	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:F:79:ARG:C	1:F:80:GLU:HG2	2.42	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:125:SER:HB2	1:F:128:ASP:CG	2.41	0.45
1:F:233:VAL:HG11	1:F:240:ILE:HG13	1.99	0.45
1:F:257:VAL:C	1:F:259:MET:H	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:198:MET:HE1	1:B:272:TYR:CD1	2.52	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: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:I:276:LEU:HD11	1:I:285:SER:HB2	2.00	0.44
1:I:346:PHE:C	1:I:347:SER:HG	2.26	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:266:ILE:HA	1:K:273:MET:HE3	2.00	0.44
1:K:368:LYS:HE3	1:L:383:ASP:HA	2.00	0.44
1:B:273:MET:HE3	1:B:287:TYR:CE2	2.53	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: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:123:GLU:CD	1:C:124:VAL:H	2.26	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: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:K:346:PHE:O	1:K:347:SER:OG	2.31	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:I:19:ASN:CG	1:I:20:GLU:H	2.26	0.43
1:I:198:MET:HE2	1:I:275:TYR:CD1	2.54	0.43
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:218:SER:OG	1:H:278:ASP:OD2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:128:ASP:OD1	1:E:128:ASP:N	2.47	0.42
1:K:257:VAL:C	1:K:259:MET:H	2.26	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ILE:HD13	1:F:105:LEU:HD23	2.02	0.42
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: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:A:259:MET:HE2	1:A:292:ASN:ND2	2.34	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:G:314:ALA:O	1:G:409:VAL:HG23	2.19	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:125:SER:C	1:L:127:GLU:H	2.28	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: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:L:273:MET:HE1	1:L:287:TYR:CE2	2.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:259:MET:HE1	1:H:295:PHE:CD2	2.55	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: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:D:362:LEU:O	1:D:363:VAL:C	2.62	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: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: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:59:GLU:C	1:F:61:ASN:H	2.28	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:J:353:ARG:C	1:J:354:LYS:HG2	2.46	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:F:308:SER:C	1:F:310:ARG:H	2.28	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:256:LEU:HD21	1:G:295:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:LEU:O	1:H:278:ASP:HB3	2.21	0.41
1:H:273:MET:HE3	1:H:273:MET:HB3	1.91	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:246:TRP:CD2	1:J:372:VAL:HG22	2.56	0.41
1:L:321:ASP:C	1:L:323:MET:H	2.28	0.41
1:F:308:SER:O	1:F:309:LYS:HB2	2.20	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:59:GLU:C	1:E:61:ASN:N	2.79	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: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:F:352:TYR:C	1:F:354:LYS:H	2.29	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:77:GLY:C	1:B:79:ARG:H	2.29	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:O	1:G:143:GLY:N	2.50	0.40
1:G:139:LEU:HD12	1:G:180:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:154:LEU:O	1:L:158:LEU:N	2.40	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: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:E:197:ASP:OD2	1:E:275:TYR:OH	2.22	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: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:B:218:SER:OG	1:B:278:ASP:OD2	2.36	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%)	10	42
1	B	415/418 (99%)	345 (83%)	67 (16%)	3 (1%)	18	54
1	C	415/418 (99%)	352 (85%)	59 (14%)	4 (1%)	12	45
1	D	415/418 (99%)	342 (82%)	65 (16%)	8 (2%)	6	34
1	E	415/418 (99%)	349 (84%)	63 (15%)	3 (1%)	18	54
1	F	415/418 (99%)	350 (84%)	59 (14%)	6 (1%)	9	39
1	G	415/418 (99%)	350 (84%)	64 (15%)	1 (0%)	43	75
1	H	415/418 (99%)	345 (83%)	66 (16%)	4 (1%)	12	45
1	I	415/418 (99%)	355 (86%)	56 (14%)	4 (1%)	12	45
1	J	415/418 (99%)	357 (86%)	56 (14%)	2 (0%)	24	60
1	K	415/418 (99%)	347 (84%)	61 (15%)	7 (2%)	7	36
1	L	415/418 (99%)	346 (83%)	61 (15%)	8 (2%)	6	34
All	All	4980/5016 (99%)	4184 (84%)	741 (15%)	55 (1%)	11	44

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 ⓘ

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%)	356 (100%)	0	100	100
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%)	356 (100%)	0	100	100
1	E	356/357 (100%)	356 (100%)	0	100	100
1	F	356/357 (100%)	356 (100%)	0	100	100
1	G	356/357 (100%)	356 (100%)	0	100	100
1	H	356/357 (100%)	356 (100%)	0	100	100
1	I	356/357 (100%)	356 (100%)	0	100	100
1	J	356/357 (100%)	356 (100%)	0	100	100
1	K	356/357 (100%)	356 (100%)	0	100	100
1	L	356/357 (100%)	356 (100%)	0	100	100
All	All	4272/4284 (100%)	4272 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	51	GLN
1	A	104	ASN
1	A	188	ASN
1	A	249	GLN
1	A	292	ASN
1	A	316	GLN
1	A	345	GLN
1	A	350	ASN
1	E	61	ASN
1	E	96	GLN
1	E	345	GLN
1	F	104	ASN
1	F	188	ASN
1	F	201	ASN
1	F	249	GLN
1	F	264	GLN
1	F	415	GLN
1	I	296	HIS

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Mol	Chain	Res	Type
1	K	327	ASN
1	K	344	GLN
1	B	201	ASN
1	B	350	ASN
1	B	415	GLN
1	C	121	ASN
1	C	161	GLN
1	C	177	HIS
1	C	344	GLN
1	C	415	GLN
1	G	51	GLN
1	G	188	ASN
1	G	249	GLN
1	G	344	GLN
1	H	61	ASN
1	H	161	GLN
1	H	201	ASN
1	D	41	ASN
1	D	104	ASN
1	D	344	GLN
1	D	345	GLN
1	J	22	GLN
1	J	104	ASN
1	J	344	GLN
1	L	185	ASN
1	L	344	GLN
1	L	384	ASN

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 oligosaccharides 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, 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	417/418 (99%)	-0.06	4 (0%) 79 61	102, 138, 187, 246	0
1	B	417/418 (99%)	0.06	5 (1%) 76 58	109, 162, 217, 242	0
1	C	417/418 (99%)	0.01	0 100 100	111, 146, 199, 249	0
1	D	417/418 (99%)	-0.07	3 (0%) 84 68	114, 148, 198, 244	0
1	E	417/418 (99%)	-0.08	1 (0%) 91 81	108, 144, 199, 236	0
1	F	417/418 (99%)	-0.06	2 (0%) 87 73	102, 145, 204, 231	0
1	G	417/418 (99%)	-0.08	2 (0%) 87 73	107, 161, 212, 246	0
1	H	417/418 (99%)	-0.12	0 100 100	110, 171, 220, 235	0
1	I	417/418 (99%)	-0.12	3 (0%) 84 68	106, 139, 191, 236	0
1	J	417/418 (99%)	-0.01	2 (0%) 87 73	116, 150, 208, 259	0
1	K	417/418 (99%)	0.00	4 (0%) 79 61	109, 166, 214, 240	0
1	L	417/418 (99%)	-0.02	4 (0%) 79 61	112, 177, 228, 245	0
All	All	5004/5016 (99%)	-0.05	30 (0%) 85 70	102, 151, 214, 259	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	272	TYR	5.0
1	E	15	VAL	3.3
1	A	100	ILE	3.0
1	K	363	VAL	2.9
1	B	244	PHE	2.9
1	L	353	ARG	2.7
1	A	272	TYR	2.7
1	B	313	ASN	2.4
1	L	276	LEU	2.4
1	A	363	VAL	2.4
1	G	2	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	418	GLY	2.3
1	J	358	GLU	2.3
1	F	402	SER	2.3
1	I	363	VAL	2.2
1	D	277	ILE	2.2
1	L	287	TYR	2.2
1	G	300	GLN	2.2
1	J	364	SER	2.2
1	K	226	LEU	2.2
1	A	103	PHE	2.1
1	B	220	PHE	2.1
1	K	406	ASP	2.1
1	B	225	ALA	2.1
1	F	359	ALA	2.1
1	D	4	ILE	2.1
1	I	105	LEU	2.1
1	L	15	VAL	2.1
1	D	183	TRP	2.0
1	K	243	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.